Chapter 6

Schrodinger Wave equation

1-Dimensional Quantum Systems

The Coordinate Representation

To form a *representation* of an abstract linear vector space we must carry out these steps:

1. Choose a complete, orthonormal set of basis vectors $\{|\alpha_k\rangle\}$.
2. Construct the identity operator $\hat{I}$ as a sum over the one-dimensional subspace projection operators $|\alpha_k\rangle\langle\alpha_k|$

$$\hat{I} = \sum_k |\alpha_k\rangle\langle\alpha_k|$$

3. Write an arbitrary vector $|\psi\rangle$ as a linear combination or superposition of basis vectors using the identity operator

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_k |\alpha_k\rangle\langle\alpha_k|\right)|\psi\rangle = \sum_k \langle\alpha_k|\psi\rangle|\alpha_k\rangle$$

It is clear from this last equation, that knowledge about the behavior(say in time) of the expansion coefficients $\langle\alpha_k|\psi\rangle$ will tell us the behavior of the state vector $|\psi\rangle$ and allow us to make predictions. Remember also, that the expansion coefficient is the probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\alpha_k\rangle$.

A particular representation that has become very important in the study of many systems using Quantum Mechanics is formed using the eigenstates of the position operator as a basis.

It is called the *coordinate or position representation*.

The eigenstates $\{|\vec{x}\rangle\}$ of the position operator $(\hat{x}, \hat{y}, \hat{z}) = \hat{\mathbf{Q}}$ satisfy

$$\hat{x}\,|\vec{x}\rangle = x\,|\vec{x}\rangle \quad , \quad \hat{y}\,|\vec{x}\rangle = y\,|\vec{x}\rangle \quad , \quad \hat{z}\,|\vec{x}\rangle = z\,|\vec{x}\rangle$$

where the eigenvalues (x, y, z) are **continuous** variables in the range $[-\infty,\infty]$.

They form the basis of the coordinate representation.

As we mentioned earlier(all the mathematical details are in the book), in this case, all summations in earlier lectures now become integrals in the continuous spectrum case and we have

$$\hat{I} = \int |\vec{x}\rangle\langle\vec{x}|\, d\vec{x} \qquad , \qquad \text{where } d\vec{x} = dxdydz$$

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \int (|\vec{x}\rangle\langle\vec{x}|)\,|\psi\rangle\, d\vec{x} = \int \langle\vec{x}\,|\,\psi\rangle\,|\vec{x}\rangle\, d\vec{x}$$

The expansion coefficient in the coordinate representation is given by

$$\psi(\vec{x}) = \langle\vec{x}\,|\,\psi\rangle$$

Since the inner product is defined for all states $|\vec{x}\rangle$, this new object is clearly a function of the eigenvalues (x, y, z).

As we will see, it is the probability amplitude for finding the particle to be in the neighborhood of the point $\vec{x}$ in 3-dimensional space if it is in the state $|\psi\rangle$.

It is called the **wave function**.

The bra vector or linear functional corresponding to $|\psi\rangle$ is

$$\langle\psi| = \langle\psi|\,\hat{I} = \int \langle\psi|\,(|\vec{x}\rangle\langle\vec{x}|)\, d\vec{x} = \int \langle\psi\,|\,\vec{x}\rangle\langle\vec{x}|\, d\vec{x} = \int \langle\vec{x}\,|\,\psi\rangle^*\langle\vec{x}|\, d\vec{x}$$

The normalization condition takes the form

$$\langle\psi\,|\,\psi\rangle = 1 = \langle\psi|\,\hat{I}\,|\psi\rangle = \int \langle\psi\,|\,\vec{x}\rangle\,\langle\vec{x}\,|\,\psi\rangle\; d\vec{x}$$

$$= \int |\,\langle\vec{x}\,|\,\psi\rangle\,|^2\, d\vec{x} = \int |\psi(\vec{x})|^2\, d\vec{x}$$

$$= \int \psi^*(\vec{x})\psi(\vec{x})\, d\vec{x}$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I}\,|\phi\rangle = \int (|\vec{x}\rangle\,\langle\vec{x}|)\,|\phi\rangle\; d\vec{x} = \int \langle\vec{x}\,|\,\phi\rangle\,|\vec{x}\rangle\; d\vec{x}$$

is given by

$$\langle\phi\,|\,\psi\rangle = \left(\int \langle\vec{x}\,|\,\phi\rangle^*\,\langle\vec{x}|\; d\vec{x}\right)\left(\int \langle\vec{x}\,'\,|\,\psi\rangle\,|\vec{x}\,'\rangle\; d\vec{x}\,'\right)$$

$$= \int d\vec{x} \int d\vec{x}\,'\,\langle\vec{x}\,|\,\phi\rangle^*\,\langle\vec{x}\,'\,|\,\psi\rangle\,\langle\vec{x}\,|\,\vec{x}\,'\rangle$$

We assume the *normalization* condition

$$\langle\vec{x}\,|\,\vec{x}\,'\rangle = \delta(\vec{x} - \vec{x}\,')$$

(position eigenvectors are *not* normalizable).

This normalization condition actually follows (we did not need to assume it) from the expansion in basis states.

We have

$$|\psi\rangle = \int \langle \vec{x}\,' \,|\, \psi \rangle \, |\vec{x}\,'\rangle \, d\vec{x}\,'$$

$$\langle \vec{x} \,|\, \psi \rangle = \int \langle \vec{x}\,' \,|\, \psi \rangle \, \langle \vec{x} \,|\, \vec{x}\,' \rangle \, d\vec{x}\,'$$

$$\psi(\vec{x}) = \int \psi(\vec{x}\,') \, \langle \vec{x} \,|\, \vec{x}\,' \rangle \, d\vec{x}\,'$$

which implies the delta-function normalization according to calculus rules.

Thus, the delta function normalization follows from the completeness property of the projection operators or vice versa.

Using this result we get

$$\langle \phi \,|\, \psi \rangle = \int d\vec{x} \int d\vec{x}\,' \, \langle \vec{x} \,|\, \phi \rangle^* \, \langle \vec{x}\,' \,|\, \psi \rangle \, \delta(\vec{x} - \vec{x}\,')$$

$$= \int \langle \vec{x} \,|\, \phi \rangle^* \, \langle \vec{x} \,|\, \psi \rangle \, d\vec{x} = \int \phi^*(\vec{x}) \psi(\vec{x}) \, d\vec{x}$$

We formally write the $\hat{\mathbf{Q}}$ operator using the expansion in eigenvalues and projection operators as

$$\hat{\mathbf{Q}} = \int \vec{x} \, |\vec{x}\rangle \, \langle \vec{x}| \, d\vec{x}$$

This represents three integrals, one for each coordinate.

We will also need the properties of the linear momentum operator.

The eigenstates $\{|\vec{p}\rangle\}$ of the momentum operator $(\hat{p}_x, \hat{p}_y, \hat{p}_z) = \hat{\mathbf{P}}$ satisfy

$$\hat{p}_x \, |\vec{p}\rangle = p_x \, |\vec{p}\rangle \quad , \quad \hat{p}_y \, |\vec{p}\rangle = p_y \, |\vec{p}\rangle \quad , \quad \hat{p}_z \, |\vec{p}\rangle = p_z \, |\vec{p}\rangle$$

where the eigenvalues (p_x, p_y, p_z) are continuous variables in the range $[-\infty, \infty]$.

They form the basis of the *momentum representation*.

We then have

$$\hat{I} = \frac{1}{(2\pi\hbar)^3} \int |\vec{p}\rangle \langle \vec{p}| \, d\vec{p}$$

$$|\psi\rangle = \hat{I}\,|\psi\rangle = \frac{1}{(2\pi\hbar)^3} \int (|\vec{p}\rangle \langle \vec{p}|)\,|\psi\rangle \, d\vec{p} = \frac{1}{(2\pi\hbar)^3} \int \langle \vec{p}\,|\,\psi\rangle \, |\vec{p}\rangle \, d\vec{p}$$

The expansion coefficient in the momentum representation is

$$\Psi(\vec{p}) = \langle \vec{p}\,|\,\psi\rangle$$

It is the probability amplitude for finding the particle with momentum $\vec{p}$ (in the neighborhood of) if it is in the state $|\psi\rangle$.

The bra vector or linear functional corresponding to $|\psi\rangle$ is

$$\langle\psi| = \langle\psi|\,\hat{I} = \frac{1}{(2\pi\hbar)^3} \int \langle\psi|\,(|\vec{p}\rangle \langle \vec{p}|)\, d\vec{p} = \frac{1}{(2\pi\hbar)^3} \int \langle \vec{p}\,|\,\psi\rangle^* \langle \vec{p}| \, d\vec{p}$$

The normalization condition takes the form

$$\begin{aligned}\langle \psi\,|\,\psi\rangle = 1 = \langle\psi|\,\hat{I}\,|\psi\rangle &= \frac{1}{(2\pi\hbar)^3} \int \langle \psi\,|\,\vec{p}\rangle \langle \vec{p}\,|\,\psi\rangle \, d\vec{p} \\ &= \frac{1}{(2\pi\hbar)^3} \int |\langle \vec{p}\,|\,\psi\rangle|^2 \, d\vec{p} \frac{1}{(2\pi\hbar)^3} = \int |\Psi(\vec{p})|^2 \, d\vec{p} \\ &= \frac{1}{(2\pi\hbar)^3} \int \Psi^*(\vec{p})\Psi(\vec{p}) \, d\vec{p}\end{aligned}$$

The probability amplitude for a particle in the state $|\psi\rangle$ to behave like it is in the state $|\phi\rangle$, where

$$|\phi\rangle = \hat{I}\,|\phi\rangle = \frac{1}{(2\pi\hbar)^3} \int (|\vec{p}\rangle \langle \vec{p}|)\,|\phi\rangle \, d\vec{p} = \frac{1}{(2\pi\hbar)^3} \int \langle \vec{p}\,|\,\phi\rangle \, |\vec{p}\rangle \, d\vec{p}$$

is given by

$$\langle\phi|\psi\rangle = \left(\frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}|\phi\rangle^* \langle\vec{p}|\, d\vec{p}\right)\left(\frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}\,'|\psi\rangle |\vec{p}\,'\rangle\, d\vec{p}\,'\right)$$

$$= \frac{1}{(2\pi\hbar)^6}\int d\vec{p}\int d\vec{p}\,' \langle\vec{p}|\phi\rangle^* \langle\vec{p}\,'|\psi\rangle \langle\vec{p}|\vec{p}\,'\rangle$$

The normalization condition follows from

$$|\psi\rangle = \frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}\,'|\psi\rangle |\vec{p}\,'\rangle\, d\vec{p}\,'$$

$$\langle\vec{p}|\psi\rangle = \frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}\,'|\psi\rangle \langle\vec{p}|\vec{p}\,'\rangle\, d\vec{p}\,'$$

$$\Psi(\vec{x}) = \frac{1}{(2\pi\hbar)^3}\int \Psi(\vec{p}\,') \langle\vec{p}|\vec{p}\,'\rangle\, d\vec{p}\,'$$

which implies that

$$\frac{1}{(2\pi\hbar)^3}\langle\vec{p}|\vec{p}\,'\rangle = \delta(\vec{p}-\vec{p}\,')$$

Using this result we get

$$\langle\phi|\psi\rangle = \frac{1}{(2\pi\hbar)^6}\int d\vec{p}\int d\vec{p}\,' \langle\vec{p}|\phi\rangle^* \langle\vec{p}\,'|\psi\rangle \langle\vec{p}|\vec{p}\,'\rangle$$

$$= \frac{1}{(2\pi\hbar)^3}\int d\vec{p}\int d\vec{p}\,' \langle\vec{p}|\phi\rangle^* \langle\vec{p}\,'|\psi\rangle \delta(\vec{p}-\vec{p}\,')$$

$$= \frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}|\phi\rangle^* \langle\vec{p}\psi\rangle\, d\vec{p} = \frac{1}{(2\pi\hbar)^3}\int \Phi^*(\vec{p})\Psi(\vec{p})\, d\vec{p}$$

We formally write the $\hat{\mathbf{P}}$ operator using the expansion in eigenvalues and projection operators as

$$\hat{\mathbf{P}} = \int \vec{p}\,|\vec{p}\rangle\,\langle\vec{p}|\;d\vec{p}$$

We will now derive the *connections* between the two representations.

We have

$$\psi(\vec{x}) = \langle\vec{x}\,|\,\psi\rangle = \langle\vec{x}|\,\hat{I}\,|\psi\rangle = \frac{1}{(2\pi\hbar)^3}\int \langle\vec{x}\,|\,\vec{p}\rangle\,\langle\vec{p}\,|\,\psi\rangle\;d\vec{p}$$

$$= \frac{1}{(2\pi\hbar)^3}\int \langle\vec{x}\,|\,\vec{p}\rangle\,\Psi(\vec{p})\,d\vec{p}$$

and

$$\Psi(\vec{p}) = \langle\vec{p}\,|\,\psi\rangle = \langle\vec{p}|\,\hat{I}\,|\psi\rangle = \int \langle\vec{p}\,|\,\vec{x}\rangle\,\langle\vec{x}\,|\,\psi\rangle\;d\vec{x}$$

$$= \int \langle\vec{x}\,|\,\vec{p}\rangle^*\,\psi(\vec{x})\,d\vec{x}$$

Fourier transforms are defined by

$$g(\vec{p}) = \int e^{-i\vec{p}\cdot\vec{x}/\hbar} f(\vec{x})\,d\vec{x} \quad , \quad f(\vec{x}) = \frac{1}{(2\pi\hbar)^3}\int e^{i\vec{p}\cdot\vec{x}/\hbar} g(\vec{p})\,d\vec{p}$$

which gives us the possible result

$$\langle\vec{x}\,|\,\vec{p}\rangle = e^{i\vec{p}\cdot\vec{x}/\hbar}$$

It is not a unique choice, however.

It is the choice, however, that allows Quantum mechanics *to make predictions that agree with experiment*.

It is Nature's choice!

We might even say that this choice is *another postulate*.

Now, we can use these results to determine the expectation values of operators involving the position and momentum operators.

Since we are interested in the coordinate representation we need only determine the following quantities.

The position operator calculations are straightforward

$$\langle \vec{x}| \hat{\mathbf{Q}} |\psi\rangle = \vec{x} \langle \vec{x} | \psi\rangle \text{ and } \langle \vec{x}| f(\hat{\mathbf{Q}}) |\psi\rangle = f(\vec{x}) \langle \vec{x} | \psi\rangle$$

For the momentum operator we write

$$\begin{aligned}\langle \vec{x}| \hat{\mathbf{P}} |\psi\rangle &= \frac{1}{(2\pi\hbar)^3} \int \langle \vec{x}| \hat{\mathbf{P}} |\vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p} \\ &= \frac{1}{(2\pi\hbar)^3} \int \langle \vec{x}| \vec{p} |\vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p} \\ &= \frac{1}{(2\pi\hbar)^3} \int \vec{p} \langle \vec{x} | \vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p}\end{aligned}$$

Now using

$$\langle \vec{x} | \vec{p}\rangle = e^{i\vec{p}\cdot\vec{x}/\hbar}$$

we have

$$\vec{p} \langle \vec{x} | \vec{p}\rangle = -i\hbar\nabla \langle \vec{x} | \vec{p}\rangle = \langle \vec{x}| \hat{\mathbf{P}} |\vec{p}\rangle$$

and thus

$$\begin{aligned}\langle \vec{x}| \hat{\mathbf{P}} |\psi\rangle &= \frac{1}{(2\pi\hbar)^3} \int \vec{p} \langle \vec{x} | \vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p} \\ &= (-i\hbar\nabla) \frac{1}{(2\pi\hbar)^3} \int (-i\hbar\nabla) \langle \vec{x} | \vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p} \\ &= \frac{1}{(2\pi\hbar)^3} \int \langle \vec{x} | \vec{p}\rangle \langle \vec{p} | \psi\rangle \, d\vec{p} \\ &= -i\hbar\nabla \langle \vec{x} | \psi\rangle\end{aligned}$$

In a similar manner, we can also show that

$$\langle \vec{x} | \hat{\mathbf{P}}^2 | \psi \rangle = (-i\hbar\nabla)^2 = -\hbar^2\nabla^2 \langle \vec{x} | \psi \rangle$$

Alternatively, we can show that the gradient is the correct result using the symmetry transformation ideas we developed earlier.

The momentum operator is the generator of displacements in space.

We showed earlier that

$$e^{-i\vec{a}\cdot\hat{\mathbf{P}}/\hbar} |\vec{x}\rangle = |\vec{x} + \vec{a}\rangle$$

Therefore, we have

$$\begin{aligned} \psi(\vec{x} + \vec{a}) = \langle \vec{x} + \vec{a} | \psi \rangle &= \langle \vec{x} | e^{i\vec{a}\cdot\hat{\mathbf{P}}/\hbar} | \psi \rangle \\ &= e^{-\vec{a}\cdot\nabla} \langle \vec{x} | \psi \rangle = e^{-\vec{a}\cdot\nabla} \psi(\vec{x}) \end{aligned}$$

Since

$$e^{-\vec{a}\cdot\nabla} = 1 - \vec{a}\cdot\nabla + \frac{(\vec{a}\cdot\nabla)^2}{2!} - \ldots$$

we have the standard Taylor series for $\psi(\vec{x} + \vec{a})$.

Therefore, the gradient representation of the momentum operator makes sense.

We now use these results to derive the Schrodinger wave equation.

The Schrodinger wave equation is the partial differential equation that corresponds to the eigenvector/eigenvalue equation for the Hamiltonian operator or the energy operator.

The resulting states are the energy eigenstates.

We already saw that energy eigenstates are stationary states and thus have simple time dependence.

This property will allow us to find the time dependence of amplitudes for very complex systems in a straightforward way.

We have

$$\hat{H}\,|\psi_E\rangle = E\,|\psi_E\rangle$$

where E = a number and $\hat{H}$ = the energy operator = (kinetic energy + potential energy) operators, i.e.,

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} + V(\hat{\mathbf{Q}}) \qquad \text{non-relativistic QM}$$

We then have

$$\langle \vec{x}|\left(\frac{\hat{\mathbf{P}}^2}{2m} + V(\hat{\mathbf{Q}})\right)|\psi_E\rangle = E\,\langle \vec{x}\,|\,\psi_E\rangle$$

$$\langle \vec{x}|\,\frac{\hat{\mathbf{P}}^2}{2m}\,|\psi_E\rangle + \langle \vec{x}|\,V(\hat{\mathbf{Q}})\,|\psi_E\rangle = E\,\langle \vec{x}\,|\,\psi_E\rangle$$

$$-\frac{\hbar^2}{2m}\nabla^2\,\langle \vec{x}\,|\,\psi_E\rangle + V(\vec{x})\,\langle \vec{x}\,|\,\psi_E\rangle = E\,\langle \vec{x}\,|\,\psi_E\rangle$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x}) + V(\vec{x})\psi_E(\vec{x}) = E\psi_E(\vec{x})$$

which is the *time-independent Schrodinger wave equation*.

The quantity

$$\psi_E(\vec{x}) = \langle \vec{x}\,|\,\psi_E\rangle$$

is the wave function or the energy eigenfunction in the position representation corresponding to energy E.

Now the energy eigenfunctions have a simple time dependence, as we can see from the following.

Since

$$\hat{U}(t)\,|\psi_E\rangle = e^{-i\hat{H}t/\hbar}\,|\psi_E\rangle = e^{-iEt/\hbar}\,|\psi_E\rangle$$

we have

$$|\vec{x}\rangle\,\hat{U}(t)\,|\psi_E\rangle = \psi_E(\vec{x},t) = e^{-iEt/\hbar}\,\langle\vec{x}\,|\,\psi_E\rangle$$

$$\psi_E(\vec{x},t) = e^{-iEt/\hbar}\psi_E(\vec{x},0)$$

Therefore,

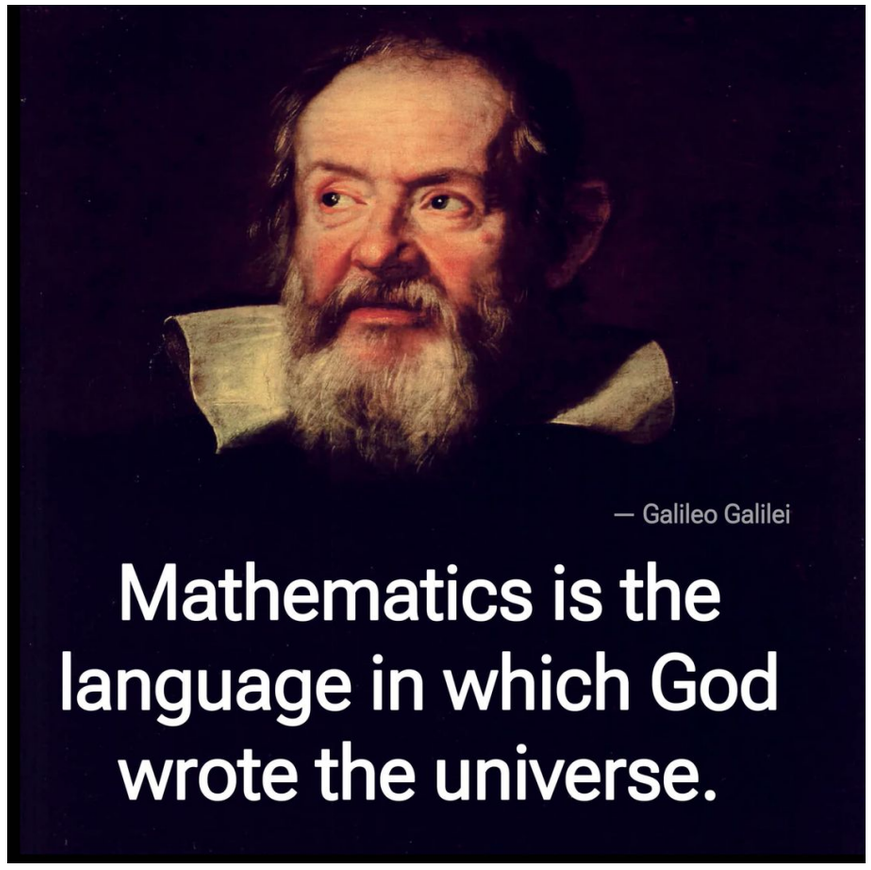
$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x},t) + V(\vec{x})\psi_E(\vec{x},t) = E\psi_E(\vec{x},t)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x},t) + V(\vec{x})\psi_E(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi_E(\vec{x},t)$$

which is the *time-dependent Schrodinger wave equation*.

We will have much more to say about these equations and how to use them later on.

For now, however, let us look at these ideas in a couple of different ways to try and get a better understanding of what they mean.



Remember what we said in lecture last time:

Thus, the mathematical sum over all projection operators being equal to the identity operator is physically equivalent to the sum over all possible intermediate states and it turns into a sum over all the amplitudes for indistinguishable ways in this interpretation.

$$\hat{I} = |R\rangle\langle R| + |L\rangle\langle L|$$

$$|x\rangle = |R\rangle\langle R|x\rangle + |L\rangle\langle L|x\rangle$$

$$\langle y|x\rangle = \langle y|\hat{I}|x\rangle = \langle R|x\rangle\langle y|R\rangle + \langle L|x\rangle\langle y|L\rangle$$

I would substitute "**Nature**" for "God.

Time-independent Schrodinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x}) + V(\vec{x})\psi_E(\vec{x}) = E\psi_E(\vec{x})$$

$$\psi_E(\vec{x}) = \langle \vec{x}|\psi_E\rangle$$

Time-dependent Schrodinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x},t) + V(\vec{x})\psi_E(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi_E(\vec{x},t)$$

$$\psi_E(\vec{x},t) = e^{-iEt/\hbar}\psi_E(\vec{x},0)$$

stop

The Free Particle and Wave Packets

Let us assume that the potential energy term in the one-particle Schrodinger equation is equal to zero.

The solution, in this case, is called a *free particle*.

We can easily see the form of the solution as a function of space and time as follows: the Hamiltonian of the system is

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} \text{ with } \hat{H}|\psi_E\rangle = E|\psi_E\rangle$$

This means that $[\,\hat{H}, \hat{\mathbf{P}}\,] = 0$ and thus $\hat{H}$ and $\hat{\mathbf{P}}$ share a common set of eigenvectors(eigenfunctions now).

The eigenvectors(eigenfunctions) corresponding to linear momentum $\hat{\mathbf{P}}$ are easy to find from our earlier derivations.

We have

$$\hat{\mathbf{P}}\,|\vec{p}\rangle = \hat{\mathbf{P}}\,|\psi_E\rangle = \vec{p}\,|\vec{p}\rangle = \vec{p}\,|\psi_E\rangle$$

$$\langle\vec{x}|\,\hat{\mathbf{P}}\,|\psi_E\rangle = \vec{p}\,\langle\vec{x}\,|\,\psi_E\rangle = \vec{p}e^{i\vec{p}\cdot\vec{x}/\hbar}$$

$$= -i\hbar\nabla e^{i\vec{p}\cdot\vec{x}/\hbar} = -i\hbar\nabla\,\langle\vec{x}\,|\,\psi_E\rangle$$

which says that the eigenfunctions are

$$\langle\vec{x}\,|\,\vec{p}\rangle = e^{i\vec{p}\cdot\vec{x}/\hbar} = \psi_E(\vec{x}) = \langle\vec{x}\,|\,\psi_E\rangle = \langle\vec{x}\,|\,E\rangle$$

We can see that this satisfies the time-independent Schrodinger equation with no potential term.

This solution is also called a *plane-wave*.

If we assume that at time $t = 0$, the state of the particle is

$$\psi_E(\vec{x}, 0) = e^{i\vec{p}\cdot\vec{x}/\hbar}$$

then the time dependence is given by

$$|\vec{x}, t\rangle = \hat{U}(t)\,|\vec{x}, 0\rangle = e^{-iEt/\hbar}\,|\vec{x}, 0\rangle$$

$$\langle\vec{x}, t\,|\,\psi_E\rangle = e^{-iEt/\hbar}\,\langle\vec{x}, 0\,|\,\psi_E\rangle$$

$$\psi_E(\vec{x}, t) = e^{-iEt/\hbar}\psi_E(\vec{x}, 0) = e^{-iEt/\hbar}e^{i\vec{p}\cdot\vec{x}/\hbar} = e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$$

where $E = p^2/2m$.

Now we can write the position state vector the as a linear combination of momentum state vectors or correspondingly we can write position space wave function as a linear combination of momentum eigenfunctions or plane waves (since they are a basis).

$$|\psi_E\rangle = \frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}\,|\,\psi_E\rangle\,|\vec{p}\rangle\; d\vec{p}$$

$$\langle\vec{x}\,|\,\psi_E\rangle = \psi_E(\vec{x}) = \frac{1}{(2\pi\hbar)^3}\int \langle\vec{p}\,|\,\psi_E\rangle\,\langle\vec{x}\,|\,\vec{p}\rangle\; d\vec{p}$$

$$\psi_E(\vec{x},0) = \frac{1}{(2\pi\hbar)^3}\int e^{i\vec{p}\cdot\vec{x}/\hbar}\Psi_E(\vec{p},0)\, d\vec{p}$$

We note that in the state $|\vec{p}\rangle$, which is an eigenvector of $\hat{\mathbf{P}}$, the momentum has the value $\vec{p}$ with probability = 1 (a certainty), which is the meaning of an eigenvector!

However, the probability of finding the particle in this state at the point $\vec{x}$ is independent of $\vec{x}$, i.e.,

$$|\langle\vec{x}\,|\,\vec{p}\rangle|^2 = |e^{i\vec{p}\cdot\vec{x}/\hbar}|^2 = 1$$

This means that the particle is equally probable to have any value of momentum.

The momentum is completely uncertain in a position eigenstate.

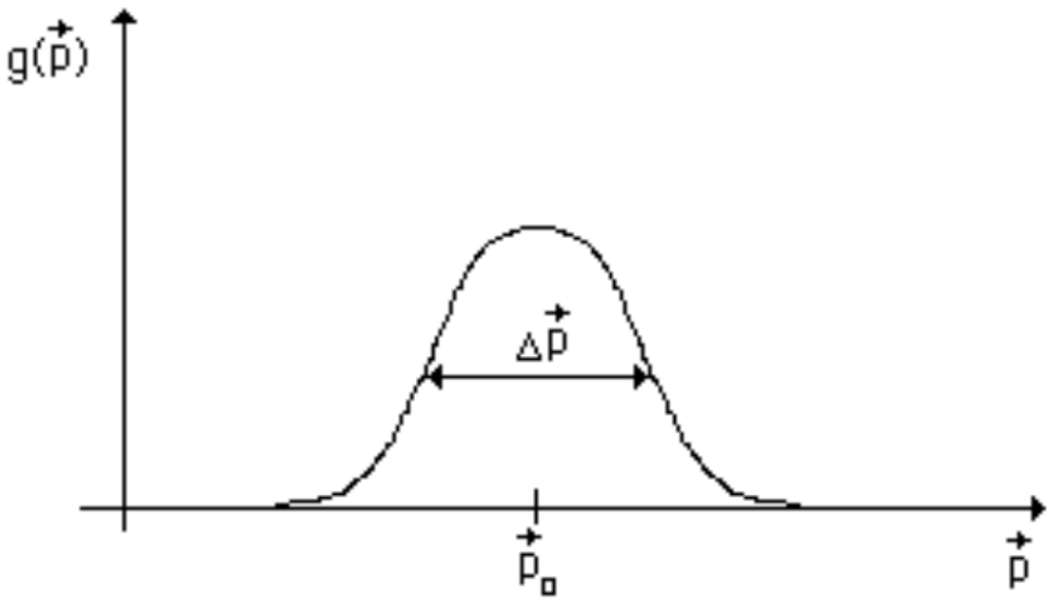
If we consider an intermediate case in which the particle is reasonably well localized in position space, and at the same time, has a fairly well defined momentum, then the wave function for such a state is called a *wave packet*.

Suppose that the function $|\Psi_E(\vec{p},0)|$ is peaked about the value $\vec{p}_0$, with a width $\approx \Delta\vec{p}$.

In particular, at $t = 0$, we choose

$$\Psi_E(\vec{p},0) = g(\vec{p})e^{i\alpha(\vec{p})}$$

where $g(\vec{p})$, called the weight function, takes the form of a real, nonnegative function such as shown in the Figure, and the phase $\alpha(\vec{p})$ is real.



Weight Function

We then have

$$\psi_E(\vec{x},t) = \frac{1}{(2\pi\hbar)^3}\int g(\vec{p})e^{i(\vec{p}\cdot\vec{x}-Et+\hbar\alpha(\vec{p}))/\hbar}\,d\vec{p}$$

as the wave function of a particle whose momentum is approximately $\vec{p}_0$.

This means that most of the time, if we measure the momentum of the particle in this state, then we would find a value within $\Delta\vec{p}$ of $\vec{p}_0$.

We now determine **how** this particle moves in time and **why** we have called this expression a wave packet.

If for some position $\vec{x}$ (which is a parameter in the integral) the phase of the exponential term is *not slowly varying* for some values of integration variable $\vec{p}$, then the integral will equal zero.

This occurs because the exponential term is a very rapidly oscillating function (since $\hbar$ is very small), i.e., if you multiply a very rapidly varying function by a function of the assumed form of $g(\vec{p})$, then *on the averag*e the integrand is zero.

In effect, we are seeing destructive interference between the plane waves.

If, however, $\vec{x}$ is a point such that the phase of the exponential remains fairly constant over the same range of $\vec{p}$ where the function $g(\vec{p})$ is nonzero, then we will get a nonzero value for the integral and the particle will have some nonzero probability of being at that point.

One way to make this work is as follows:

1. At time t, assume the point $\vec{x}_t$ makes the phase *stationary* near $\vec{p}_0$. By stationary we mean

$$\nabla_{\vec{p}}(\vec{p}\cdot\vec{x}_t - Et + \hbar\alpha(\vec{p}))_{\vec{p}=\vec{p}_0} = 0$$

   or we are near an extremum of the phase and hence the phase will be slowly varying.

2. We will then get strong *constructive* interference between the plane waves and $\psi_E(\vec{x},t)$ will be nonzero.

Solving the stationary phase equation for $\vec{x}_t$ we find, using $E = p^2/2m$

$$(\vec{x}_t - \nabla_{\vec{p}}(E)t + \hbar(\nabla_{\vec{p}}\alpha(\vec{p})))_{\vec{p}=\vec{p}_0} = 0$$

$$\vec{x}_t = ((\vec{p}E)t + \hbar(\nabla_{\vec{p}}\alpha(\vec{p})))_{\vec{p}=\vec{p}_0}$$

$$= \frac{\vec{p}_0}{m}t - \hbar(\nabla_{\vec{p}}\alpha(\vec{p})) = \frac{\vec{p}_0}{m}t + \vec{x}_0$$

Therefore, the point $\vec{x}_t$, which is essentially the center of the wave packet, moves in time with a constant velocity $\vec{v} = \vec{p}_0/m$.

This is exactly the velocity one expects for a free particle of momentum $\vec{p}_0$ and mass m.

It is called the *group velocity* of the wave packet.

This procedure is called the *stationary phase method*.

How localized is this wave packet(*particle*) or what is the spatial extent of the packet?

We will have a nonzero integral and hence a nonzero probability for the particle to be at a particular point as long as we have constructive interference or as long as the exponential undergoes less than one oscillation as $\vec{p}$ varies over the region for which the function $g(\vec{p})$ is also large.

The change in the phase of the exponential as we vary the x-component of $\vec{p}$ is approximately

$$\Delta\phi = \Delta(\vec{p}\cdot\vec{x} - Et + \hbar\alpha(\vec{p}))_{\vec{p}=\vec{p}_0} = \frac{1}{\hbar}\Delta p_x \frac{\partial}{\partial p_x}(\vec{p}\cdot\vec{x} - Et + \hbar\alpha(\vec{p}))_{\vec{p}=\vec{p}_0}$$

$$= \frac{1}{\hbar}\Delta p_x \left(x - \frac{\partial}{\partial p_x}(Et + \hbar\alpha(\vec{p})\right)_{\vec{p}=\vec{p}_0} = \frac{1}{\hbar}\Delta p_x (x - x_t)$$

As long as $\Delta\phi \leq 2\pi$ we will get constructive interference and the integral will be nonzero.

This tells us the extent of the wave packet in the x-direction about the point x_t.

We get

$$|x - x_t| \geq \frac{2\pi\hbar}{\Delta p_x} \text{ or } |x - x_t|\Delta p_x \geq h$$

or

$$\Delta x \Delta p_x \geq h$$

Similarly we can show that $\Delta y \Delta p_y \geq h$ and $\Delta z \Delta p_z \geq h$.

These relations between the spatial extent of the wave packet or the uncertainty in its position, and the uncertainty in the particle momentum, are often called the *Heisenberg uncertainty principle*.

We will see later that the uncertainty principle involves more than just these simple properties of a wave packet.

We will also develop more details about wave packets later on the lectures.

Note that there is no uncertainty relation between

$$\Delta x \text{ and } \Delta y, \Delta z, \Delta p_y, \Delta p_z$$
$$\Delta y \text{ and } \Delta x, \Delta z, \Delta p_x, \Delta p_z$$
$$\Delta z \text{ and } \Delta x, \Delta y, \Delta p_x, \Delta p_y$$

What is the difference between these pairs of variables?

The difference is in their commutators.

It turns out, in this example of the wave packet, that only those observables that are represented by non-commuting operators have nonzero uncertainty relations.

This result has nothing to do with wave packets, Schrodinger equations, wave functions or Fourier transforms, although all of these quantities can be used to show that uncertainty relations exist.

The existence of uncertainty relations between non-commuting observables was actually built into the theory of Quantum Mechanics when we assumed that we were in an abstract linear vector space.

All linear vector spaces have a property called the Schwarz inequality and it always leads to such uncertainty relations for non-commuting operators.

So the Heisenberg uncertainty principle, to which much mysticism has been attached, is really an assumption and little more than a lemma that follows from the original assumption of a vector space.

Derivation of the Uncertainty Relations in General

Given two Hermitian operators $\hat{A}$ and $\hat{B}$ we define the two new operators

$$\hat{D}_A = \hat{A} - \langle \hat{A} \rangle \text{ and } \hat{D}_B = \hat{B} - \langle \hat{B} \rangle$$

where $\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle$ equals the average or expectation value in the state $|\psi\rangle$.

In the statistical analysis of data, we use a quantity called the standard or mean-square deviation as a measure of the uncertainty of an observed quantity.

It is defined, for a set of *N* measurements of the quantity Δq by

$$(\Delta q)^2 = (\text{standard deviation})^2 = \frac{1}{N}\sum_{i=1}^{N}(q_i - q_{average})^2$$

$$= \frac{1}{N}\sum_{i=1}^{N}(q_i)^2 - \frac{1}{N}\sum_{i=1}^{N}(q_i q_{average}) - \frac{1}{N}\sum_{i=1}^{N}(q_{average} q_i) + \frac{1}{N}\sum_{i=1}^{N}(q_{average})^2$$

$$= (q^2)_{average} - (q_{average})^2$$

where we have used

$$q_{average} = \frac{1}{N}\sum_{i=1}^{N} q_i$$

In analogy, we define the mean-square deviations for $\hat{A}$ and $\hat{B}$ as

$$(\Delta\hat{A})^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{D}_A^2\rangle$$
$$(\Delta\hat{B})^2 = \langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2 = \langle(\hat{B} - \langle\hat{B}\rangle)^2\rangle = \langle\hat{D}_B^2\rangle$$

We then have

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 = \langle\hat{D}_A^2\rangle\langle\hat{D}_B^2\rangle$$

Now we assume that

$$[\hat{D}_A, \hat{B}] = [\hat{A}, \hat{B}] = [\hat{D}_A, \hat{D}_B] = i\hat{C}$$

where $\hat{C}$ is also a Hermitian operator and we let

$$|\alpha\rangle = \hat{D}_A|\psi\rangle = (\hat{A} - \langle\hat{A}\rangle)|\psi\rangle \text{ and } |\beta\rangle = \hat{D}_B|\psi\rangle = (\hat{B} - \langle\hat{B}\rangle)|\psi\rangle$$

Then we have

$$(\Delta\hat{A})^2 = \langle\hat{D}_A^2\rangle = \langle\psi|\hat{D}_A^2|\psi\rangle = (\langle\psi|\hat{D}_A)(\hat{D}_A|\psi\rangle) = \langle\alpha|\alpha\rangle$$
$$(\Delta\hat{B})^2 = \langle\hat{D}_B^2\rangle = \langle\psi|\hat{D}_B^2|\psi\rangle = (\langle\psi|\hat{D}_B)(\hat{D}_B|\psi\rangle) = \langle\beta|\beta\rangle$$

The Schwarz inequality says that for any two vectors we must have the relation

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

We therefore have

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 = \langle\hat{D}_A^2\rangle\langle\hat{D}_B^2\rangle = \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$
$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq |\langle\psi|\hat{D}_A\hat{D}_B|\psi\rangle|^2 = |\langle\hat{D}_A\hat{D}_B\rangle|^2$$

Now

$$|\langle \hat{D}_A \hat{D}_B \rangle|^2 = |\langle \Delta\hat{A}\Delta\hat{B} \rangle|^2 = |\langle \frac{1}{2}[\Delta\hat{A}, \Delta\hat{B}] + \frac{1}{2}\{\Delta\hat{A}, \Delta\hat{B}\} \rangle|^2$$

$$= |\langle \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{2}\{\hat{A}, \hat{B}\} \rangle|^2$$

where

$$[\Delta\hat{A}, \Delta\hat{B}]^\dagger = -[\Delta\hat{A}, \Delta\hat{B}] \rightarrow \text{ anti-Hermitian } \rightarrow \text{ expectation value is imaginary}$$

$$\{\Delta\hat{A}, \Delta\hat{B}\}^\dagger = \{\Delta\hat{A}, \Delta\hat{B}\} \rightarrow \text{ Hermitian } \rightarrow \text{ expectation value is real}$$

Therefore,

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq |\langle \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{2}\{\hat{A}, \hat{B}\} \rangle|^2$$

$$\geq \frac{1}{4}|\langle i\hat{C} \rangle + a|^2$$

where a is a real number.

Then

$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq \frac{1}{4}|a|^2 + \frac{1}{4}|\langle \hat{C} \rangle|^2 \geq \frac{1}{4}|\langle \hat{C} \rangle|^2$$

since $|a|^2/4 \geq 0$.

This is the Heisenberg uncertainty principle.

It is simply the Schwarz inequality!!

The standard form in most texts follows from $[\ \hat{x}, \hat{p}_x\ ] = \mathrm{i}\,\hbar$, which gives $\Delta\hat{x}\Delta\hat{p}_x \geq \frac{\hbar}{2}$

We note that if $[\ \hat{A}, \hat{B}\ ] = \mathrm{i}\,\hat{C} = 0$, we then get

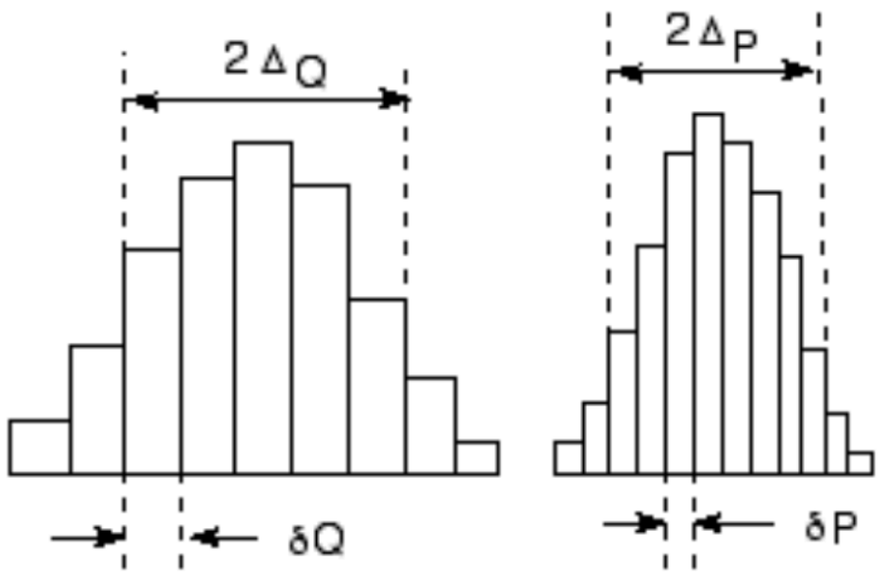
$$(\Delta\hat{A})^2(\Delta\hat{B})^2 \geq 0$$

or commuting observables do not have an uncertainty principle!

The Meaning of the Indeterminacy Relations

What is the significance of indeterminacy relations in the world of experimental physics?

Consider the experimental results shown in the Figure below:



Experimental Data

These are frequency distributions for the results of independent measurements of Q and P on an ensemble if similarly prepared systems, i.e., on each of a large number of similarly prepared systems one performs a single measurement (either Q or P).

The histograms are the statistical distribution of the results.

The standard deviations (variances) as shown must satisfy (according to the theory) the relation

$$\Delta_Q \Delta_P \geq \frac{\hbar}{2}$$

They must be distinguished from the resolution of the individual measurements, δQ and δP.

Let me emphasize these points:

1. The quantities Δ_Q and Δ_P are *not* errors of measurement. The *errors* or preferably the *resolutions* of the Q and P measuring instruments are δ_Q and δ_P. They are logically unrelated to Δ_Q and Δ_P and to the uncertainty relations except for the practical requirement that if

$$\delta_Q > \Delta_Q \ (or\ \delta_P > \Delta_P) \tag{6.71}$$

   then it will not be possible to determine Δ_Q (or Δ_P) in the experiment and the experiment cannot test the uncertainty relation.

2. The experimental test of the indeterminacy relation *does not* involve simultaneous measurements of Q and P, but rather it involves the measurement of one or the other of these dynamical variables on each independently prepared representative of the particular state being studied.

Why am I being so picky here?

The quantities ΔQ and ΔP as defined here are often misinterpreted as the errors of individual measurements.

This probably arises because Heisenberg's original paper on this subject, published in 1927, was based on an early version of quantum mechanics that predates the systematic formulation and statistical interpretation of quantum mechanics as it exists now.

The derivation, as carried out here was not possible in 1927!

Time-Energy Uncertainty Relations

The use of time-energy uncertainty relations in most textbooks is simply incorrect.

Let us now derive the most we can say about such relations.

Earlier, we showed that

$$\frac{d\langle \hat{Q} \rangle_t}{dt} = Tr\left(\hat{W}_0 \frac{d\hat{Q}_H(t)}{dt} \right) = Tr\left[\frac{i}{\hbar} \hat{W}_0 [\hat{H}, \hat{Q}_H(t)] + \hat{W}_0 \left(\frac{\partial \hat{Q}}{\partial t} \right)_H \right]$$

in the Heisenberg picture.

So we can write in general that for any operator $\hat{Q}$

$$\frac{d\langle \hat{Q} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{Q}, \hat{H}] \rangle + \langle \frac{\partial \hat{Q}}{\partial t} \rangle$$

Now consider a system whose Hamiltonian $\hat{H}$ does not explicitly depend on time and let $\hat{Q}$ be another observable of this system which does not depend on time explicitly so that

$$\frac{d\langle \hat{Q} \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{Q}, \hat{H}] \rangle$$

We consider the dynamical state of the system at a given time *t*.

Let $|\psi\rangle$ be the vector representing that state.

Call ΔQ and ΔE the root-mean-square deviations of and $\hat{H}$, respectively.

Applying the Schwarz inequality (as earlier) to the vectors $(\hat{Q} - \langle \hat{Q} \rangle)|\psi\rangle$ and $(\hat{H} - \langle \hat{H} \rangle)|\psi\rangle$ and carrying out the same manipulations, we find after some calculations

$$\Delta Q \Delta E \geq \frac{1}{2} |\langle [\hat{Q}, \hat{H}] \rangle|$$

the equality being realized when $|\psi\rangle$ satisfies the equation

$$(\hat{Q} - \alpha)\,|\psi\rangle = i\gamma(\hat{H} - \epsilon)\,|\psi\rangle$$

where α, γ, and ε are arbitrary real constants.

We then have

$$\frac{\Delta Q}{|\frac{d\langle \hat{Q} \rangle}{dt}|} \Delta E \geq \frac{\hbar}{2}$$

or

$$\tau_Q \Delta E \geq \frac{\hbar}{2}$$

where we have defined

$$\tau_Q = \frac{\Delta Q}{|\frac{d\langle \hat{Q} \rangle}{dt}|}$$

τ_Q appears as a time characteristic of the evolution of the expectation value of $\hat{Q}$.

It is the time required for the center of the center $\langle \hat{Q} \rangle$ of the statistical distribution of $\hat{Q}$ to be displaced by an amount equal to its width ΔQ.

In other words, the time necessary for this statistical distribution to be appreciably modified.

In this way we can define a characteristic evolution time for each dynamical variable of the system.

Let τ be the shortest of the times thus defined.

τ may be considered as the characteristic time of evolution of the system itself, that is, whatever the measurement carried out on the system at an instant of time t', the statistical distribution of the results is essentially the same as would be obtained at the instant t, as long as the difference $|t - t'|$ is less than τ.

This time τ and the energy spread ΔE satisfy the time-energy uncertainty relation

$$\tau \Delta E \geq \frac{\hbar}{2}$$

If, in particular, the system is in a stationary state where $d\langle \hat{Q} \rangle/dt = 0$ no matter what $\hat{Q}$, and consequently τ is infinite, then $\Delta E = 0$ according to the above relation.

Ordinary time t is just a parameter in non-relativistic QM and not an operator!

We cannot say that

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

which is an equation that has no meaning!

The Wave Function and Its Meaning

The Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(\vec{x},t) + V(\vec{x})\psi_E(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi_E(\vec{x},t)$$

has the mathematical form similar to that of a type of equation called a *wave equation*.

Since other wave equations imply the existence of real physical fields or waves propagating in real three dimensional space, a possible interpretation of the Schrodinger wave function $\psi_{\mathrm{E}}(\vec{\mathrm{x}},t)$ is that of a wave in real, three dimensional space.

We might also associate the wave field with a particle or a particle could be identified with a wave packet solution to the Schrodinger equation, as we did earlier in our discussion.

These are all misinterpretations!!!

We are being misled here because we are working with a simple system, namely, a single particle in three-dimensional space.

To see that these interpretations are not valid, we must look at the more complicated case of a system of N particles.

We now generalize to a coordinate representation for the system of N particles as follows:

1. Choose as a basis the set of vectors that is a common set of eigenvectors for the N position operators $\hat{\mathbf{Q}}^{(1)}, \hat{\mathbf{Q}}^{(2)}, \ldots, \hat{\mathbf{Q}}^{(\mathbf{N})}$ corresponding to the N particles.

2. Assuming that each position operator satisfies an eigenvalue/eigenvector equation of the form

$$\hat{Q}^{(i)} \left|\vec{x}^{(i)}\right\rangle = \vec{x}^{(i)} \left|\vec{x}^{(i)}\right\rangle \quad , \quad i = 1, 2, \ldots, N$$

and that each of the sets of single particle eigenvectors forms a basis for the 3-dimensional subspace of the single particle. The basis states for the N particle system are then the *direct product* states among the N sets of single particle eigenvectors. We write them as

$$\left|\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)}\right\rangle = \left|\vec{x}^{(1)}\right\rangle \otimes \left|\vec{x}^{(2)}\right\rangle \otimes \ldots \otimes \left|\vec{x}^{(N)}\right\rangle$$

The state vector $|\Psi\rangle$ representing an N particle system is then represented in the $3N$-dimensional configuration space corresponding to the $3N$ coordinates of the N particles by

$$\Psi(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)}) = \left\langle \vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)} \middle| \Psi \right\rangle$$

The Hamiltonian for the N particle system is given by

$$\hat{H} = \sum_{n=1}^{N} \hat{H}_n + \hat{U}(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)})$$

where

$$\hat{H}_n = \text{ single particle Hamiltonian for the } n^{th} \text{ particle}$$

$$= -\frac{\hbar^2}{2m_n}\nabla_n^2 + V(\vec{x}^{(n)})$$

and $\hat{U}(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)})$ = the interparticle interaction potential energy.

The equation of motion(the N-particle Schrodinger equation) is then

$$\hat{H}\Psi(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)}) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)})$$

As we shall now see, this N particle equation does not allow any of the interpretations that might seem to be valid for the single particle Schrodinger equation.

If we associated a physical wave in real, three dimensional space with a particle or if a particle were to be identified with a wave packet, then there would have to be N interacting waves in the real, three dimensional space where we actually measure things.

It is clear, however, that the N particle Schrodinger equation says that this is NOT the case.

There is only one wave function in an abstract $3N$-dimensional configuration space.

We are able to make the incorrect interpretation in the one particle case because it just happens, in that case, that the real, 3-dimensional has a one-to-one correspondence to the 3-dimensional configuration space of the Schrodinger equation.

The proper interpretation of Ψ is that it is a statistical state function.

It is nothing more than a function that enables us to calculate probability distributions for all observables and their expectation values.

The important physical quantities are the probabilities and the NOT the function used to calculate them.

$$|\Psi(\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots, \vec{x}^{(N)})|^2 = \text{ probability density in configuration space for}$$

$$\text{particle 1 to be at } \vec{x}^{(1)}$$

$$\text{particle 2 to be at } \vec{x}^{(2)}$$

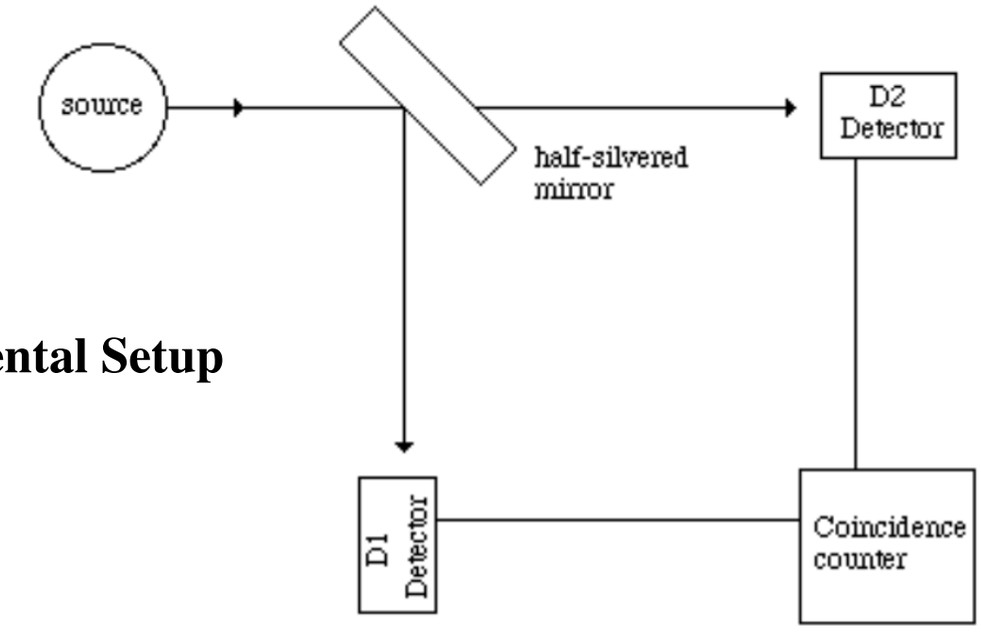
$$\ldots$$

$$\ldots$$

$$\text{particle N to be at } \vec{x}^{(N)}$$

We can demonstrate the necessity for a purely statistical interpretation for the *N*-particle wave function as follows.

Consider the experiment with photons shown in the Figure.



Experimental Setup

We have a source which emits light(photons).

This light falls on a half-silvered mirror, which allows 1/2 of the light to be transmitted though and 1/2 to be reflected as shown.

The transmitted and reflected light is detected with the two photomultipliers $D1$ and $D2$, respectively.

Finally signals generated by the detectors when they record a photon hit, are sent to a coincidence counter, which records a count when it receives two signals at the same time (one from each detector) to within some specified accuracy.

Now, suppose that the source can be described as an emitter of identical localized wave packets ($|\Psi|^2$ is nonzero only over a finite region of space).

Assume that these packets are emitted at random times, at an average rate R per second and that no more than one packet exists in a small interval Δ.

The probability of an emission in any short interval of length Δt is then

$$p = R\Delta t$$

In each of these intervals, the detectors either see a photon or they do not.

The experimental arrangement guarantees that over long periods of time each detector sees 1/2 of the emitted photons.

We can learn more about the details of what is happening as the detectors record photon hits by monitoring the temporal response of the two detectors, in particular, we can ask whether the detectors have both recorded photon hits during the same interval.

The experimental procedure is to send light into the system and record the number of coincidences relative to number of individual counts of the detectors.

The results are analyzed in terms of an anti-coincidence parameter A given by

$$A = \frac{P_c}{P_1 P_2}$$

where

P_1 = experimentally measured probability of detector 1 responding

P_2 = experimentally measured probability of detector 2 responding

P_c = experimentally measured probability of coincidences

If light is composed of single particles (photons) and photons are not divisible and $|\Psi(\vec{x},t)|^2$ = the probability per unit volume at time t that the photon will be located within some small volume about the point $\vec{x}$, then the two detectors should never both record a hit in the same interval (they are mutually exclusive events) and thus $P_c = A = 0$.

As we shall see later on when we analyze the space-time behavior of wave packets, if the photon is a wave packet, then the packet will split into two equal parts, one on each path.

This means that both detectors will always record hits during the same interval and thus $P_c = 1$.

The probability of a detector recording a count is proportional to the amount of the wave amplitude in the region of the detector, in particular, to

$$\int_{\substack{detector \\ volume}} |\Psi|^2 \, d\vec{x}$$

For a symmetrical, equal path device, this is exactly $p/2$ for each detector.

If the detectors are far apart, the respective triggerings are independent (we assume that a spacelike interval exists between the events).

Therefore, the probability of coincidence is given by

$$P_c = \frac{p^2}{4}$$

Experiments of this type were carried out by Clauser(1974) and Grangier, Roger and Aspect(1986).

They obtained $A = 0$.

This confirmed that light is photons or single particles with a statistical interpretation of the wave function and not particles represented by wave packets or wave fields of some kind.

One-Dimensional Systems

The time-independent Schrodinger equation in 1-dimension is

$$-\frac{\hbar^2}{2m}\nabla^2\psi_E(x) + V(x)\psi_E(x) = E\psi_E(x)$$

The solutions $\psi_E(x)$ are the energy eigenstates (eigenfunctions).

As we have seen, their time dependence is given by

$$\psi_E(x,t) = e^{-iEt/\hbar}\psi_E(x,0) \text{ where } \psi_E(x,0) = \langle x \,|\, E\rangle$$

and

$$\hat{H}\,|E\rangle = E\,|E\rangle \text{ where } \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

We are thus faced with solving an ordinary differential equation with boundary conditions.

Since $\psi_E(x)$ is physically related to a probability amplitude and hence to a measurable probability, we assume that $\psi_E(x)$ is continuous.

Using this assumption, we can determine the general continuity properties of $d\psi_E(x)/dx$.

The continuity property at a particular point, say $x = x_0$, is derived as follows:

$$\int_{x_0-\epsilon}^{x_0+\epsilon} \frac{d^2\psi_E(x)}{dx^2}\,dx = \int_{x_0-\epsilon}^{x_0+\epsilon} d\left(\frac{d\psi_E(x)}{dx}\right)$$

$$= -\frac{2m}{\hbar^2}\left[E\int_{x_0-\epsilon}^{x_0+\epsilon}\psi_E(x)\,dx - \int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx\right]$$

Taking the limit as $\varepsilon \to 0$ we have

$$\lim_{\epsilon\to 0}\left(\left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0+\epsilon} - \left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0-\epsilon}\right)$$

$$= -\frac{2m}{\hbar^2}\left[E\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon}\psi_E(x)\,dx - \lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx\right]$$

or

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx$$

where we have used the continuity of $\psi_E(x)$ to set

$$\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon}\psi_E(x)\,dx = 0$$

This make it clear that whether or not $d\psi_E(x)/dx$ has a discontinuity depends directly on the properties of the potential energy function.

If $V(x)$ is continuous at $x = x_0$ (harmonic oscillator example later), i.e., if

$$\lim_{\epsilon\to 0}[V(x_0+\epsilon) - V(x_0-\epsilon)] = 0$$

then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx = 0$$

and $d\psi_E(x)/dx$ is continuous at $x = x_0$.

If $V(x)$ has a *finite* discontinuity (jump) at $x = x_0$ (finite square well and square barrier examples later), i.e., if

$$\lim_{\epsilon\to 0}[V(x_0+\epsilon) - V(x_0-\epsilon)] = \text{ finite}$$

then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx = 0$$

and $d\psi_E(x)/dx$ is continuous at $x = x_0$.

Finally, if $V(x)$ has an infinite jump at $x = x_0$ (infinite square well and delta-function examples later), then we have two choices:

1. if the potential is infinite over an extended range of x (the infinite well), then we must force $\psi_E(x) = 0$ in that region and use only the continuity of $\psi_E(x)$ as a boundary condition at the edge of the region

2. if the potential is infinite at a single point, i.e., $V(x) = A\delta(x - x_0)$, then

$$\begin{aligned}\Delta\left(\frac{d\psi_E(x)}{dx}\right) &= \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} V(x)\psi_E(x)\,dx \\ &= \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} A\delta(x-x_0)\psi_E(x)\,dx \\ &= \frac{2mA}{\hbar^2}\lim_{\epsilon\to 0}\psi_E(x_0) = \frac{2mA}{\hbar^2}\psi_E(x_0)\end{aligned}$$

and, thus, $d\psi_E(x)/dx$ is discontinuous at $x = x_0$.

The last thing we must worry about is the validity of our probability interpretation of $\psi_E(x)$, i.e.,

$$\psi_E(x) = \langle x \,|\, \psi_E \rangle = \text{probability amplitude for the particle in the state } |\psi_E\rangle \text{ to be found at } x$$

which says that we must also have

$$\langle \psi_E \,|\, \psi_E \rangle = \int_{-\infty}^{\infty} |\psi_E(x)|^2 \, dx < \infty$$

This means that we must be able to normalize the wave functions and make the total probability that the particle is somewhere on the x-axis equal to one.

A wide range of interesting physical systems can be studied using 1-dimensional potential energy functions.

We will consider potentials in the form of square wells and square barriers, delta-functions, linear functions and parabolic functions.

We will now learn how to work with potentials in 1-dimension by doing a variety of different examples.

Along the way we will learn some very clever techniques and tricks and expand our understanding of the physics and mathematics of Quantum Mechanics.

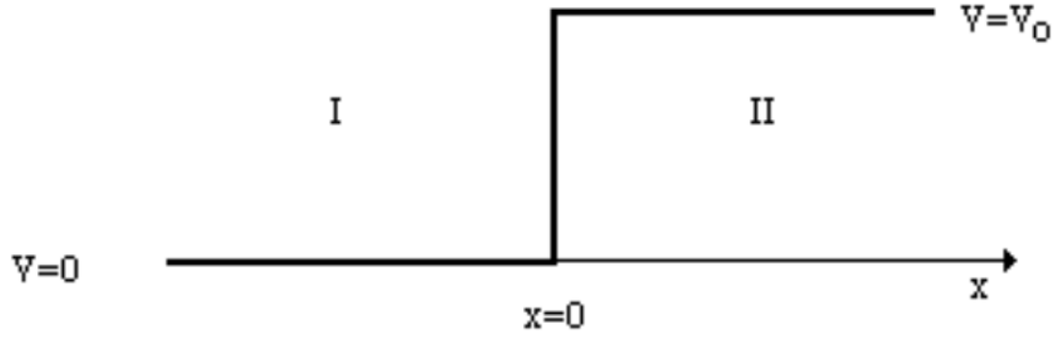
We start with a simple system to illustrate the process for solving the Schrodinger equation.

One-Dimensional Barrier

Consider the potential energy function

$$V(x) = \begin{cases} 0 & x \le 0 \\ V_0 & x \ge 0 \end{cases}$$

which looks like the Figure below.



Finite Step barrier

Since there are no infinite jumps in the potential energy function, both $\psi(x)$ and $d\psi(x)/dx$ are continuous everywhere.

We have two distinct regions to consider, which are labeled I and II in the Figure.

In region I, $V(x) = 0$ and the Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I(x)}{dx^2} = E\psi_I(x)$$

Let us define k by

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

There are two possible solutions to this equation in region I, namely,

$$\psi_I(x) = e^{\pm ikx}$$

each with energy

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

The most general solution is a linear combination of the two possible solutions

$$\psi_I(x) = Ae^{+ikx} + Be^{-ikx}$$

This is a linear combination of two waves.

Since this is an energy eigenstate it has a time dependence

$$e^{-iEt/\hbar}$$

If we insert the time dependence we have

$$\psi_I(x,t) = Ae^{+i(kx-\omega t)} + Be^{-i(kx+\omega t)} \quad , \quad \omega = \frac{E}{\hbar}$$

The first term is a traveling wave moving in the $+x$ direction with phase velocity ω/k and the second term is a traveling wave moving in the $-x$ direction with a phase velocity ω/k.

We can think of this solution in region I as representing an incident wave moving in the $+x$ direction with amplitude A and a reflected wave moving in the $-x$ direction with an amplitude B.

The reflection takes place at the potential discontinuity much the same as a reflection occurs for light on the interface between air and glass.

We will show this clearly using wave packets later in this section.

The wave packets will also allow us to relate these results to particle motion.

In region II, $V(x) = V_0$ and Schrodinger's equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} = (E - V_0)\psi_{II}(x)$$

If we define

$$\gamma^2 = \frac{2m}{\hbar^2}(E - V_0)$$

We then again have two possible solutions

$$\psi_{II}(x) = e^{\pm i\gamma x}$$

Two cases arise

$$E > V_0 \rightarrow \gamma \text{ is real} \rightarrow \text{traveling wave solutions}$$

$$E < V_0 \rightarrow \gamma \text{ is imaginary} \rightarrow \text{real exponential solutions}$$

We first consider $E > V_0$, γ real. We then have the general solution in region II

$$\psi_{II}(x) = Ce^{+i\gamma x} + De^{-i\gamma x}$$

Now the actual physical experiment we are considering must always restrict the possibilities (always remember that we are physicists and not just solving an abstract mathematical problem).

If we assume the incident wave is traveling in the $+x$ direction in region I (coming in from $x = -\infty$), then the existence of a wave in region I traveling in the $-x$ direction makes sense.

It is a reflected wave (reflection occurs at $x = 0$).

In region II, however, we cannot physically have a wave traveling in the $-x$ direction (what is its source?).

We can, however, have a wave traveling in the $+x$ direction.

It is the transmitted wave (again think of an analogy to an air-glass interface).

So, on physical grounds, we will assume that $D = 0$.

The real difference between mathematics and physics appears here!!

We then have the solutions for $E > V_0$, γ real

$$\psi_I(x) = Ae^{+ikx} + Be^{-ikx} \qquad x < 0 \quad , \quad k^2 = \frac{2m}{\hbar^2}E$$

$$\psi_{II}(x) = Ce^{+i\gamma x} \qquad x > 0 \quad , \quad \gamma^2 = \frac{2m}{\hbar^2}(E - V_0)$$

We now use the continuity conditions at $x = 0$.

$$\psi_I(0) = \psi_{II}(0) \text{ and } \frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx}$$

which give the equations

$$A + B = C \text{ and } ik(A - B) = i\gamma C$$

which imply the solutions

$$\frac{C}{A} = \frac{2k}{k + \gamma} \text{ and } \frac{B}{A} = \frac{k - \gamma}{k + \gamma}$$

We can see the physical content by looking more deeply at the probability ideas associated with the Schrodinger equation.

For a one-particle state, the Schrodinger equation formalism says that

$$\int_\Omega \psi^*(x)\psi(x)\, d^3x = \text{ probability particle is located in volume } \Omega$$

The time rate of change of this probability is

$$\frac{\partial}{\partial t}\int_\Omega \psi^*(x)\psi(x)\,d^3x = \int_\Omega \left[\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right] d^3x$$
$$= \frac{i\hbar}{2m}\int_\Omega \left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] d^3x$$
$$= \frac{i\hbar}{2m}\int_\Omega \nabla\cdot\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] d^3x$$

where we have used the time-dependent Schrodinger equation and its complex conjugate

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = i\hbar\frac{\partial\psi}{\partial t} \text{ and } -\frac{\hbar^2}{2m}\nabla^2\psi^* + V(\vec{x})\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t}$$

Since the volume Ω is arbitrary, this result implies a continuity equation of the form

$$\frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 + \nabla\cdot\vec{J}(\vec{x},t) = 0$$

where

$$\vec{J}(\vec{x},t) = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$$

is called the *probability flux vector* or the *probability current density*.

Using the barrier solutions for $E > V_0$, γ real, we have (for x-components)

$$J_I(x,t) = \frac{i\hbar}{2m}(A^*e^{-ikx} + B^*e^{ikx})(ikAe^{ikx} - ikBe^{-ikx})$$
$$- \frac{i\hbar}{2m}(Ae^{ikx} + Be^{-ikx})(ikA^*e^{-ikx} - ikB^*e^{ikx})$$
$$= \frac{\hbar k}{m}\left[|A|^2 - |B|^2\right] = J_{I+} - J_{I-}$$

$$J_{II}(x,t) = \frac{i\hbar}{2m}\left[(C^* e^{-i\gamma x})(i\gamma C e^{i\gamma x}) - (C e^{i\gamma x})(-i\gamma C^* e^{-i\gamma x})\right]$$
$$= \frac{\hbar\gamma}{m}|C|^2 = J_{II+}$$

We then define the reflection and transmission probabilities in terms of the current as

$$R = \frac{J_{I-}}{J_{I+}} = \frac{|B|^2}{|A|^2} \text{ and } T = \frac{J_{II+}}{J_{1+}} = \frac{\gamma}{k}\frac{|C|^2}{|A|^2}$$

Now, physically, we identify

$$|A|^2 = \text{incident beam intensity}$$
$$|B|^2 = \text{reflected beam intensity}$$
$$|C|^2 = \text{transmitted beam intensity}$$

and therefore

R = probability that an incident wave will be reflected

T = probability that an incident wave will be transmitted

We find

$$R = \frac{(k-\gamma)^2}{(k+\gamma)^2} \text{ and } T = \frac{4k\gamma}{(k+\gamma)^2}$$

Notice that

$$R + T = 1$$

which makes physical sense since the total probability for the wave to go somewhere must equal one.

In the book, I now recast the case $E > V_0$ in terms of the wave packet formalism derived earlier.

This allows us to make particle interpretations.

I will skip that section in these lectures.

Now what happens if $E = p^2/2m < V_0$?

We then have the solutions (let $A = 1$)

$$x < 0 \qquad \psi_I = e^{ikx} + Re^{-ikx}$$

$$x > 0 \qquad \psi_{II} = Se^{-\beta x}$$

where $\hbar k = \sqrt{2mE}$ and $\hbar\beta = \sqrt{2m(V_0 - E)}$.

We have excluded the mathematical solution $e^{\beta x}$ for $x > 0$ because it would cause the integral

$$\int_{-\infty}^{\infty} |\psi|^2 \, dx$$

to diverge, which means it is a *non-normalizable* or *unphysical solution*.

This is an example of a solution not being well-behaved.

At $x = 0$, we have the continuity conditions which give

$$1 + R = S \text{ and } 1 - R = -\frac{\beta}{ik}S \text{ or}$$

$$S = \frac{2ik}{ik - \beta} \text{ and } R = \frac{ik + \beta}{ik - \beta}$$

Since the solution for $x > 0$ is not a traveling wave, there is no transmitted packet.

The incident wave packet analysis is the same as before.

The reflected wave packet analysis is different because $R(p)$ is not a real function.

In fact,

$$|R|^2 = 1 \rightarrow R = e^{i\phi} = \frac{ip + \sqrt{2mV_0 - p^2}}{ip - \sqrt{2mV_0 - p^2}}$$

$$= \frac{ip + \sqrt{2mV_0 - p^2}}{ip - \sqrt{2mV_0 - p^2}} \frac{ip + \sqrt{2mV_0 - p^2}}{ip + \sqrt{2mV_0 - p^2}}$$

or

$$e^{i\phi} = \frac{p^2 - mV_0 - ip\sqrt{2mV_0 - p^2}}{mV_0} = \cos\phi + i\sin\phi$$

with

$$\cos\phi = \frac{p^2 - mV_0}{mV_0} \text{ and } \sin\phi = -\frac{p\sqrt{2mV_0 - p^2}}{mV_0}$$

Therefore, we have as wave packet representations

$$\psi_{inc}(x,t) = \int_0^\infty \frac{dp}{2\pi\hbar} f(p) f(p) e^{i(px - Et)/\hbar} \text{ where } E = \frac{p^2}{2m},\ p = \hbar k$$

$$\psi_{refl}(x,t) = \int_0^\infty \frac{dp}{2\pi\hbar} f(p) f(p) e^{-i(px + Et - \hbar\phi(p))/\hbar}$$

$$\text{where } E = \frac{p^2}{2m},\ p = \hbar k$$

The stationary phase argument implies

$$x = \frac{p_0}{m} t = v_0 t \text{ for the incident packet}$$

which says that the incident packet arrives at x = 0 at t = 0 and

$$x = -\frac{p_0}{m}t + \hbar \left.\frac{\partial\phi(p)}{\partial p}\right|_{p=p_0} \quad \text{for the reflected packet}$$

This says that the reflected wave packet leaves $x = 0$ at

$$t = t_{delay} = \frac{\hbar m}{p_0} \left.\frac{\partial\phi(p)}{\partial p}\right|_{p=p_0}$$

which is NOT the same time that the incident packet arrived!

Continuing we have

$$\frac{\partial \cos\phi(p)}{\partial p} = -\sin\phi(p)\frac{\partial\phi(p)}{\partial p} = \frac{2p}{mV_0}$$

$$\frac{\partial\phi(p)}{\partial p} = \frac{2}{\sqrt{2mV_0 - p_0^2}}$$

which gives

$$t_{delay} = \frac{m\hbar}{p_0}\frac{2}{\sqrt{2mV_0 - p_0^2}} = \frac{2m}{p_0}\frac{1}{\beta}$$

Now, we found that

$$\psi_{II}(x) = Se^{-\beta x}$$

which says that the probability amplitude is significantly different from zero up to a distance $d = 1/\beta$ approximately.

In other words,

$$\psi_{II}(x = 1/\beta) = \frac{1}{e}\psi_{II}(x = 0) \rightarrow |\psi_{II}(x = 1/\beta)|^2 \approx \frac{1}{7}|\psi_{II}(x = 0)|^2$$

Therefore, to a good approximation, we have the striking result $t_{\text{delay}} = 2d/v_0$.

What does this mean?

It seems as if there is a nonzero probability for finding the particle in the classically forbidden region $x > 0$, where K = kinetic energy = $E - V_0 < 0$ since $\psi_{\text{II}}(x) = e^{-\beta x} \neq 0$ there.

Since K cannot be less than zero, it seems like we must have a violation of conservation of energy if the particle were actually found in the region $x > 0$.

This is NOT the case, however.

If we observe the particle in this forbidden region, then it will no longer be in a state with $E < V_0$.

The act of measuring the location of the particle must necessarily introduce an uncertainty in p and hence in E.

The particle seems to have an appreciable probability to exist in the region up to a distance $d = 1/\beta$.

If we observe the particle on the right, we have then localized it such that $\Delta x \approx 1/\beta$.

This says that we have introduced an uncertainty in p

$$\Delta p \geq \frac{\hbar}{\Delta x} \approx \hbar\beta$$

and a corresponding energy uncertainty

$$\Delta E \approx \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2\beta^2}{2m} = V_0 - E$$

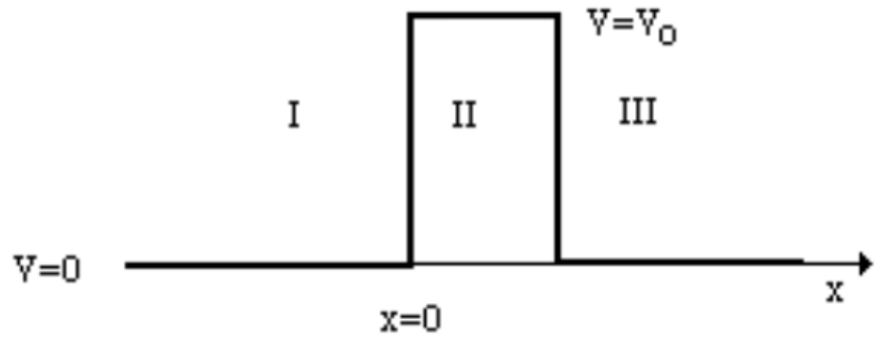
This implies that E is now uncertain enough that we can no longer claim that energy conservation has been violated!

Quantum mechanics has a way of covering its own tracks!

Tunneling

We now change the potential energy function so that the barrier (step) is not infinitely thick (which prevented a traveling wave from existing for $E < V_0$, $x > 0$.

The new potential energy function is shown in the Figure below.



Finite Step - Finite Width barrier

For $E > V_0$ the results are similar to infinitely thick barrier and no new physical ideas appear.

For $E < V_0$, however, we get some very interesting new physical results.

As we shall see, it turns out that a real traveling wave can appear on the other side of the barrier (even though there are no sources on that side) in this case.

This is called **quantum tunneling**.

Let us see how it works.

We have three regions I, II and III to consider as shown in the Figure.

We get the solutions

$$x \le 0 \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$$

$$\psi_I = A_1 e^{ikx} + B_1 e^{-ikx} \quad , \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \ , \ k \text{ real}$$

$$0 \le x \le a \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + V_0\psi_{II} = E\psi_{II}$$

$$\psi_{II} = Ce^{\gamma x} + De^{-\gamma x} \quad , \quad V_0 - E = \frac{p^2}{2m} = \frac{\hbar^2\gamma^2}{2m} \ , \ \gamma \text{ real}$$

$$x \ge a \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}$$

$$\psi_{III} = A_2e^{ikx} + B_2e^{-ikx} \quad , \quad E = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m} \ , \ k \text{ real}$$

The probability current does not vanish at $x = \pm\infty$, which implies that we must assume the existence of distant sources and sinks of probability(or particles).

We have two sets of continuity equations (at $x = 0$ and $x = a$).

At $x = 0$ we get

$$\psi_I(0) = \psi_{II}(0) \rightarrow A_1 + B_1 = C + D$$

$$\frac{d\psi_I(0)}{dx}\frac{d\psi_{II}(0)}{dx} \rightarrow ik(A_1 - B_1) = \gamma(C - D)$$

and at $x = a$ we get

$$\psi_{II}(a) = \psi_{III}(a) \rightarrow Ce^{\gamma a} + De^{-\gamma a} = A_2e^{ika} + B_2e^{-ika}$$

$$\frac{d\psi_{II}(a)}{dx}\frac{d\psi_{III}(a)}{dx} \rightarrow \gamma(Ce^{\gamma a} - De^{-\gamma a}) = ik(A_2e^{ika} - B_2e^{-ika})$$

We can restate these equations in matrix form.

At $x = 0$ we get

$$\begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{M}_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \gamma & -\gamma \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = \hat{M}_2 \begin{pmatrix} C \\ D \end{pmatrix}$$

and at $x = a$ we get

$$\begin{pmatrix} e^{\gamma a} & e^{-\gamma a} \\ \gamma e^{\gamma a} & -\gamma e^{-\gamma a} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = \hat{M}_3 \begin{pmatrix} C \\ D \end{pmatrix}$$

$$= \begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \hat{M}_4 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

The transmission/reflection properties of the barrier are given by the coefficients A_1, B_1, A_2, B_2, which we assume are related by a transfer matrix $\hat{Y}$, where

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{Y}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

We then have

$$\hat{M}_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{M}_2 \begin{pmatrix} C \\ D \end{pmatrix} \rightarrow \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{M}_1^{-1}\hat{M}_2 \begin{pmatrix} C \\ D \end{pmatrix}$$

$$\hat{M}_3 \begin{pmatrix} C \\ D \end{pmatrix} = \hat{M}_4 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} \rightarrow \begin{pmatrix} C \\ D \end{pmatrix} = \hat{M}_3^{-1}\hat{M}_4 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

or

$$\hat{Y} = \hat{M}_1^{-1}\hat{M}_2\hat{M}_3^{-1}\hat{M}_4$$

A great deal of algebra gives

$$Y_{11} = e^{ika}\left[\cosh\gamma a + \frac{1}{2}i\sinh\gamma a\left(\frac{\gamma}{k} - \frac{k}{\gamma}\right)\right]$$

$$Y_{12} = \frac{1}{2}e^{-ika}\sinh\gamma a\left(\frac{\gamma}{k} + \frac{k}{\gamma}\right)$$

$$Y_{21} = -\frac{1}{2}ie^{ika}\sinh\gamma a\left(\frac{\gamma}{k} + \frac{k}{\gamma}\right)$$

$$Y_{22} = e^{-ika}\left[\cosh\gamma a - \frac{1}{2}i\sinh\gamma a\left(\frac{\gamma}{k} - \frac{k}{\gamma}\right)\right]$$

If we have sources only on the left of the barrier, then we must choose $B_2 = 0$.

The currents are

$$J_{LEFT}(x,t) = \frac{\hbar k}{m}\left[|A_1|^2 - |B_1|^2\right]$$
$$= J_{LEFT+}(x,t) - J_{LEFT-}(x,t) \qquad x < 0$$

$$J_{RIGHT}(x,t) = J_{RIGHT+}(x,t) = \frac{\hbar k}{m}|A_2|^2 \qquad x > 0$$

The reflection and transmission probabilities are given by

$$R = \frac{|B_1|^2}{|A_1|^2} = \frac{|Y_{21}|^2}{|Y_{11}|^2} \quad , \quad T = \frac{|A_2|^2}{|A_1|^2} = \frac{1}{|Y_{11}|^2}$$

Algebra shows $R+T = 1$ as it must in order to conserve probability (or particles).

Evaluating the expression for T we get

$$T = \frac{1}{1 + \frac{V_0^2\sinh^2\gamma a}{4E(V_0 - e)}} \quad , \quad \gamma^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

The fact that $T > 0$ for $E < V_0$ implies the existence of tunneling.

The probability amplitude leaks through the barrier.

It is important to realize that the fact that $T > 0$, **DOES NOT** say that particles or wave packets passed through the barrier.

No measurement can be done on the system that will allow us to observe a particle in the region $0 < x < a$ with $E < V_0$, since this would violate energy conservation.

It is **ONLY** probability that is leaking through.

If this causes the probability amplitude and hence the probability to be nonzero on the other side of the barrier, than it *must be possible for us to observe* the particle on the other side, i.e., we can observe the particle on the left side of the barrier with $E < V_0$, but we can never observe it in the region of the barrier with $E < V_0$.

That is what is being said here.

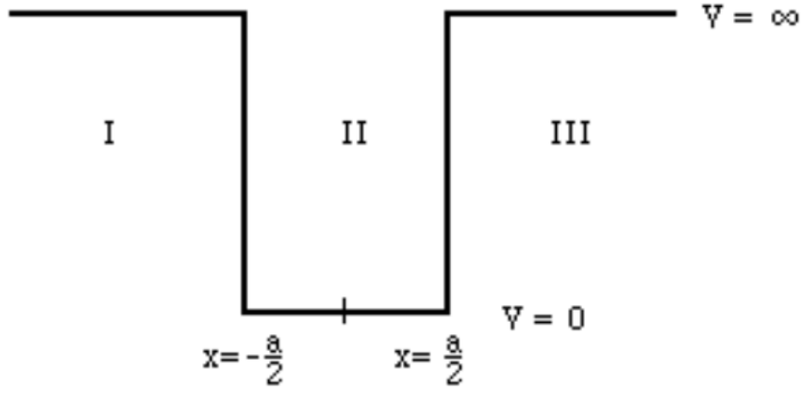
Bound States

Infinite Square Well

We now consider the potential energy function

$$V(x) = \begin{cases} 0 & -\frac{a}{2} \le x \le \frac{a}{2} \\ \infty & |x| \ge \frac{a}{2} \end{cases}$$

This is the so-called *infinite square well* shown in the Figure.



Infinite Square Well

This is an example of a potential that is infinite in an extended region.

Therefore, we must require that the wave function $\psi(x) = 0$ in these regions or the Schrodinger equation makes no sense mathematically.

In this case we have

$$\psi_I(x) = 0 \text{ and } \psi_{III}(x) = 0$$

In region II we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

and

$$\psi_{II}(x) = Ae^{ikx} + Be^{-ikx}$$

The continuity of the wavefunction at $x = \pm a/2$ says that we must have

$$\psi_{II}\left(-\frac{a}{2}\right) = Ae^{-ika/2} + Be^{ika/2} = 0$$

$$\psi_{II}\left(\frac{a}{2}\right) = Ae^{ika/2} + Be^{-ika/2} = 0$$

which imply that

$$\frac{B}{A} = -e^{-ika} = -e^{ika}$$

This is an equation for the allowed values(values corresponding to a valid solution) of k.

This equation is

$$e^{2ika} = 1$$

The allowed values of *k* form a discrete spectrum of energy eigenvalues (quantized energies) given by

$$2k_n a = 2n\pi \rightarrow k_n = \frac{n\pi}{a} \rightarrow E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}\ ,\ n = 1, 2, 3, 4, \ldots$$

The corresponding wave functions are

$$\begin{aligned}\psi_{II}^{(n)}(x) &= A_n(e^{ik_n x} - e^{-ik_n a}e^{-ik_n x}) \\ &= A_n e^{-ik_n a/2}(e^{ik_n(x+a/2)} - e^{-ik_n(x+a/2)}) \\ &= \tilde{A}_n \sin k_n(x + a/2)\end{aligned}$$

where $\tilde{A}_n$ is determined bv the normalization condition

$$\int_{-a/2}^{a/2} |\psi_n(x)|^2\, dx = 1$$

Substituting the value of k_n we get

$$\begin{aligned}\psi_{II}^{(1)}(x) &= \tilde{A}_1 \sin k_1(x + a/2) = \tilde{A}_1 \sin \pi(x + a/2)/a \\ &= \tilde{A}_1 \sin(\pi x/a + \pi/2) = \tilde{A}_1 \cos(\pi x/a)\end{aligned}$$

$$\begin{aligned}\psi_{II}^{(2)}(x) &= \tilde{A}_2 \sin k_2(x + a/2) = \tilde{A}_2 \sin 2\pi(x + a/2)/a \\ &= \tilde{A}_2 \sin(2\pi x/a + \pi) = \tilde{A}_2 \sin(2\pi x/a)\end{aligned}$$

$$\begin{aligned}\psi_{II}^{(3)}(x) &= \tilde{A}_3 \sin k_3(x + a/2) = \tilde{A}_3 \sin 3\pi(x + a/2)/a \\ &= \tilde{A}_3 \sin(3\pi x/a + 3\pi/2) = \tilde{A}_3 \cos(3\pi x/a)\end{aligned}$$

or

$$\psi_{II}(x) = \begin{cases} \sin(n\pi x/a) & \text{n even} \\ \cos(n\pi x/a) & \text{n odd} \end{cases} \qquad n = 1, 2, 3, 4, \ldots$$

We have mathematically solved the ordinary differential equation problem, now what is the physical meaning of these results?

We find a discrete spectrum of allowed energies corresponding to bound states of the Hamiltonian; *the energy is quantized*.

Bound states designate states which are localized in space, i.e., the probability is large only over restricted regions of space and goes to zero far from the potential region.

The *lowest* energy value or lowest energy *level* or *ground state energy* is

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2} > 0$$

with

$$\psi_1(x) = \begin{cases} A\cos(n\pi x/a) & |x| \le \frac{a}{2} \\ 0 & |x| \ge \frac{a}{2} \end{cases} \qquad n = 1, 2, 3, 4, \ldots$$

This minimum energy is not zero because of the Heisenberg uncertainty principle.

Since the particle has a nonzero amplitude for being in the well, we say that it is localized such that $\Delta x \approx a$ and thus

$$\Delta p \ge \frac{\hbar}{\Delta x} \approx \frac{\hbar}{a}$$

This says that the kinetic energy (or energy in this case because the potential energy equals zero in region II) must have a minimum value given approximately by

$$E_{min} = K_{min} \approx \frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2}$$

Let us look more closely at the wave functions.

The integer $n-1$ corresponds to the number of nodes (zeros) of the wave function (other than the well edges).

They also have the property

$$\psi(-x) = \psi(x) \text{ for n odd and } \psi(-x) = -\psi(x) \text{ for n even}$$

The above discrete transformation of the wave function corresponds to the *parity* operator $\hat{\mathcal{P}}$ where we have

$$\hat{\mathcal{P}}\psi(x) = \psi(-x) = \psi(x) \text{ means even parity}$$

$$\hat{\mathcal{P}}\psi(x) = \psi(-x) = -\psi(x) \text{ means odd parity}$$

Let us look more generally at the parity operation.

Suppose that the potential energy function obeys the rule $V(\vec{\mathrm{x}}) = V(-\vec{\mathrm{x}})$ and let $\psi(\vec{\mathrm{x}})$ be a solution of the Schrodinger equation with energy E

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x}) = E\psi(\vec{x})$$

Now let $\vec{\mathrm{x}} \rightarrow -\vec{\mathrm{x}}$ to get the equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(-\vec{x})\right)\psi(-\vec{x}) = E\psi(-\vec{x})$$

or

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(-\vec{x}) = E\psi(-\vec{x})$$

This says that, if $\psi(\vec{x})$ is a solution of the Schrodinger equation with energy E, then $\psi(-\vec{x})$ is also a solution of the Schrodinger equation with the same energy E.

This says that the combinations

$$\psi(\vec{x}) \pm \psi(-\vec{x})$$

are also solutions of the Schrodinger equation with the same energy E.

Now

$$\psi(\vec{x}) + \psi(-\vec{x}) \rightarrow \text{ an even parity solution}$$
$$\psi(\vec{x}) - \psi(-\vec{x}) \rightarrow \text{ an odd parity solution}$$

This says that if $V(\vec{x}) = V(-\vec{x})$ (a symmetric potential), then we can always choose solutions that have a definite parity (even or odd).

We formally define the *parity operator* by the relation

$$\langle \vec{x} | \hat{\mathcal{P}} | \psi \rangle = \langle -\vec{x} | \psi \rangle$$

Since

$$\langle \vec{x} | \hat{\mathcal{P}}^2 | \psi \rangle = \langle -\vec{x} | \hat{\mathcal{P}} | \psi \rangle = \langle \vec{x} | \psi \rangle$$

we must have

$$\hat{\mathcal{P}}^2 = \hat{I}$$

which means the eigenvalues of $\hat{\mathcal{P}}$ are ±1 as we indicated earlier.

This also says that $\hat{\mathcal{P}}^{-1} = \hat{\mathcal{P}}$.

We can show $[\ \hat{H}\ ,\ \hat{\mathcal{P}}\ ] = 0$ for symmetric potentials by

$$\hat{\mathcal{P}}\hat{H}\,|E\rangle = \hat{\mathcal{P}}E\,|E\rangle = E\hat{\mathcal{P}}\,|E\rangle = \pm E\,|E\rangle$$

$$\hat{H}\hat{\mathcal{P}}\,|E\rangle = \pm\hat{H}\,|E\rangle = \pm E\,|E\rangle$$

$$(\hat{\mathcal{P}}\hat{H} - \hat{H}\hat{\mathcal{P}})\,|E\rangle = 0$$

$$[\hat{H}, \hat{\mathcal{P}}] = 0$$

since $|E\rangle$ is an arbitrary state.

As we saw earlier, this commutator relationship says that

$$\hat{H}\hat{\mathcal{P}} = \hat{\mathcal{P}}\hat{H}$$

$$\hat{\mathcal{P}}\hat{H}\hat{\mathcal{P}} = \hat{\mathcal{P}}^2\hat{H} = \hat{H}$$

$$\hat{\mathcal{P}}^{-1}\hat{H}\hat{\mathcal{P}} = \hat{H}$$

which means that $\hat{H}$ is invariant under the $\hat{\mathcal{P}}$ transformation.

We have used $\hat{\mathcal{P}}^2 = \hat{I}$ in this derivation.

It also says that

$$\hat{H}(\hat{\mathcal{P}}\,|E\rangle) = \hat{\mathcal{P}}\hat{H}\,|E\rangle = E(\hat{\mathcal{P}}\,|E\rangle)$$

or $\hat{\mathcal{P}}\,|E\rangle$ is an eigenstate of $\hat{H}$ with energy E as we stated above.

The concept of parity invariance and the fact that $\hat{H}$ and $\hat{\mathcal{P}}$ share a common set of eigenfunctions can greatly simplify the solution of the Schrodinger equation in many cases.

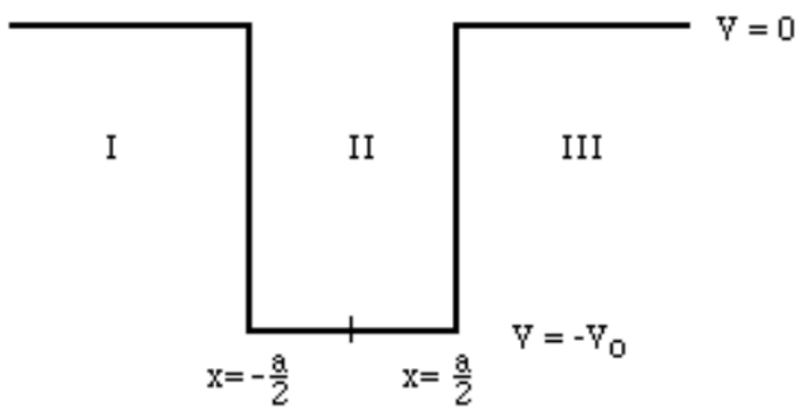
stop

The Finite Square Well

We now consider the potential energy function

$$V(x) = \begin{cases} -V_0 & |x| \le \frac{a}{2} \\ 0 & |x| \ge \frac{a}{2} \end{cases}$$

This is the so-called *finite square well* (in one dimension) and it is shown in the Figure below.



Finite Square Well

The solutions are:

Region I : $x < \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I \ , 0 \ge E \ge -V_0 \ , \hbar^2 k^2 = 2m|E| \ , E = -|E|$$

with solutions

$$\psi_I(x) = Ae^{-kx} + Be^{kx}$$

Since $x = -\infty$ is included in this region, we must exclude the e^{-kx} term by choosing $A = 0$, which gives

$$\psi_I(x) = Be^{kx} \qquad x < -\frac{a}{2}$$

Region II: $-\frac{a}{2} \leq x \leq \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} - V_0\psi_{II} = E\psi_{II}\ , 0 \geq E \geq -V_0\ , p^2 = 2m(V_0 - |E|)\ , E = -|E|$$

with solutions

$$\psi_{II}(x) = Ce^{ipx/\hbar} + De^{-ipx/\hbar}$$

Region III: $x > \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}\ , 0 \geq E \geq -V_0\ , \hbar^2k^2 = 2m|E|\ , E = -|E|$$

with solutions

$$\psi_{III}(x) = Fe^{kx} + Ge^{-kx}$$

Since x = +∞ is included in this region, we must exclude the e^{kx} term by choosing $F = 0$, which gives

$$\psi_{III}(x) = Ge^{-kx}$$

These results represent a general solution to the problem.

There seems to be 4 unknown constants, namely, B, C, D, and G.

However, since $V(x) = V(-x)$, parity is conserved and we can choose even and odd solutions, or solutions of definite parity.

Even parity implies $\psi(x) = \psi(-x)$ or $G = B$ and $C = D$.

This solution is

$$\psi(x) = \begin{cases} C\cos px/\hbar & |x| \le \frac{a}{2} \\ Be^{-kx} & x > \frac{a}{2} \\ Be^{kx} & x < -\frac{a}{2} \end{cases}$$

Odd parity implies $\psi(x) = -\psi(-x)$ or $G = -B$ and $D = -C$.

This solution is

$$\psi(x) = \begin{cases} C\sin px/\hbar & |x| \le \frac{a}{2} \\ Be^{-kx} & x > \frac{a}{2} \\ -Be^{kx} & x < -\frac{a}{2} \end{cases}$$

Thus, by using parity we reduce the number of unknowns in the problem to two for each type of solution.

We now impose the continuity conditions of the wave function and its derivative only at $x = a/2$ for both solutions.

Since these are definite parity solutions the continuity condition at $x = -a/2$ will give no new information and is not needed.

Even Parity Results

$$C\cos pa/2\hbar = Be^{-ka/2} \text{ and } -\frac{p}{\hbar}C\sin pa/2\hbar = -kBe^{-ka/2}$$

or

$$\frac{B}{C} = e^{ka/2}\cos pa/2\hbar = \frac{p}{\hbar k}e^{ka/2}\sin pa/2\hbar$$

so that

$$p\tan pa/2\hbar = \hbar k$$

This last equation is a transcendental equation for E and its solutions determine the allowed E values for the even parity states for this potential energy function.

These E values are the even parity energies or energy levels of a particle in the finite square well potential.

Odd Parity Results

$$C\sin pa/2\hbar = Be^{-ka/2} \text{ and } \frac{p}{\hbar}C\cos pa/2\hbar = -kBe^{-ka/2}$$

or

$$\frac{B}{C} = e^{ka/2}\sin pa/2\hbar = \frac{p}{\hbar k}e^{ka/2}\cos pa/2\hbar$$

so that

$$p\cot pa/2\hbar = -\hbar k$$

Again, this last equation is a transcendental equation for E and its solutions determine the allowed E values for the odd parity states for this potential energy function.

These E values are the odd parity energies or energy levels of a particle in the finite square well potential.

In general, at this stage of the solution, we must either devise a clever numerical or graphical trick to find the solutions of the transcendental equations or resort to a computer.

The first thing one should always do is change variables to get rid of as many extraneous constants as possible.

In this case we let

$$\beta = ka = \frac{a}{\hbar}\sqrt{2m|E|} \quad , \quad \alpha = \gamma a = \frac{p}{\hbar}a = \frac{a}{\hbar}\sqrt{2m(V_0 - |E|)}$$

The first useful equation we can derive is

$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} = \text{ constant for a given well}$$

This is the equation of a circle of radius

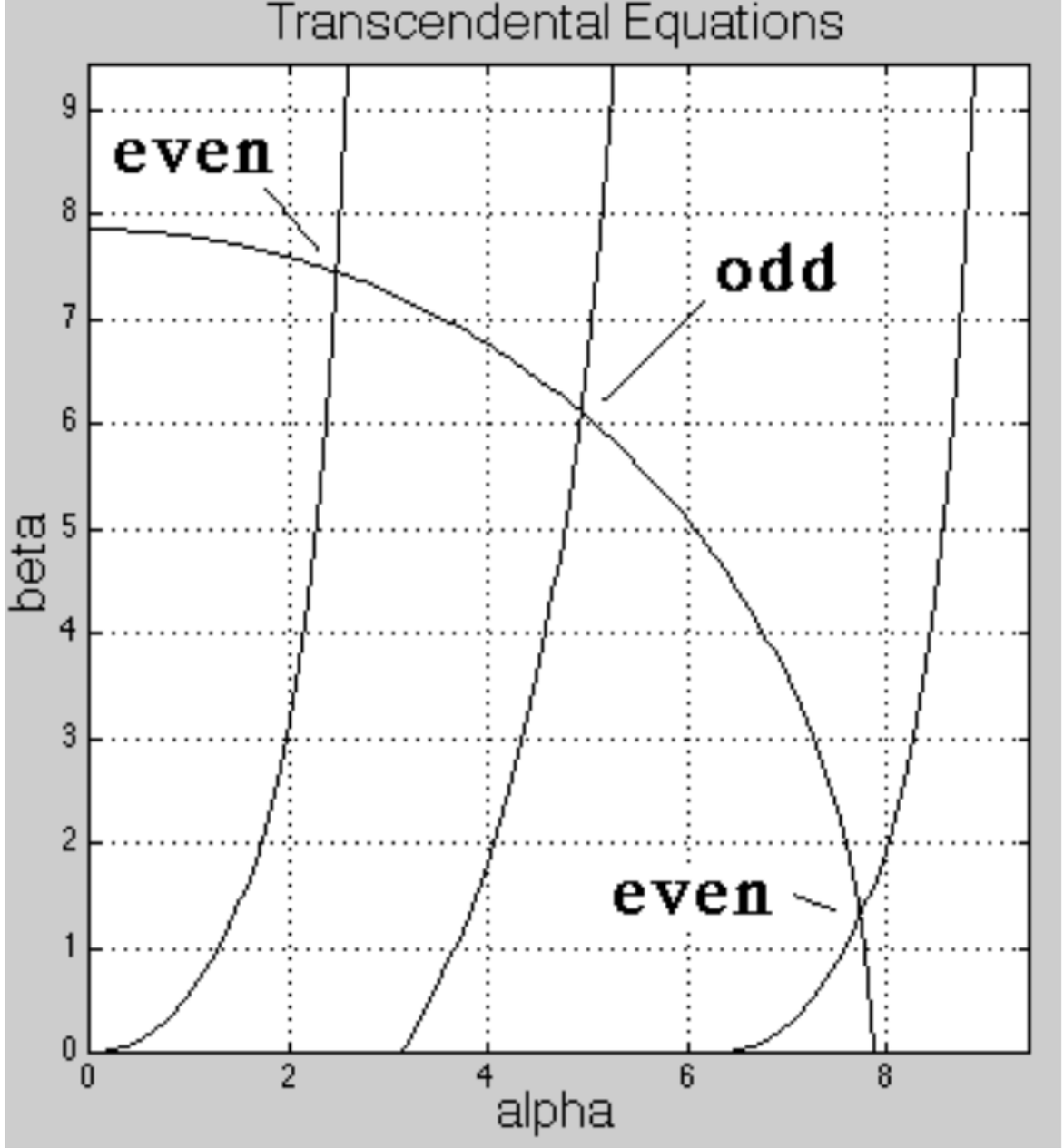
$$\sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

With these new variables the two transcendental equations are

$$\beta = \alpha \tan\frac{\alpha}{2} \text{ for even parity and } \beta = -\alpha \cot\frac{\alpha}{2} \text{ for odd parity}$$

We can find solutions graphically by plotting as shown in the Figure on the next slide for the case (effectively a choice of the quantity $V_0\, a^2$)

$$\text{circle radius } = \sqrt{\frac{2mV_0a^2}{\hbar^2}} = \frac{5\pi}{2}$$



Solutions for $\sqrt{\frac{2mV_0a^2}{\hbar^2}} = \frac{5\pi}{2}$

The solutions correspond to the intersections of the circle (fixed for a given well) and the curves represented by the two transcendental equations.

They are shown in the Figure.

For the choice of potential well shown in the figure we have 2 even parity solutions and 1 odd parity solution.

These correspond to the allowed energy levels for this particular well and the corresponding wave functions and energies represent bound states of the well.

We can also do a straight numerical solution for even parity by rearranging the equations as follows:

$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} \text{ and } \beta = \alpha \tan\frac{\alpha}{2}$$

$$\alpha^2\left(1 + \tan^2\frac{\alpha}{2}\right) = \frac{2mV_0a^2}{\hbar^2}$$

$$\alpha^2 - \frac{25\pi^2}{4}\cos^2\frac{\alpha}{2} = f(\alpha) = 0$$

The numerical solution of this equation can be carried out by any standard technique (Newton-Raphson method, for instance) for finding the zeros of the function f(α).

For this case we get

$$\alpha = 2.4950 \text{ and } 7.1416$$

which is clearly in agreement with the graphical result.

Transmission Resonances

As we have seen the spectrum of energies for the square well is made up of a **finite** number of bound-state levels.

The most important feature of a bound-state wave function is that it is localized in space, i.e., it falls off exponentially as we move away from the well.

Another interesting feature of the square well has to do with the continuous part of its energy spectrum.

All energy states with $E > 0$ are allowed.

Again there are three regions to consider, labeled in the same way as earlier.

We will again assume that we have a wave incident from the left (from $x = -\infty$) with unit intensity

$$\psi_I(x) = e^{ikx} + Be^{-ikx} \text{ where } E = \frac{\hbar^2 k^2}{2m}$$

where B is the amplitude for the reflected wave.

In region II, which is over the well, we have the solution

$$\psi_{II}(x) = Ce^{ik_1 x} + De^{-ik_1 x} \text{ where } E + V_0 = \frac{\hbar^2 k_1^2}{2m}$$

In region III, we only have a transmitted wave as the solution

$$\psi_{III}(x) = Fe^{ikx} \text{ where } E = \frac{\hbar^2 k^2}{2m}$$

Again, we must match the wave functions and their derivatives at $x = \pm a/2$.

This gives us 4 equations for the 4 unknown coefficients.

Usually an author now says that *lots of algebra* gives us the transmission coefficient and writes down the answer.

Let us actually do it just once.

Continuity of the wave function and its derivative at $x = -a/2$ gives

$$e^{-ika/2} + Be^{ika/2} = Ce^{-ik_1 a/2} + De^{ik_1 a/2}$$
$$ike^{-ika/2} - ikBe^{ika/2} = ik_1 Ce^{-ik_1 a/2} - ik_1 De^{ik_1 a/2}$$

Continuity of the wave function and its derivative at $x = +a/2$ gives

$$Fe^{ika/2} = Ce^{ik_1 a/2} + De^{-ik_1 a/2}$$
$$ikFe^{ika/2} = ik_1 Ce^{ik_1 a/2} - ik_1 De^{-ik_1 a/2}$$

Then

$$ik_1 e^{-ika/2} + ik_1 Be^{ika/2} = ik_1 Ce^{-ik_1 a/2} + ik_1 De^{ik_1 a/2}$$
$$ike^{-ika/2} - ikBe^{ika/2} = ik_1 Ce^{-ik_1 a/2} - ik_1 De^{ik_1 a/2}$$
$$ik_1 Fe^{ika/2} = ik_1 Ce^{ik_1 a/2} + ik_1 De^{-ik_1 a/2}$$
$$ikFe^{ika/2} = ik_1 Ce^{ik_1 a/2} - ik_1 De^{-ik_1 a/2}$$

Solving for C and D we get

$$2ik_1 Ce^{-ik_1 a/2} = i(k + k_1)e^{-ika/2} - i(k - k_1)Be^{ika/2}$$
$$2ik_1 De^{ik_1 a/2} = -i(k - k_1)e^{-ika/2} + i(k + k_1)Be^{ika/2}$$
$$2ik_1 Ce^{ik_1 a/2} = i(k + k_1)Fe^{ika/2}$$
$$2ik_1 De^{-ik_1 a/2} = -i(k - k_1)Fe^{ika/2}$$

Rearranging we have

$$C = \left(\frac{k+k_1}{2k_1}\right) Fe^{-ik_1 a/2} e^{ika/2} = e^{ik_1 a/2}\left[\left(\frac{k+k_1}{2k_1}\right) e^{-ika/2} - \left(\frac{k-k_1}{2k_1}\right) Be^{ika/2}\right]$$
$$D = -\left(\frac{k-k_1}{2k_1}\right) Fe^{ik_1 a/2} e^{ika/2} = e^{-ik_1 a/2}\left[-\left(\frac{k-k_1}{2k_1}\right) e^{-ika/2} + \left(\frac{k+k_1}{2k_1}\right) Be^{ika/2}\right]$$

Therefore

$$\left(\frac{k+k_1}{2k_1}\right) Fe^{-ik_1 a} e^{ika/2} - \left(\frac{k+k_1}{2k_1}\right) e^{-ika/2} = -\left(\frac{k-k_1}{2k_1}\right) Be^{ika/2}$$
$$-\left(\frac{k-k_1}{2k_1}\right) Fe^{ik_1 a} e^{ika/2} + \left(\frac{k-k_1}{2k_1}\right) e^{-ika/2} = \left(\frac{k+k_1}{2k_1}\right) Be^{ika/2}$$

Dividing we get

$$\frac{\left(\frac{k+k_1}{2k_1}\right)Fe^{-ik_1a}e^{ika/2}-\left(\frac{k+k_1}{2k_1}\right)e^{-ika/2}}{-\left(\frac{k-k_1}{2k_1}\right)Fe^{ik_1a}e^{ika/2}+\left(\frac{k-k_1}{2k_1}\right)e^{-ika/2}}=\frac{-\left(\frac{k-k_1}{2k_1}\right)}{\left(\frac{k+k_1}{2k_1}\right)}$$

$$(k+k_1)^2\left[Fe^{-ik_1a}e^{ika/2}-e^{-ika/2}\right]=-(k-k_1)^2\left[-Fe^{ik_1a}e^{ika/2}+e^{-ika/2}\right]$$

or

$$\left[(k+k_1)^2e^{-ik_1a}-(k-k_1)^2e^{ik_1a}\right]e^{ika/2}F$$
$$=-(k-k_1)^2e^{-ika/2}+(k+k_1)^2e^{-ika/2}$$

Finally we solve for the transmission coefficient F to get

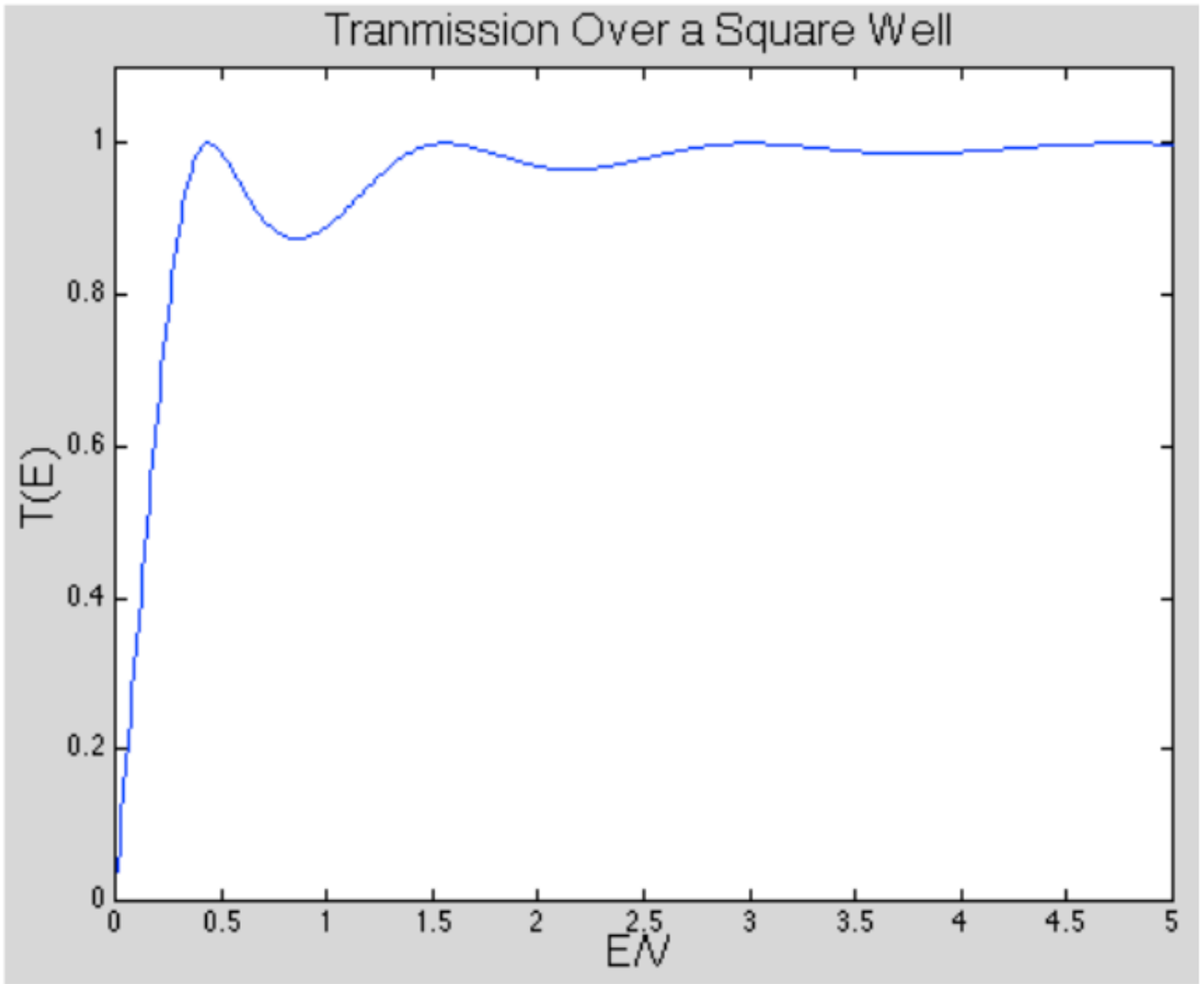
$$F=\frac{(k+k_1)^2-(k-k_1)^2}{(k+k_1)^2e^{-ik_1a}-(k-k_1)^2e^{ik_1a}}e^{-ika}$$
$$=\frac{4kk_1}{(k^2+k_1^2)(e^{-ik_1a}-e^{ik_1a})+2kk_1(e^{-ik_1a}+e^{ik_1a})}e^{-ika}$$
$$=\frac{e^{-ika}}{\cos k_1a-\frac{i}{2}\left(\frac{k}{k_1}+\frac{k_1}{k}\right)\sin k_1a}$$

and the transmission probability

$$T(E)=|F(E)|^2=\frac{1}{1+\frac{\sin^2\sqrt{\frac{2m}{\hbar^2}V_0a^2(1+\frac{E}{V_0})}}{4\left(\frac{E}{V_0}\right)\left(1+\frac{E}{V_0}\right)}}$$

A plot of $T(E)$ versus E is shown below for the case

$$\frac{2mV_0a^2}{\hbar^2} = \frac{25\pi^2}{4}$$



Transmission over a Square Well

The peaks are called *resonances*.

They occur when $T(E) = 1$ or

$$\sin^2 \sqrt{\frac{2m}{\hbar^2} V_0 a^2 (1 + \frac{E}{V_0})} = 0$$

or when

$$\sqrt{\frac{2m}{\hbar^2}V_0a^2(1+\frac{E}{V_0})} = n\pi$$
$$\frac{E}{V_0} = \frac{n^2\pi^2}{\frac{2m}{\hbar^2}V_0a^2} - 1 = \frac{4n^2}{25} - 1 \geq 0$$
$$\frac{E}{V_0} = 0.44, 1.56, 3.00, ...$$

in agreement with the diagram.

To a particle of these particular energies, the potential looks completely transparent; there is no reflected particle

$$R(E) = |B(E)|^2 = 0$$

All of the incident wave is transmitted into region III.

A special feature of these amplitudes, not derivable from non-relativistic quantum mechanics, relates the properties of the transmission probability and the bound state energies of the well.

The transmission amplitude $F(E)$ is a function of the energy E.

It was derived for $E > 0$.

If we assume that it is an analytic function of E, then it has some interesting properties.

In particular, in the regions of $E < 0$ and real, $F(E)$ has poles (goes to infinity) at E values that correspond to the bound state energies of the well.

$F(E)$ being infinite corresponds to having a transmitted wave without having an incident wave.

This is exactly the condition to have a bound state, where the transmitted(and reflected) wave does not propagate, but instead fall off exponentially.

The poles of $F(E)$ occur when

$$\cos k_1 a = \frac{i}{2}\left(\frac{k}{k_1} + \frac{k_1}{k}\right)\sin k_1 a$$
$$k_1 \cot \frac{k_1 a}{2} = ik \text{ and } k_1 \tan \frac{k_1 a}{2} = -ik$$

which are the same transcendental equations we had earlier for the bound states of the corresponding finite square well.

This property can be used to find bound state energies after solving the trans- mission problem for a given potential.

The book discusses wave packets and time delays.

Delta-Function Potentials

We now consider the potential energy function

where

$$V(x) = A\delta(x-a)$$
$$\delta(x-a) = 0 \quad x \neq a$$
$$\int_{-\infty}^{\infty} f(x)\delta(x-a)\,dx = f(a)$$

and solve the corresponding Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

As we discussed earlier the wave function $\psi(x)$ is assumed to be continuous for physical reasons relating to the probability interpretation.

The derivative of the wave function, however, is not continuous at $x = a$ for this potential.

We can see this as follows.

We have

$$-\frac{\hbar^2}{2m}\int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2\psi(x)}{dx^2}dx + A\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)V(x)\psi(x)dx = E\int_{a-\varepsilon}^{a+\varepsilon}\psi(x)dx$$

In the limit $\varepsilon \longrightarrow 0$, using the continuity of $\psi(x)$, we get

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_{a+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{a-\varepsilon}\right] = E\psi(a)\int_{a-\varepsilon}^{a+\varepsilon}dx - A\psi(a)$$

so that

$$\text{discontinuity}\left(\frac{d\psi}{dx}\right)_{x=a} = \Delta\left(\frac{d\psi}{dx}\right) = \frac{2mA}{\hbar^2}\psi(a)$$

For simplicity we choose $a = 0$.

We then have two regions to consider

region I $\quad x < 0$

region II $\quad x > 0$

and the derivative is discontinuous at $x = 0$.

Transmission Problem

We first carry out the calculation of the transmission and reflection probabilities.

We assume that $A > 0$ (we have a delta function barrier), $E > 0$ and an incident wave of unit intensity coming in from the left.

In region I we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I \rightarrow \psi_I(x) = e^{ikx} + Be^{-ikx} \text{ with } E = \frac{\hbar^2 k^2}{2m} > 0$$

We have both an incident and a reflected wave.

In region II we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E\psi_{II} \rightarrow \psi_{II}(x) = Ce^{ikx} \text{ with } E = \frac{\hbar^2 k^2}{2m} > 0$$

There is only a transmitted wave.

The boundary conditions (at $x = 0$) give

$$\psi_I(0) = \psi_{II}(0) \rightarrow 1 + B = C$$

$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = \frac{2m}{\hbar^2}A\psi_{II}(0) \rightarrow ikC - ik(1 - B) = \frac{2m}{\hbar^2}AC$$

The solutions are

$$C = \frac{ik}{ik - \frac{mA}{\hbar^2}} \text{ and } B = \frac{\frac{mA}{\hbar^2}}{ik - \frac{mA}{\hbar^2}}$$

We then have

$$T = \text{ transmission probability } = |C|^2 = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}}$$

$$R = \text{ reflection probability } = |B|^2 = \frac{1}{1 + \frac{2\hbar^2 E}{mA^2}}$$

We note that $T + R = 1$ as it must for the probability interpretation to make sense.

From our previous discussion, we suspect that the energy values of the poles of the transmission probability correspond to the bound state energies for the delta function well problem ($A < 0$).

For the single delta function potential, T has a single pole at

$$E = -\frac{mA^2}{2\hbar^2}$$

Bound-State Problem

We let $A \rightarrow -A,\ A > 0$.

In region I we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = -|E|\,\psi_I \rightarrow \psi_I(x) = Be^{\alpha x}$$

with

$$E = -|E| = -\frac{\hbar^2\alpha^2}{2m} < 0$$

We have excluded the positive exponential term since it would diverge in region II as $x \rightarrow +\infty$.

The boundary conditions give

$$\psi_I(0) = \psi_{II}(0) \rightarrow B = C$$

$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = -\frac{2m}{\hbar^2}A\psi_I(0) \rightarrow -\alpha C - \alpha B = -\frac{2m}{\hbar^2}AB$$

The resulting equation for α gives the allowed the bound state energies.

We have

$$\alpha = \frac{mA}{\hbar^2} \rightarrow \text{ only 1 solution only } \rightarrow \text{ 1 bound state}$$

$$E = -|E| = -\frac{\hbar^2\alpha^2}{2m} = -\frac{mA^2}{2\hbar^2}$$

which is the same value as we obtained from the pole of the transmission probability.

We also note that the solution has definite parity (even) since $\psi(x) = \psi(-x)$.

This must occur since $V(x) = V(-x)$ and hence parity commutes with the Hamiltonian.

As we also saw in the square well case, if only one solution exists then it is always an even parity solution.

Double Delta Function Potential

We now tackle a more realistic and hence more complex system, namely the double delta function potential energy function given by

$$V(x) = u\left[\delta\left(x + \frac{\ell}{2}\right) + \delta\left(x - \frac{\ell}{2}\right)\right]$$

We again start by considering the barrier transmission problem for $u > 0$.

Transmission problem

There are three regions to consider

region I	$x < \frac{\ell}{2}$
region II	$-\frac{\ell}{2} < x < \frac{\ell}{2}$
region III	$x > \frac{\ell}{2}$

The solutions in the three regions are

$$\begin{array}{lll} \text{region I} & x < \frac{\ell}{2} & \psi_I(x) = Ae^{ikx} + Be^{-ikx} \\ \text{region II} & -\frac{\ell}{2} < x < \frac{\ell}{2} & \psi_{II}(x) = Ce^{ikx} + De^{-ikx} \\ \text{region III} & x > \frac{\ell}{2} & \psi_{III}(x) = Fe^{ikx} \end{array} \qquad E = \frac{\hbar^2 k^2}{2m} > 0$$

The boundary conditions (the derivatives are discontinuous at $x = \pm \ell/2$)give the equations

$$x = -\frac{\ell}{2} \qquad Ae^{-ik\frac{\ell}{2}} + Be^{ik\frac{\ell}{2}} = Ce^{-ik\frac{\ell}{2}} + De^{ik\frac{\ell}{2}}$$

$$\text{ik}\left(Ce^{-ik\frac{\ell}{2}} - De^{ik\frac{\ell}{2}}\right) - ik\left(Ae^{-ik\frac{\ell}{2}} - Be^{ik\frac{\ell}{2}}\right)$$

$$= \frac{2mu}{\hbar^2}\left(Ce^{-ik\frac{\ell}{2}} + De^{ik\frac{\ell}{2}}\right)$$

$$x = +\frac{\ell}{2} \qquad Ce^{ik\frac{\ell}{2}} + De^{-ik\frac{\ell}{2}} = Fe^{ik\frac{\ell}{2}}$$

$$\text{ik}\left(Fe^{ik\frac{\ell}{2}}\right) - ik\left(Ce^{ik\frac{\ell}{2}} - De^{-ik\frac{\ell}{2}}\right) = \frac{2mu}{\hbar^2}\left(Fe^{ik\frac{\ell}{2}}\right)$$

We are interested in calculating the transmission probability

$$T(E) = \frac{|F|^2}{|A|^2}$$

Much algebra gives these results

$$C = (1 - \frac{mu}{ik\hbar^2})F \text{ and } D = \frac{mu}{ik\hbar^2}e^{ik\ell}F$$

$$\frac{F}{A} = \frac{1}{\left[1 - \frac{mu^2}{2\hbar^2 E}(1 - \cos 2k\ell)\right]^2 + i\left[\frac{ku}{E} + \frac{mu^2}{2\hbar^2 E}\sin 2k\ell\right]}$$

$$= \frac{1}{\left[1 - \frac{mu}{ik\hbar^2}\right]^2 - \left[\frac{mu}{ik\hbar^2}\right]^2 e^{2ik\ell}}$$

The poles of the transmission probability occur for the zeroes of the denominator.

If we let $u = -|u|$ and $E = -|E| < 0$ and $k = i\gamma$, the poles are given by

$$\left[1 - \frac{m|u|}{\gamma\hbar^2}\right]^2 - \left[\frac{m|u|}{\gamma\hbar^2}\right]^2 e^{-2\gamma\ell} = 0$$

Some rearranging and algebra gives

$$e^{\gamma\frac{\ell}{2}} = \frac{m|u|}{\gamma\hbar^2}(e^{\gamma\frac{\ell}{2}} \pm e^{-\gamma\frac{\ell}{2}})$$

as the transcendental equation for the bound state energies of the double delta function well.

We will solve this transcendental equation graphically.

Again, it is always best to first clean up the equation as much as possible by changing variables.

There are no rules for this part.

We let $$\beta = \gamma\frac{\ell}{2} \text{ and } \varepsilon = \frac{m|u|\ell}{2\hbar^2}$$

The transcendental equation then becomes

$$e^{-2\beta} = \pm\left(\frac{\beta}{\varepsilon} - 1\right) \qquad \pm \begin{matrix} \text{+1 parity} \\ \text{-1 parity} \end{matrix}$$

The book shows how to get the same result by actually solving the bound-state problem directly.

I will skip that.

Graphical Solution

Since

$$\varepsilon = \frac{m\,|u|\,\ell}{2\hbar^2}$$

is fixed by the choice of the parameters of the potential, we have transcendental equations for β.

The solutions give us the energy eigenvalues.

We can simplify the graphical solution with one more change of variables.

We let

$$\frac{\beta}{\varepsilon} = \eta$$

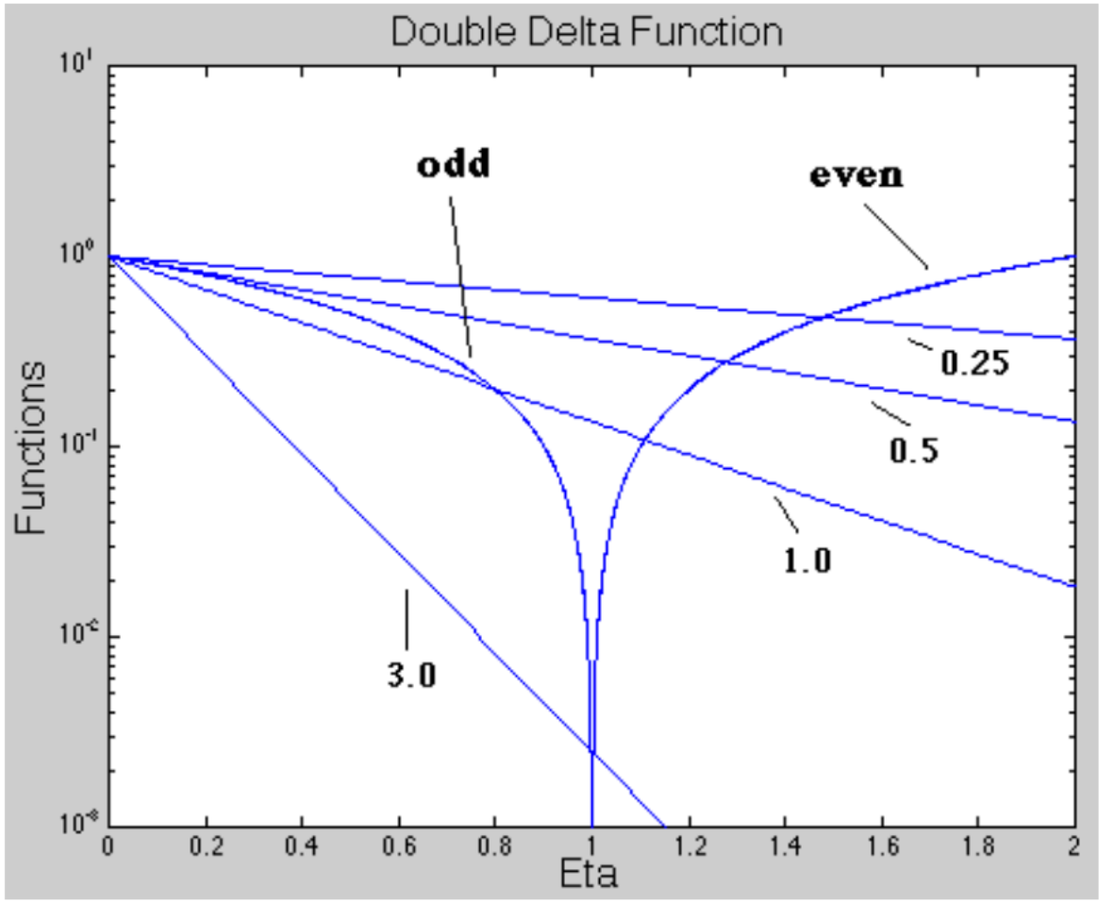
and get

$$\begin{array}{ll} \text{even parity} & e^{-2\epsilon\eta} = \eta - 1 \\ \text{odd parity} & e^{-2\epsilon\eta} = 1 - \eta \end{array}$$

Procedure:

1. plot $1-\eta$ versus η and $\eta - 1$ versus η
2. plot $e^{-2\epsilon\eta}$ versus η for several values of ϵ
3. the intersections are the even and odd solutions

In the Figure on the next slide, we plot the exponential function for several values of ε.



Double delta Function Bound States

As can be seen, the properties of the solutions are:

1. Even solutions always exist
2. Odd solutions do not always exists (see the $\epsilon = 0.25$ line, which only intersects the even curve)
3. As $\epsilon \to 0$ which corresponds to $\ell \to \infty$ we get $E_{odd} = E_{even}$. Physically, the wells are separating so that they no longer influence each other and the system behaves like two separate wells.

We will look at this property again later when we consider a translationally invariant infinite line of delta functions.

The interaction between the wells coupled to the translations invariance will lead to energy bands as in real solids.

Problems: Chapter 6: 1, 2, 4, 6,30

1. Delta function in a well

A particle of mass m moving in one dimension is confined to a space $0 < x < L$ by an infinite well potential. In addition, the particle experiences a delta function potential of strength λ given by $\lambda\delta(x - L/2)$ located at the center of the well as shown in Figure 6.1 below.

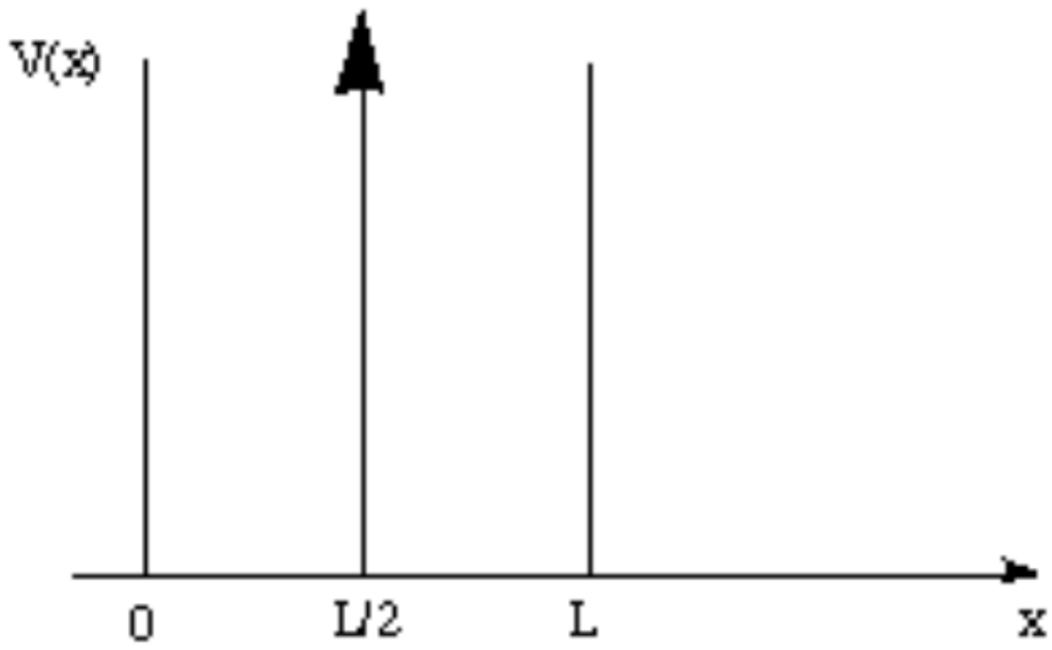


Figure 6.1: Potential Diagram

Find a transcendental equation for the energy eigenvalues E in terms of the mass m, the potential strength λ, and the size of the well L.

We have two regions to consider:

Region I: $0 \leq x \leq L/2$ The solution is

$$\psi_I(x) = A_1 \sin kx$$

which already incorporates the boundary condition $\psi_I(x = 0) = 0$.

Region II: $L/2 \leq x \leq L$ The solution is

$$\psi_{II}(x) = A_2 \sin k(x - L)$$

which already incorporates the boundary condition $\psi_{II}(x = L) = 0$.

At $x = L/2$, we have

$$\psi_I(x = L/2) = \psi_{II}(x = L/2) \rightarrow A_1 = A_2$$

The first derivative is discontinuous at $x = L/2$ and we have

$$\psi'_{II}(x = L/2) - \psi'_I(x = L/2) = \frac{2m\lambda}{\hbar^2}\psi_I(x = L/2)$$

or

$$-A_1 k \cos\frac{kL}{2} - A_1 k \cos\frac{kL}{2} = \frac{2m\lambda}{\hbar^2}\sin\frac{kL}{2} \rightarrow \tan\frac{kL}{2} = -\frac{\hbar^2}{m\lambda}k$$

Therefore, we have a transcendental equation for

$$k \rightarrow E = \frac{\hbar^2 k^2}{2m}$$

2. Properties of the wave function

A particle of mass m is confined to a one-dimensional region $0 \leq x \leq a$ (an infinite square well potential). At $t = 0$ its normalized wave function is

$$\psi(x, t = 0) = \sqrt{\frac{8}{5a}}\left(1 + \cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right)$$

For an infinite square well we have

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \; n = 1, 2, 3, ...$$

And any arbitrary wave function can be expanded in this basis, that is,

$$\psi(x,t) = \sum_n A_n e^{-iE_n t/\hbar}\psi_n(x)$$

We have

$$\psi(x,t=0) = \sqrt{\frac{8}{5a}}\left(1+\cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right)$$

This can be written

$$\begin{aligned}\psi(x,t=0) &= \sqrt{\frac{8}{5a}}\left(1+\cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right)\\ &= \sqrt{\frac{8}{5a}}\sin\left(\frac{\pi x}{a}\right)+\sqrt{\frac{2}{5a}}\sin\left(\frac{2\pi x}{a}\right)\\ &= \sqrt{\frac{4}{5}}\psi_1(x)+\sqrt{\frac{1}{5}}\psi_2(x)\end{aligned}$$

which is a sum of eigenfunctions.

(a) What is the wave function at a later time $t = t_0$?

At time t we then have

$$\psi(x,t_0) = \sqrt{\frac{4}{5}}e^{-iE_1 t_0/\hbar}\psi_1(x)+\sqrt{\frac{1}{5}}e^{-iE_2 t_0/\hbar}\psi_2(x)$$

(b) What is the average energy of the system at $t = 0$ and $t = t_0$?

The average energy does not change so that

$$\langle E\rangle = \langle\psi|\,\hat{H}\,|\psi\rangle = \sum_n E_n\,|A_n|^2 = E_1\,|A_1|^2+E_2\,|A_2|^2 = \frac{4}{5}E_1+\frac{1}{5}E_2 = \frac{4\pi^2\hbar^2}{5ma^2}$$

(c) What is the probability that the particle is found in the left half of the box(i.e., in the region $0 \leq x \leq a/2$ at $t = t_0$?

The probability that the particle is in the region $0 \leq x \leq a/2$ at $t = t_0$ is

$$P(0 \leq x \leq a/2; t_0) = \int_0^{a/2} |\psi(x, t_0|^2 \, dx$$

where

$$|\psi(x, t_0|^2 = e^{-iE_1 t_0/\hbar} \left| e^{-iE_1 t_0/\hbar} \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) \left(1 + \cos\left(\frac{\pi x}{a}\right) e^{-i(E_2 - E_1)t_0/\hbar}\right) \right|^2$$

$$= \frac{8}{5a} \sin^2\left(\frac{\pi x}{a}\right) \left(1 + \cos^2\left(\frac{\pi x}{a}\right) + 2\cos\left(\frac{\pi x}{a}\right) \cos \frac{3\pi^2 \hbar^2}{2ma^2} t_0\right)$$

so that

$$P(0 \leq x \leq a/2; t_0) = \frac{1}{2} + \frac{16}{15\pi} \cos \frac{3\pi^2 \hbar^2}{2ma^2} t_0$$

4. Step and Delta Functions

Consider a one-dimensional potential with a step-function component and an attractive delta function component just at the edge of the step, namely,

$$V(x) = V\Theta(x) - \frac{\hbar^2 g}{2m} \delta(x)$$

(a) For $E > V$, compute the reflection coefficient for particle incident from the left. How does this result differ from that of the step barrier alone at high energy?

(a) For $E > V$, compute the reflection coefficient for particle incident from the left. How does this result differ from that of the step barrier alone at high energy?

The wave function will be of the form

$$\psi(x) = \begin{cases} e^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ikx} & x > 0 \end{cases}$$

with

$$k = \sqrt{\frac{2mE}{\hbar}} \quad , \quad q = \sqrt{\frac{2m(E-V)}{\hbar}}$$

Continuity of the wave function at $x = 0$ gives

$$1 + B = C$$

Integrating the Schrodinger equation over the infinitesimal interval around the origin gives

$$-\frac{\hbar^2}{2m}\left(\psi'(0+) - \psi'(0-)\right) = \frac{\hbar^2 g}{2m}\psi(0)$$
$$1 - B = -\frac{i}{k}(g + iq)C$$

From the two relationships between B and C we obtain

$$C = \frac{2}{1+q/k-ig/k}$$
$$B = \frac{1-q/k+ig/k}{1+q/k-ig/k}$$

The reflection coefficient is

$$\Re = \left|\frac{j_r}{j_l}\right| = \frac{(\hbar k/m)\,|B|^2}{\hbar k/m} = \left|\frac{1 - q/k + ig/k}{1 + q/k - ig/k}\right|^2 = \frac{(1-q/k)^2 + g^2/k^2}{(1+q/k)^2 + g^2/k^2}$$

In the high energy limit we have

$$\Re = \frac{g\hbar^2}{8mE}$$

For the pure step barrier we have (in the same limit)

$$\Re = \frac{V^2}{8E^2}$$

which drops off faster with energy.

(b) For $E < 0$ determine the energy eigenvalues and eigenfunctions of any bound-state solutions.

In order to study the case of negative energy, $E < 0$, it is convenient to introduce the notation

$$\kappa_- = \sqrt{\frac{2m\,|E|}{\hbar^2}} \quad , \quad \kappa_+ = \sqrt{\frac{2m(V + |E|)}{\hbar^2}}$$

Then we can write the bound-state wave function as

$$\psi(x) = \begin{cases} Ae^{\kappa_- x} & x < 0 \\ Ae^{-\kappa_+ x} & x > 0 \end{cases}$$

The discontinuity at the origin implies that

$$-\tfrac{\hbar^2}{2m}(-A\kappa_+ - A\kappa_-) = \tfrac{\hbar^2 g}{2m} A$$
$$\kappa_+ + \kappa_- = g$$

This then gives

$$E = -\frac{m}{2\hbar^2 g^2}\left(\frac{\hbar^2 g^2}{2m} - V\right)^2$$

and

$$\kappa_{\pm}^2 = \frac{m^2}{\hbar^4 g^2}\left(\frac{\hbar^2 g^2}{2m} \pm V\right)^2$$

and

$$A = \sqrt{\frac{2\kappa_+ \kappa_-}{g}}$$

6. A confined particle

A particle of mass m is confined to a space $0 < x < a$ in one dimension by infinitely high walls at $x = 0$ and $x = a$. At $t = 0$ the particle is initially in the left half of the well with a wave function given by

$$\psi(x,0) = \begin{cases} \sqrt{2/a} & 0 < x < a/2 \\ 0 & a/2 < x < a \end{cases}$$

(a) Find the time-dependent wave function $\psi(x,t)$.

The eigenfunctions and eigenvalues of $\hat{H}$ for this system are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \; n = 1, 2, 3, ...$$

We then have

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-iE_n t/\hbar}$$

We evaluate the a_n coefficients using the initial wavefunction

$$\psi(x,0) = \sum_{n=1}^{\infty} a_n \psi_n(x)$$

$$\int_0^a \psi(x,0)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \int_0^a \psi_n(x)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \delta_{nk} = a_k$$

so that

$$a_k = \int_0^a \psi(x,0)\psi_k(x)dx = \frac{2}{a}\int_0^{a/2} \sin\frac{k\pi x}{a}dx = \frac{2}{k\pi}\left(1-\cos\frac{k\pi}{2}\right)$$

Therefore,

$$\psi(x,t) = \frac{2}{\pi}\sqrt{\frac{2}{a}}\sum_{n=1}^{\infty}\frac{1}{n}\left(1-\cos\frac{n\pi}{2}\right)\sin\frac{n\pi x}{a}e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}$$

(b) What is the probability that the particle is in the nth eigenstate of the well at time t?

The probability of being in the nth eigenstate is

$$P_n = |a_n|^2 = \frac{4}{n^2\pi^2}\left(1-\cos\frac{n\pi}{2}\right)^2$$

(c) Derive an expression for average value of particle energy. What is the physical meaning of your result?

We have

$$\langle E\rangle = \langle\psi|\,\hat{H}\,|\psi\rangle = \sum_n E_n P_n = \sum_n E_n |a_n|^2 = \frac{2\hbar^2}{ma^2}\sum_n\left(1-\cos\frac{n\pi}{2}\right)^2$$

which does not converge! It takes an infinite amount of energy to form the initial wavefunction because of the sharp edges!

30. Things about particles in box

A particle of mass m moves in a one-dimensional box Infinite well) of length ℓ with the potential

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < \ell \\ \infty & x > \ell \end{cases}$$

At $t = 0$, the wave function of this particle is known to have the form

$$\psi(x,0) = \begin{cases} \sqrt{30/\ell^5}\, x(\ell - x) & 0 < x < \ell \\ 0 & \text{otherwise} \end{cases}$$

(a) Write this wave function as a linear combination of energy eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{\pi n x}{\ell}\right) \quad , \quad E_n = n^2 \frac{\pi^2 \hbar^2}{2m\ell^2} \quad , \quad n = 1, 2, 3, \ldots.$$

We have

$$\psi(x,0) = \sum_n^\infty a_n \psi_n(x)$$

which gives

$$\int \psi_k^*(x)\psi(x,0)\, dx = \sum_n^\infty a_n \int \psi_k^*(x)\psi_n(x)\, dx = \sum_n^\infty a_n \delta_{nk} = a_k$$

Therefore

$$\begin{aligned} a_k &= \sqrt{60/\ell^6}\int_0^\ell x(\ell-x)\sin\frac{\pi k x}{\ell}\,dx \\ &= \sqrt{\frac{60}{\ell^6}}\frac{\ell^3}{k^3\pi^3}(2-\cos k\pi + k\pi\sin k\pi) \\ &= \frac{8\sqrt{15}}{k^3\pi^3} \quad k=1,3,5,..... \end{aligned}$$

and $a_k = 0$ for $k = 2, 4, ...$

Therefore,

$$\psi(x,0) = \sum_{m\ odd}\frac{8\sqrt{15}}{m^3\pi^3}\psi_m(x)$$

(b) What is the probability of measuring E_n at $t = 0$?

$$P(E_n) = |a_n|^2 = \begin{cases} \frac{960}{m^6\pi^6} & m = 1,3,5,..... \\ 0 & \text{otherwise} \end{cases}$$

NOTE: Since

$$\sum_n P(E_n) = 1$$

we have

$$\frac{960}{\pi^6}\sum_{n\ odd}\frac{1}{n^6} = 1 \rightarrow \sum_{n\ odd}\frac{1}{n^6} = \frac{\pi^6}{960} = 1.00145$$

(c) What is $\psi(x, t > 0)$?

$$\psi(x,t>0) = \sum_{m\ odd} a_m\psi_m(x)e^{-iE_m t/\hbar}$$

Harmonic Oscillators

We now turn our attention to a physical system with a harmonic oscillator potential energy function

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega_0^2 x^2$$

We will first solve this system by going to the position representation and solving the Schrodinger equation using differential equation techniques.

We will review all of our methods, introduce Hermite polynomials and define generating functions along the way.

After that we will introduce an algebraic method for solving this system that does not make any reference to the position representation.

Later, we will generalize this algebraic method for use in other types of systems.

Differential Equation Method

The Hamiltonian for the system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2$$

The energy eigenvalue equation is

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

We put this into the position representation by these steps:

$$\langle x|\,\hat{H}\,|\psi\rangle = \langle x|\,E\,|\psi\rangle = E\,\langle x\mid\psi\rangle = E\psi(x)$$

$$\langle x|\left(\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega_0^2\hat{x}^2\right)|\psi\rangle = E\psi(x)$$

$$\langle x|\,\frac{\hat{p}^2}{2m}\,|\psi\rangle + \frac{1}{2}m\omega_0^2\,\langle x|\,\hat{x}^2\,|\psi\rangle = E\psi(x)$$

$$\frac{1}{2m}(-i\hbar\frac{d}{dx})^2\,\langle x\mid\psi\rangle + \frac{1}{2}m\omega_0^2x^2\,\langle x\mid\psi\rangle = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\frac{1}{2}m\omega_0^2x^2\psi(x) = E\psi(x)$$

The last line is the standard 1-dimensional time-independent Schrodinger equation for the harmonic oscillator potential.

When solving such equations it is useful to rewrite it in dimensionless form.

We do this by making these substitutions (the choice is an art, not a science)

$$\alpha^4 = \frac{m^2\omega_0^2}{\hbar^2}\ ,\ q{=}\alpha x \text{ and } \lambda = \frac{2E}{\hbar\omega_0}$$

The harmonic oscillator Schrodinger equation becomes

$$\frac{d^2\psi}{dq^2}+(\lambda-q^2)\psi = 0$$

The solution of such equations is greatly aided by examining and extracting the behavior of ψ in the asymptotic regions $q \to \pm\infty$.

For sufficiently large q the equation becomes

$$\frac{d^2\psi}{dq^2} - q^2\psi = 0$$

which is satisfied by functions of the form

$$q^n e^{\pm\frac{1}{2}q^2} \quad \text{for any finite value of } n$$

Since the probability interpretation of the function requires us to be able to normalize it, i.e., we must have

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty$$

This rules out the positive exponential.

This result suggests that we try a solution of the form

$$\psi(q) = H(q)e^{-\frac{1}{2}q^2}$$

where $H(q)$ is a polynomial of finite order in q and we have explicitly extracted the asymptotic behavior.

Substituting into the original differential equation gives a new differential equation for $H(q)$

$$\frac{d^2H}{dq^2} - 2q\frac{dH}{dq} + (\lambda - 1)H = 0$$

We now use the standard Frobenius series substitution method to solve this equation.

We assume a solution of the form

$$H(q) = q^s \sum_{j=0}^{\infty} a_j q^j \text{ where } a_0 \neq 0 \text{ and } s \geq 0$$

The nonnegative restriction on s is required in order to guarantee that the solution is well-behaved at $q = 0$ (we need to be able to normalize the wave function).

If we substitute this guess into the differential equation for H we get

$$q^s \sum_{j=0}^{\infty} a_j (j+s)(j+s-1) q^{j-2} - 2q^s \sum_{j=0}^{\infty} a_j (j+s) q^j + (\lambda - 1) q^s \sum_{j=0}^{\infty} a_j q^j = 0$$

$$\begin{aligned} q^s \left[a_0 s(s-1) q^{-2} + a_1 s(s+1) q^{-1} + \left(a_2 (s+2)(s+1) - a_0 (2s+1-\lambda) \right) q^0 \right] \\ + \left(a_3 (s+3)(s+2) - a_1 (2s+3-\lambda) \right) q^1 + \ldots\ldots + \\ \left(a_{j+2} (s+j+2)(s+j+1) - (2s+2j+1-\lambda) a_j \right) q^j + \ldots\ldots = 0 \end{aligned}$$

Now for a power series to be identically zero, the coefficient of each power must be zero separately.

We thus have

$$\begin{aligned} s(s-1)a_0 &= 0 \\ s(s+1)a_1 &= 0 \\ (s+2)(s+1)a_2 - (2s+1-\lambda)a_0 &= 0 \\ (s+3)(s+2)a_3 - (2s+3-\lambda)a_1 &= 0 \\ &\ldots\ldots \\ (s+j+2)(s+j+1)a_{j+2} - (2s+2j+1-\lambda)a_j &= 0 \end{aligned}$$

Now we assumed that $a_0 \neq 0$, $s \geq 0$.

Therefore the equations says that we must have $s = 0$ or $s = 1$ and that $s = 0$ or $a_1 = 0$, or both.

The remaining equations give a_2 in terms of a_0, a_3 in terms of a_1, and, in general, a_{j+2} in terms of a_j.

Whether the series will have a finite or an infinite number of terms depends on the choice of s, a_1, and the eigenvalue λ.

If the series does not terminate, then its asymptotic behavior can be inferred from the coefficients of the high power terms.

From the last recursion formula we have

$$\frac{a_{j+2}}{a_j} \underset{j\to\infty}{\to} \frac{2}{j}$$

This ratio is the same as that of the series for $q^n e^{q^2}$ with any finite value of n.

This implies that the solution we have found for the wave function

$$\psi(q) = H(q)e^{-\frac{1}{2}q^2}$$

will diverge at large q.

Since we cannot have that happen and still retain the probability interpretation, the series must terminate ($H(q)$ must be a polynomial as I mentioned earlier).

From the last recursion formula we can see that if we choose

$$\lambda = 2s + 2j + 1$$

for some j, then the series will terminate ($a_{j+2} = 0$).

Since $a_0 \neq 0$ this cutoff procedure requires that j equals an even integer.

This means that the odd series will not terminate unless we choose $a_1 = 0$.

The index s can still be either 0 or 1 .

Corresponding to these two values, λ is equal to $2j+1$ or $2j+3$, where j is an even integer.

We can express both cases in terms of an integer n as

$$\lambda_n = 2n + 1$$

This gives us the energy eigenvalues

$$E_n = \frac{\lambda_n}{2}\hbar\omega_0 = \left(n + \frac{1}{2}\right)\hbar\omega_0$$

As in the square well examples, we have a *zero point energy*.

It corresponds to the lowest or ground state energy value

$$E_0 = \frac{1}{2}\hbar\omega_0$$

The eigenfunctions have a definite parity, as they should since $V(x) = V(-x)$.

From the definition of n, we can see that for a given solution

$$n = \text{ highest value of } s + j$$

If we denote the corresponding polynomials by $H_n(q)$ we see that $H_n(q)$ is of degree n in q.

Therefore, since the exponential is an even function, we have

n = even → even parity solution

n = odd → odd parity solution

The polynomial of order n, $H_n(q)$, is a solution of the original equation with $\lambda = 2n + 1$

$$\frac{d^2H_n}{dq^2} - 2q\frac{dH_n}{dq} + 2nH_n = 0$$

It is called the Hermite polynomial.

We could find the exact forms of the polynomials from the recursion relations.

However, it more instructive to introduce the idea of a generating function.

We define

$$S(q,s) = e^{q^2-(s-q)^2} = e^{-s^2+2sq} = \sum_{n=0}^{\infty} G_n(q)\frac{s^n}{n!}$$

The functions $G_n(q)$ defined in this way are polynomials in q.

Now we have

$$\frac{\partial S}{\partial q} = 2se^{-s^2+2sq} = \sum_{n=0}^{\infty} G_n(q)\frac{2s^{n+1}}{n!} = \sum_{n=0}^{\infty} \frac{dG_n(q)}{dq}\frac{s^n}{n!}$$

$$\frac{\partial S}{\partial s} = (-2s+2q)e^{-s^2+2sq} = \sum_{n=0}^{\infty} G_n(q)\frac{(-2s+2q)s^n}{n!} = \sum_{n=0}^{\infty} G_n(q)\frac{s^{n-1}}{(n-1)!}$$

Equating equal powers of q in each of these equation we get

$$\frac{dG_n}{dq} = 2nG_{n-1} \text{ and } G_{n+1} = 2qG_n - 2nG_{n-1}$$

The lowest order differential equation, which involves only $G_n(q)$, that we can construct out of this pair of equation is

$$\frac{d^2G_n}{dq^2} = 2n\frac{dG_{n-1}}{dq}, \frac{dG_{n+1}}{dq} = 2(n+1)G_n$$

$$\frac{dG_{n+1}}{dq} = 2\mathrm{q}\frac{dG_n}{dq} + 2G_n - 2\mathrm{n}\frac{dG_{n-1}}{dq}$$

$$\frac{d^2G_n}{dq^2} = 2\mathrm{q}\frac{dG_n}{dq} + 2G_n - \frac{dG_{n+1}}{dq} = 2\mathrm{q}\frac{dG_n}{dq} + 2G_n - 2(n+1)G_n$$

$$\frac{d^2G_n}{dq^2} - 2\mathrm{q}\frac{dG_n}{dq} - 2nG_n = 0$$

which is the Hermite polynomial equation.

So $G_n(q) = H_n(q)$ and we have

$$S(q,s) = e^{q^2-(s-q)^2} = e^{-s^2+2sq} = \sum_{n=0}^{\infty} H_n(q)\frac{s^n}{n!}$$

We then have

$$\frac{\partial^n S(q,s)}{\partial s^n} = e^{q^2}\frac{\partial^n e^{-(s-q)^2}}{\partial s^n} = (-1)^n e^{q^2}\frac{\partial^n e^{-(s-q)^2}}{\partial q^n}$$

$$= \frac{\partial^n \sum_{m=0}^{\infty} H_m(q)\frac{s^m}{m!}}{\partial s^n} = \sum_{m=n}^{\infty} H_m(q)\frac{s^{m-n}}{(m-n)!}$$

where we have used the property

$$\frac{\partial f(s-q)}{\partial s} = -\frac{\partial f(s-q)}{\partial q}$$

If we set $s = 0$ in the equation above we get

$$(-1)^n e^{q^2} \frac{\partial^n e^{-q^2}}{\partial q^n} = H_n(q)$$

We can then easily generate the polynomials

$$H_0 = 1\,,\; H_1 = 2q\,,\; H_2 = 4q^2 - 2\,,\; \ldots$$

The Schrodinger wave functions are then given by

$$\psi_n(x) = A_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$

We find the normalization constant A_n by

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx = 1 = \frac{|A_n|^2}{\alpha} \int_{-\infty}^{\infty} H_n^2(q) e^{-q^2}\, dq$$

Now we can determine all of the integrals of this type from the generating function as follows.

We have

$$\int_{-\infty}^{\infty} e^{-s^2+2sq} e^{-t^2+2tq} e^{-q^2}\, dq = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{s^n t^m}{n!m!} \int_{-\infty}^{\infty} H_n(q) H_m(q) e^{-q^2}\, dq$$

$$= \sqrt{\pi} e^{2st} = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!}$$

which says that

$$\int_{-\infty}^{\infty} H_n(q) H_m(q) e^{-q^2}\, dq = \sqrt{\pi} 2^n n! \delta_{nm}$$

The case $n = m$, gives

$$A_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2}$$

The case $n \neq m$ just corresponds to the orthogonality property of eigenfunctions of different eigenvalues.

stop

Algebraic Method

The Hamiltonian for this system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2$$

The energy eigenvalue equation is

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

The commutator between the position and momentum operators is

$$[\hat{x}, \hat{p}] = i\hbar$$

This information defines a complete solution to the problem when using algebraic methods.

We now define the two new operators (like a change of basis)

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{2m\hbar\omega_0}} \text{ and } \hat{a}^+ = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{2m\hbar\omega_0}}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}\,(\hat{a} + \hat{a}^+) \text{ and } \hat{p} = -i\sqrt{\frac{m\hbar\omega_0}{2}}\,(\hat{a} - \hat{a}^+)$$

These new operators are not Hermitian.

They are Hermitian conjugates, however.

We then have

$$[\hat{a}, \hat{a}^{+}] = 1 \text{ and } \hat{H} = \hbar\omega_0(\hat{N}_{op} + \frac{1}{2}), \hat{N}_{op} = \hat{a}^{+}\hat{a}$$

Now suppose that the vector $|n\rangle$ is an eigenvector of $\hat{N}_{op} = \hat{a}^{\dagger}\hat{a}$ with eigenvalue n

$$\hat{N}_{op}|n\rangle = n|n\rangle$$

Since $\hat{N}_{op}$ and $\hat{H}$ differ only by a constant, this implies that $|n\rangle$ is also an eigenvector of $\hat{H}$, i.e.,

$$\hat{H}|n\rangle = \hbar\omega_0(\hat{N}_{op} + \frac{1}{2})|n\rangle = \hbar\omega_0(n + \frac{1}{2})|n\rangle$$

Therefore, $|E_n\rangle = |n\rangle$ and the energy eigenvalues are

$$E_n = \hbar\omega_0(n + \frac{1}{2})$$

Our task now is to find the allowed values of n.

Now $\hat{N}_{op}^{\dagger} = (\hat{a}^{\dagger}\hat{a}) = \hat{a}^{\dagger}\hat{a} = \hat{N}_{op}$, so $\hat{N}_{op}$ is a Hermitian operator.

This means that the eigenvalues of $\hat{N}_{op}$ (and $\hat{H}$) are real numbers.

Now we also have the relation

$$n = \langle n|\hat{N}_{op}|n\rangle = \langle n|\hat{a}^{+}\hat{a}|n\rangle$$

If we let $|\phi\rangle = \hat{a}|n\rangle$, then the last equation can be written

$$n = \langle \phi \mid \phi \rangle \geq 0$$

which says that the eigenvalues of $\hat{N}_{op}$ (the values of n) are *non-negative*, *real* numbers.

Finally, using $[\hat{a}, \hat{a}^{\dagger}] = 1$, we have

$$\hat{N}_{op}\hat{a} = \hat{a}^{+}\hat{a}\hat{a} = (\hat{a}\hat{a}^{+} - 1)\hat{a} = \hat{a}(\hat{a}^{+}\hat{a} - 1) = \hat{a}(\hat{N}_{op} - 1)$$

and similarly,

$$\hat{N}_{op}\hat{a}^{+} = \hat{a}^{+}\left(\hat{N}_{op} + 1\right)$$

These operator relations imply that

$$\hat{N}_{op}\hat{a}\,|n\rangle = \hat{a}(\hat{N}_{op} - 1)\,|n\rangle = (n-1)\hat{a}\,|n\rangle$$

which says that $\hat{a}\,|n\rangle$ is an eigenstate of $\hat{N}_{op}$ with eigenvalue $n-1$ or that we can write

$$\hat{a}\,|n\rangle = \alpha\,|n-1\rangle \rightarrow \langle n|\,\hat{a}^{+} = \alpha^{*}\,\langle n-1|$$

We will assume that the eigenstates are normalized, i.e., $\langle n \mid n\rangle = 1$.

We then have

$$(\langle n|\,\hat{a}^{+})\,(\hat{a}\,|n\rangle) = |\alpha|^{2}\,\langle n-1 \mid n-1\rangle = |\alpha|^{2}$$

$$= \langle n|\,\hat{a}^{+}\hat{a}\,|n\rangle = \langle n|\,\hat{N}_{op}\,|n\rangle = n$$

which says that $\alpha = \sqrt{n}$ and we have the relation

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$$

Repeating this procedure we have

$$\hat{a}^{2}\,|n\rangle = \hat{a}\sqrt{n}\,|n-1\rangle = \sqrt{n}\hat{a}\,|n-1\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$

which implies the following:

if the eigenvalue n exists, then
so do the eigenvalues $n-1$, $n-2$, ...

This sequence cannot continue forever since we have already shown that the eigenvalues of $\hat{N}_{op}$ are non-negative.

The only way out of this dilemma is that *n* is an integer.

In this case, we would eventually arrive at some eigenstate and then get

$$\hat{a}\,|1\rangle = |0\rangle \text{ and } \hat{a}\,|0\rangle = 0$$

which says the sequence ends.

Thus, the eigenvalues of $\hat{N}_{op}$ are the *non-negative integers*.

We can also go the other way since similar algebra shows that

$$\hat{N}_{op}\hat{a}^{+}\,|n\rangle = \hat{a}^{+}(\hat{N}_{op}+1)\,|n\rangle = (n+1)\hat{a}^{+}\,|n\rangle$$

This implies that, in the same way as before,

$$\hat{a}^{+}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

Thus, the eigenvalues of N_{op} are all the non-negative integers

$$n = 0, 1, 2, 3, 4, \ldots\ldots$$

The operators $\hat{a}$ and $\hat{a}^{\dagger}$ are called lowering/raising operators from their property of lowering and raising the eigenvalues by unity.

They are also sometimes called ladder operators because they generate a ladder of equally-spaced eigenvalues.

Finally, assuming that $\langle 0 \mid 0 \rangle = 1$ we have

$$|1\rangle = \frac{\hat{a}^+}{\sqrt{1}}|0\rangle = \frac{\hat{a}^+}{\sqrt{1!}}|0\rangle$$

$$|2\rangle = \frac{\hat{a}^+}{\sqrt{2}}|1\rangle = \frac{\hat{a}^+}{\sqrt{2}}\frac{\hat{a}^+}{\sqrt{1}}|0\rangle = \frac{(\hat{a}^+)^2}{\sqrt{2!}}|0\rangle$$

$$|3\rangle = \frac{\hat{a}^+}{\sqrt{3}}|2\rangle = \frac{\hat{a}^+}{\sqrt{3}}\frac{(\hat{a}^+)^2}{\sqrt{2!}}|0\rangle = \frac{(\hat{a}^+)^3}{\sqrt{3!}}|0\rangle$$

.....

$$|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$$

and

$$E_n = \hbar\omega_0(n + \frac{1}{2})$$

Notice that we were able to derive all of these results without introducing the wave function (the position representation).

If you are desperate to see the position representation wave functions they can easily be derived from this formalism.

We have

$$0 = \langle x|\,\hat{a}\,|0\rangle = \langle x|\sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{2m\hbar\omega_0}}|0\rangle$$

$$= \sqrt{\frac{m\omega_0}{2\hbar}}x\,\langle x\mid 0\rangle + \frac{i(-i\hbar\frac{d}{dx})}{\sqrt{2m\hbar\omega_0}}\langle x\mid 0\rangle$$

This is a differential equation for $\langle x \mid 0\rangle = \psi_0(x)$ which is the ground state wave function.

We have

$$\frac{d\psi_o(x)}{dx} + \frac{m\omega_0}{\hbar} x\psi_o(x) = 0$$

which has the solution (when normalized)

$$\langle x \mid 0\rangle = \psi_o(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega_0 x^2}{2\hbar}}$$

which agrees with our earlier work.

The higher energy wave functions are obtained using

$$\begin{aligned}\langle x \mid 1\rangle = \psi_1(x) &= \langle x|\, \hat{a}^+ \,|0\rangle \\ &= \langle x| \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{2m\hbar\omega_0}} \,|0\rangle \\ &= \sqrt{\frac{2m\omega_0}{\hbar}} x \,\langle x \mid 0\rangle\end{aligned}$$

and so on.

The raising and lowering operator formalism is very powerful and will be very useful beyond non-relativistic quantum mechanics where they will allow the theory to represent the creation and annihilation of particles.

Start of Lecture #6

Like a surgeon's general warning……

As we delve deeper into theoretical aspects of quantum mechanics

some of the mathematics will get more difficult,

some of the necessary algebraic manipulations will get long and complicated, and

some of the logical paths in the derivations and/or problem solutions will get tricky to follow.

Please bear with me and hang in there as we proceed.

I am trying to give you an accurate picture of what modern theoretical physics is like and and how it uses mathematics to solve problems.

The important things in each case for this class are the conclusions we arrive at and not the particular intricacies of the associated derivations.

We will make a digression at one point for me to teach you some needed classical physics ideas.

Thanks for your patience.

Coherent States

Let us now use this formalism to do an interesting exercise and show the power of the methods.

We consider the following question: what are the eigenstates of the lowering operator $\hat{a}$?

That is, we write

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \;\text{ with }\; \alpha = |\alpha|\, e^{i\phi}$$

where $|\alpha\rangle$ is the eigenvector of $\hat{a}$ and α is the eigenvalue, which is not necessarily real since $\hat{a}$ is not Hermitian.

Since the vectors $|n\rangle$ are eigenvectors of a Hermitian operator, they form a orthonormal complete set and can be used as an orthonormal basis vector space.

We can then write

$$|\alpha\rangle = \sum_{m=0}^{\infty} b_m\,|m\rangle$$

where

$$\langle k \mid \alpha\rangle = \sum_{m=0}^{\infty} b_m \langle k \mid m\rangle = \sum_{m=0}^{\infty} b_m \delta_{km} = b_k$$

Now

$$\langle n-1|\,\hat{a}\,|\alpha\rangle = \alpha\,\langle n-1 \mid \alpha\rangle = \alpha b_{n-1}$$

and using

$$\hat{a}^{+}\,|n-1\rangle = \sqrt{n}\,|n\rangle \rightarrow \langle n-1|\,\hat{a} = \sqrt{n}\,\langle n|$$

we have

$$\langle n-1|\,\hat{a}\,|\alpha\rangle = \sqrt{n}\,\langle n \mid \alpha\rangle = \sqrt{n} b_n$$

or

$$b_n = \frac{\alpha}{\sqrt{n}} b_{n-1}$$

This says that

$$b_1 = \frac{\alpha}{\sqrt{1}} b_0 \;,\; b_2 = \frac{\alpha}{\sqrt{2}} b_1 = \frac{\alpha^2}{\sqrt{2!}} b_0$$

or

$$b_n = \frac{\alpha^n}{\sqrt{n!}} b_0$$

We thus get the final result

$$|\alpha\rangle = b_0 \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle$$

Let us now normalize this state (choose b_0). We have

$$\begin{aligned}
\langle \alpha \mid \alpha \rangle = 1 &= |b_0|^2 \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} \frac{\alpha^{*m} \alpha^k}{\sqrt{m!}\sqrt{k!}} \langle k \mid m \rangle \\
&= |b_0|^2 \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} \frac{\alpha^{*m} \alpha^k}{\sqrt{m!}\sqrt{k!}} \delta_{km} \\
&= |b_0|^2 \sum_{m=0}^{\infty} \frac{|\alpha|^2}{m!} = |b_0|^2 e^{|\alpha|^2}
\end{aligned}$$

which says that

$$b_0 = e^{-\frac{1}{2}|\alpha|^2}$$

and thus

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} |m\rangle$$

Now

$$\begin{aligned}
\langle n \mid \alpha \rangle = &\text{ probability amplitude that the system in the state} \\
&|\alpha\rangle \text{ will be found in the state } |n\rangle
\end{aligned}$$

which then says that

$$P_n = |\langle n \mid \alpha \rangle|^2 = \frac{e^{-|\alpha|^2} |\alpha|^{2n}}{n!} = \frac{e^{-N} N^n}{n!}$$

is the probability that the system in the state $|\alpha\rangle$ will be found in the state $|n\rangle$, where we have defined $N = |\alpha|^2$.

We note that

$$\langle\alpha|\,\hat{a}^{+}\hat{a}\,|\alpha\rangle = \left|\alpha^{2}\right|\langle\alpha\mid\alpha\rangle = \left|\alpha^{2}\right| = N = \langle\alpha|\,\hat{N}_{op}\,|\alpha\rangle$$

or N = the average value or expectation value of the $\hat{N}_{op}$ operator in the state $|\alpha\rangle$.

This type of probability distribution is called a **Poisson distribution**, i.e., the state $|\alpha\rangle$ has the number states or energy eigenstates distributed in a Poisson manner.

Since the states $|n\rangle$ are energy eigenstates, we know their time dependence, i.e.,

$$|n,t\rangle = e^{-i\frac{E_n}{\hbar}t}\,|n\rangle$$

Therefore, we have for the time dependence of the state $|\alpha\rangle$

$$|\alpha,t\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{m=0}^{\infty}\frac{\alpha^m}{\sqrt{m!}}\,|m,t\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{m=0}^{\infty}\frac{\alpha^m}{\sqrt{m!}}e^{-i\frac{E_m}{\hbar}t}\,|m\rangle$$

This simple operation clearly indicates the fundamental importance of the energy eigenstates when used as a basis set.

If we are able to expand an arbitrary vector representing some physical system in the energy basis, then we immediately know the time dependence of that state vector and hence we know the time dependence of all the probabilities associated with the state vector and the system.

We will use this result to solve for the time dependence of real physical systems in later discussions.

Now let us try to understand the physics contained in the $|\alpha\rangle$ state vector.

In a given energy eigenstate the expectation value of the position operator is given by

$$\langle n,t|\,\hat{x}\,|n,t\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n,t|\,(\hat{a}+\hat{a}^+)\,|n,t\rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\,e^{i\frac{E_n}{\hbar}t}(\hat{a}+\hat{a}^+)e^{-i\frac{E_n}{\hbar}t}\,|n\rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\,(\hat{a}+\hat{a}^+)\,|n\rangle$$
$$= \sqrt{\frac{\hbar}{2m\omega_0}}\,\langle n|\left(\sqrt{n}\,|n-1\rangle+\sqrt{n+1}\,|n+1\rangle\right)=0$$

i.e., it is equal to zero and is independent of time.

On the other hand, in the state $|\alpha\rangle$ we find

$$\langle \alpha,t|\,\hat{x}\,|\alpha,t\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\sum_m\sum_k b_m^* b_k e^{i\frac{(E_m-E_k)}{\hbar}t}\,\langle m|\,(\hat{a}+\hat{a}^+)\,|k\rangle$$

Now

$$\langle m|\,(\hat{a}+\hat{a}^+)\,|k\rangle = \langle m|\left(\sqrt{k}\,|k-1\rangle+\sqrt{k+1}\,|k+1\rangle\right)$$
$$= \sqrt{k}\delta_{m,k-1}+\sqrt{k+1}\delta_{m,k+1}$$

Using this result we have

$$
\begin{aligned}
&\langle \alpha, t| \hat{x} |\alpha, t\rangle \\
&\quad = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=1}^{\infty} b_{k-1}^* b_k \sqrt{k} e^{i\frac{(E_{k-1}-E_k)}{\hbar}t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\frac{(E_{k+1}-E_k)}{\hbar}t} \right) \\
&\quad = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=1}^{\infty} b_{k-1}^* b_k \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\omega_0 t} \right) \\
&\quad = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\sum_{k=0}^{\infty} b_k^* b_{k+1} \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} b_{k+1}^* b_k \sqrt{k+1} e^{i\omega_0 t} \right) \\
&\quad = \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 \left(\sum_{k=0}^{\infty} \frac{\alpha^{*k}\alpha^{k+1}}{\sqrt{(k+1)!k!}} \sqrt{k} e^{-i\omega_0 t} + \sum_{k=0}^{\infty} \frac{\alpha^{*k+1}\alpha^{k}}{\sqrt{(k+1)!k!}} \sqrt{k+1} e^{i\omega_0 t} \right) \\
&\quad = \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 \sum_k \frac{1}{k!} |\alpha|^{2k} \left(\alpha e^{-i\omega_0 t} + \alpha^* e^{i\omega_0 t} \right)
\end{aligned}
$$

Now using $\alpha = |\alpha| e^{i\phi}$ we get

$$
\begin{aligned}
\langle \alpha, t| \hat{x} |\alpha, t\rangle &= \sqrt{\frac{\hbar}{2m\omega_0}} b_0^2 2 |\alpha| \sum_k \frac{|\alpha|^{2k}}{k!} \mathrm{Real}(e^{i\phi} e^{-i\omega_0 t}) \\
&= 2x_0 |\alpha| \cos(\omega_0 t - \phi) (b_0^2 \sum_k \frac{|\alpha|^{2k}}{k!}) \quad , \quad x_0 = \sqrt{\frac{\hbar}{2m\omega_0}} \\
&= 2x_0 |\alpha| \cos(\omega_0 t - \phi)
\end{aligned}
$$

The expectation value of the position operator in the state $|\alpha\rangle$ is time-dependent and behaves like a classical oscillator.

Now let us look at these states in another way.

We consider adding a term to the Hamiltonian(the energy operator) of the form

$$V(\hat{x}) = -F_0\hat{x}$$

so that

$$\hat{H} = \hbar\omega_0(\hat{a}^+\hat{a} + \frac{1}{2}) - F_0x_0(\hat{a} + \hat{a}^+)$$

In Physics, this corresponds to putting a charged oscillator in an electric field and including the effective dipole interaction energy in the Hamiltonian.

In the corresponding classical mechanics problem, we have

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \rightarrow \text{ oscillator with equilibrium point at } x = 0$$

and if we add a linear term in x, we get

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 - F_0x$$

$$= \frac{p^2}{2m} + \frac{1}{2}k(x - \frac{F_0}{k})^2 - \frac{F_0^2}{2k}$$

a constant -> no effect

$$\rightarrow \text{ oscillator with equilibrium point at } x = \frac{F_0}{k}$$

This suggests that we look for an oscillator solution to the quantum mechanical problem.

In particular, we look for a new set of raising and lowering operators with the same commutator as the original set.

We can accomplish this by letting

$$\hat{A} = \hat{a} + \beta \text{ and } \hat{A}^{+} = \hat{a}^{+} + \beta \text{ where } \beta = \text{ a real number}$$

The commutator $[\hat{a}, \hat{a}^{\dagger}] = 1$ then implies that $[\hat{A}, \hat{A}^{\dagger}] = 1$.

The Hamiltonian becomes

$$\hat{H} = \hbar\omega_0((\hat{A}^{+} - \beta)(\hat{A} - \beta) + \frac{1}{2}) - F_0 x_0((\hat{A} - \beta) + (\hat{A}^{+} - \beta))$$

$$= \hbar\omega_0(\hat{A}^{+}\hat{A} + \frac{1}{2}) - \hbar\omega_0\beta(\hat{A} + \hat{A}^{+}) + \hbar\omega_0\beta^2 - F_0 x_0(\hat{A} + \hat{A}^{+}) + 2F_0 x_0\beta$$

We are still free to choose β.

We choose $\omega_0\beta = -F_0 x_0$, which gives

$$\hat{H} = \hbar\omega_0(\hat{A}^{+}\hat{A} + \frac{1}{2}) - \frac{F_0^2 x_0^2}{\hbar\omega_0}$$

which is just a harmonic oscillator with the energies shifted by a **constant**.

Now choose the new number states $|N\rangle$ where $\hat{A}^{\dagger}\hat{A}\,|N\rangle = N\,|N\rangle$ as before.

We then have

$$\hat{H}\,|N\rangle = (\hbar\omega_0(\hat{A}^{+}\hat{A} + \frac{1}{2}) - \frac{F_0^2 x_0^2}{\hbar\omega_0})\,|N\rangle$$

$$= (\hbar\omega_0(N + \frac{1}{2}) - \frac{F_0^2 x_0^2}{\hbar\omega_0})\,|N\rangle = E_N\,|N\rangle$$

or we get the same set of energy levels as before, except that they are all **displaced** by the same constant amount

$$-\frac{F_0^2 x_0^2}{\hbar\omega_0}$$

The new ground state is given by

$$\hat{A}\,|N=0\rangle = (\hat{a}+\beta)\,|N=0\rangle = 0$$

$$\hat{a}\,|N=0\rangle = -\beta\,|N=0\rangle = \frac{F_0 x_0}{\hbar\omega_0}\,|N=0\rangle$$

The new ground state is just an eigenstate of $\hat{a}$ with eigenvalue

$$\alpha = \frac{F_0 x_0}{\hbar\omega_0}$$

i.e., the new ground state is a *coherent state*.

These states are called *coherent* states because of their properties when they appear in the quantum mechanical theory of the laser.

We will discuss these states in many other contexts later.

Now let us get this state another way that illustrates some new powerful tools.

Using the Translation Operator

In general, a displaced state $|\lambda\rangle$ is given in terms of the displacement operator (in one dimension) by

$$|\lambda\rangle = e^{-\frac{i}{\hbar}\hat{p}\lambda}\,|0\rangle$$

For the harmonic oscillator system

$$\hat{p} = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}-\hat{a}^{+})$$

If we choose $|0\rangle$ to be the ground state of the oscillator, then we have for the corresponding displaced ground-state

$$|\lambda\rangle = e^{\sqrt{\frac{m\omega}{2\hbar}}(\hat{a}^+ - \hat{a})\lambda}\,|0\rangle$$

By Glauber's theorem (see proof below)

$$e^{(\hat{A}+\hat{B})} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A},\hat{B}]}$$

we have

$$e^{\sqrt{\frac{m\omega}{2\hbar}}(\hat{a}^+ - \hat{a})\lambda} = e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^+\lambda} e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda} e^{\frac{1}{2}\frac{m\omega}{2\hbar}[\hat{a}^+,\hat{a}]\lambda^2}$$

$$= e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^+\lambda} e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda} e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^2}$$

and thus

$$|\lambda\rangle = e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^+\lambda} e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda} e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^2}\,|0\rangle$$

Now

$$e^{-\sqrt{\frac{m\omega}{2\hbar}}\hat{a}\lambda}\,|0\rangle = \left(\hat{I} + \left(-\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}\right) + \frac{1}{2}\left(-\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}\right)^2 + \ldots\right)|0\rangle$$

$$= |0\rangle$$

where we used $\hat{a}\,|0\rangle = 0$.

Similarly, using $(\hat{a}^\dagger)^n\,|0\rangle = \sqrt{n!}\,|n\rangle$ we have

$$e^{\sqrt{\frac{m\omega}{2\hbar}}\hat{a}^{+}\lambda}|0\rangle = \left(\hat{I} + \left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}^{+}\right) + \frac{1}{2}\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\hat{a}^{+}\right)^{2} + \ldots\right)|0\rangle$$

$$= |0\rangle + \sqrt{\frac{m\omega}{2\hbar}}\lambda|1\rangle + \frac{1}{2}\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^{2}|2\rangle + \ldots$$

$$= \sum_{n=0}^{\infty} \frac{\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^{n}}{\sqrt{n!}}|n\rangle$$

or

$$|\lambda\rangle = e^{-\frac{1}{4}\frac{m\omega}{\hbar}\lambda^{2}} \sum_{n=0}^{\infty} \frac{\left(\sqrt{\frac{m\omega}{2\hbar}}\lambda\right)^{n}}{\sqrt{n!}}|n\rangle$$

Thus

$$|\lambda\rangle = \sum_{n=0}^{\infty} b_n |n\rangle$$

where

$$b_n = \frac{e^{-\frac{N}{2}} N^{\frac{n}{2}}}{\sqrt{n!}} \quad , \quad \frac{N}{2} = \frac{m\omega}{4\hbar}\lambda^{2}$$

or

$$P_n = \text{ probability of find the system in the state } |n\rangle$$

$$= |b_n|^{2} = \frac{e^{-N} N^{n}}{n!}$$

which is a **Poisson distribution**.

We, thus, obtain the coherent states once again.

Glauber's theorem proof (for those interested in the mathematics details):

For two operators $\hat{A}$ and $\hat{B}$ assume that

$$\left[(\hat{A}+\hat{B}),\left[\hat{A},\hat{B}\right]\right] = \left[\hat{A},\left[\hat{A},\hat{B}\right]\right] = \left[\hat{B},\left[\hat{A},\hat{B}\right]\right] = 0 \qquad \text{(proof in book)}$$

Now let x be a parameter and consider the operator

$$f(x) = e^{\hat{A}x}e^{\hat{B}x}$$

We then get

$$\frac{df}{dx} = \hat{A}e^{\hat{A}x}e^{\hat{B}x} + e^{\hat{A}x}\hat{B}e^{\hat{B}x} = \hat{A}e^{\hat{A}x}e^{\hat{B}x} + e^{\hat{A}x}\hat{B}e^{-\hat{A}x}e^{\hat{A}x}e^{\hat{B}x}$$

$$= \left(\hat{A} + e^{\hat{A}x}\hat{B}e^{-\hat{A}x}\right)e^{\hat{A}x}e^{\hat{B}x} = \left(\hat{A} + e^{\hat{A}x}\hat{B}e^{-\hat{A}x}\right)f(x)$$

Our assumption above implies that

$$\left[\hat{B},\hat{A}^n\right] = n\hat{A}^{n-1}\left[\hat{B},\hat{A}\right]$$

and

$$\left[\hat{B},e^{-\hat{A}x}\right] = \sum_n (-1)^n \frac{x^n}{n!}\left[\hat{B},\hat{A}^n\right]$$

$$= \sum_n (-1)^n \frac{x^n}{(n-1)!}\hat{A}^{n-1}\left[\hat{B},\hat{A}\right]$$

$$= -e^{-\hat{A}x}\left[\hat{B},\hat{A}\right]x$$

which gives

$$\left[\hat{B},e^{-\hat{A}x}\right] = \hat{B}e^{-\hat{A}x} - e^{-\hat{A}x}\hat{B} = -e^{-\hat{A}x}\left[\hat{B},\hat{A}\right]x$$

$$e^{\hat{A}x}\hat{B}e^{-\hat{A}x} = \hat{B} - \left[\hat{B},\hat{A}\right]x$$

Thus, we have

$$\frac{df}{dx} = \left(\hat{A} + e^{\hat{A}x}\hat{B}e^{-\hat{A}x}\right) f(x) = \left(\hat{A} + \hat{B} + \left[\hat{A}, \hat{B}\right] x\right) f(x)$$

Since $\left[(\hat{A}+\hat{B}), \left[\hat{A}, \hat{B}\right]\right] = 0$, we can treat them like numbers to solve the above differential equation, i.e., we do not have to be careful above operator order.

The solution is

$$f(x) = e^{\hat{A}x} e^{\hat{B}x} = e^{(\hat{A}+\hat{B})x} e^{\frac{1}{2}\left[\hat{A},\hat{B}\right]x^2}$$

Letting $x = 1$ we have the Baker-Hausdorf identity (Glauber's theorem)

$$e^{(\hat{A}+\hat{B})} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]}$$

Charged Particles in Electromagnetic Fields (Uses Classical Ideas)

First, let me introduce you to the Lagrangian.

Let us restrict our attention to one-dimensional systems. We then have

$$E = K + V$$

where

$$K = \frac{1}{2}mv^2 = \frac{1}{2}m\dot{x}^2 = \text{ kinetic energy}$$
$$V = V(x) = \text{ potential energy}$$

Now Newton's second law takes the form

$$F_x = -\frac{\partial V(x)}{\partial x} = ma_x = m\ddot{x}$$

Some algebra gives

$$m\ddot{x} = \frac{d}{dt}(m\dot{x}) = \frac{d}{dt}\left(\frac{\partial}{\partial \dot{x}}\right)\left(\frac{1}{2}m\dot{x}^2\right) = \frac{d}{dt}\left(\frac{\partial K}{\partial \dot{x}}\right)$$

Combining everything we then have

$$-\frac{\partial V}{\partial x} = \frac{d}{dt}\left(\frac{\partial K}{\partial \dot{x}}\right)$$

assuming that

$$K = K(\dot{x}) \rightarrow \frac{\partial K}{\partial x} = 0$$ no dependence on position

$$V = V(x) \rightarrow \frac{\partial V}{\partial \dot{x}} = 0$$ no dependence on velocity

we have

$$\frac{\partial (K - V)}{\partial x} = \frac{d}{dt}\left(\frac{\partial (K - V)}{\partial \dot{x}}\right)$$

or

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x}$$

where we define

$$L = K - V = \text{ Lagrangian}$$

and this equation is called **Lagrange's equation**.

It is important to realize that I have not introduced any new physical content into the theory at this point. I have only found an alternative way to write Newton's second law.

In a full derivation using the calculus of variations and the action principle, Lagrange equations can be formally derived and have a vastly larger physical content than Newton's second law.

Examples

(1) For an object falling in a gravitational field, we have

$$K = \frac{1}{2}m\dot{y}^2$$
$$V = mgy$$
$$L = K - V = \frac{1}{2}m\dot{y}^2 - mgy$$

We then have

$$\frac{\partial L}{\partial \dot{y}} = m\dot{y} \rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) = m\ddot{y}$$
$$\frac{\partial L}{\partial y} = -mg$$

so that equation of motion is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) - \frac{\partial L}{\partial y} = 0$$
$$m\ddot{y} = -mg \rightarrow \ddot{y} = -g$$

which agrees with usual result.

(2) For an object attached to a spring, we have

$$K = \frac{1}{2}m\dot{x}^2$$
$$V = \frac{1}{2}kx^2$$
$$L = K - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\dot{x}^2$$

We then have

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x} \rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial yx}\right) = m\ddot{x}$$
$$\frac{\partial L}{\partial x} = -kx$$

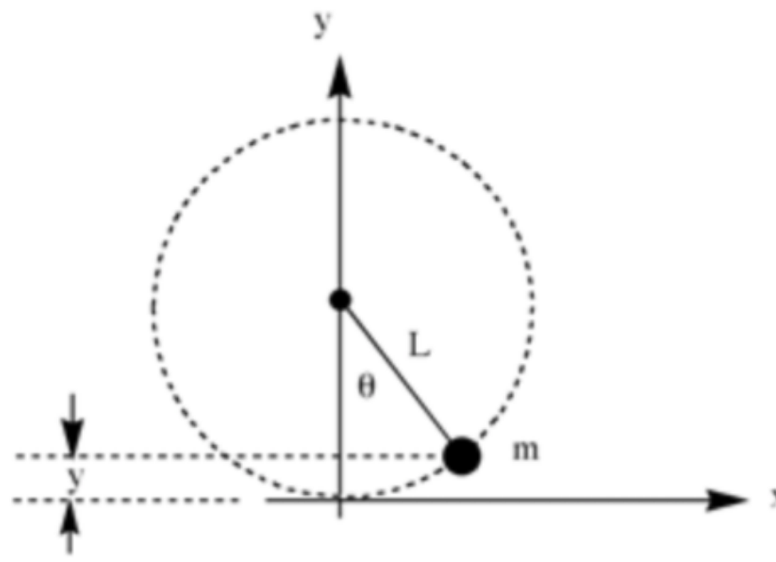
so that the equation of motion is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$$

$$m\ddot{x} = -kx \rightarrow \ddot{x} = -\frac{k}{m}x = -\omega_0^2 x$$

—> standard result….

(3) For an object attached to a string (simple pendulum) (see figure)



we have $K = \frac{1}{2}mL^2\dot{\theta}^2$

$V = mgy = mgL(1-\cos\theta)$ $\qquad L\dot{\theta} = v_\theta$

$L = K - V = \frac{1}{2}mL^2\dot{\theta}^2 - mgL(1-\cos\theta)$

We then have

$$\frac{\partial L}{\partial \dot{\theta}} = mL^2\dot{\theta} \rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) = mL^2\ddot{\theta}$$

$$\frac{\partial L}{\partial \theta} = -mgL\sin\theta$$

so that the equation of motion is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) - \frac{\partial L}{\partial \theta} = 0$$

$$mL^2\ddot{\theta} = -mgL\sin\theta \rightarrow \ddot{\theta} + \frac{g}{L}\sin\theta = 0$$

For small angles we have $\sin\theta \approx \theta$, so that our equations reduces to

$$\ddot{\theta} + \frac{g}{L}\theta = \ddot{\theta} + \omega_0^2\theta = 0$$

—> standard result….

Now we continue our discussion…….

If a charged particle moves in an electromagnetic field, the Lorentz force

Full-blown classical physics included; Just follow along for completeness.

$$\vec{F} = q\left(\vec{E} + \frac{\vec{v}}{c} \times \vec{B}\right)$$

acts on the particle, where q = charge, $\vec{E}$ = electric field, $\vec{v}$ = velocity and $\vec{B}$ = magnetic field.

The electric and magnetic fields can be expressed in terms of the **electromagnetic vector and scalar potentials**

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \text{ and } \vec{B} = \nabla \times \vec{A}$$

In order to make the transition to a quantum mechanical discussion, we must determine the Lagrangian and Hamiltonian for the charged particle in an electromagnetic field.

The appearance of the velocity vector $\vec{v}$ in the Lorentz force law means that we will need to work with a velocity-dependent potential function.

If we insert the expressions for the electric and magnetic fields into the Lorentz force law we get

$$\vec{F} = q\left(-\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} + \frac{1}{c}\vec{v} \times \left(\nabla \times \vec{A}\right)\right)$$

Using the vector identity

$$\vec{B} \times \left(\nabla \times \vec{C}\right) = \nabla\left(\vec{B} \cdot \vec{C}\right) - \left(\vec{B} \cdot \nabla\right)\vec{C} - \left(\vec{C} \cdot \nabla\right)\vec{B} - \vec{C} \times \left(\nabla \times \vec{B}\right)$$

we get

$$\vec{v} \times \left(\nabla \times \vec{A}\right) = \nabla\left(\vec{v} \cdot \vec{A}\right) - \left(\vec{v} \cdot \nabla\right)\vec{A}$$

where we have used the fact that $\vec{v}$ is not an explicit function of the position vector $\vec{r}$.

Now, the total derivative relationship is given by

$$\begin{aligned}\frac{d\vec{A}}{dt} &= \frac{\partial \vec{A}}{\partial t} + \frac{\partial \vec{A}}{\partial x}\frac{dx}{dt} + \frac{\partial \vec{A}}{\partial y}\frac{dy}{dt} + \frac{\partial \vec{A}}{\partial z}\frac{dz}{dt} \\ &= \frac{\partial \vec{A}}{\partial t} + (\vec{v} \cdot \nabla)\vec{A}\end{aligned}$$

Putting all this together we get

$$\vec{F} = q\left(-\nabla\varphi + \frac{1}{c}\nabla(\vec{v} \cdot \vec{A}) - \frac{1}{c}\frac{d\vec{A}}{dt}\right)$$

The standard Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_j}\right) - \frac{\partial L}{\partial x_j} = 0 \text{ where } L = T - V = \text{ Lagrangian}$$

works only for a potential V which **does not depend** on the velocity.

However, when the force law takes the following particular form

$$F_j = -\frac{\partial U}{\partial x_j} + \frac{d}{dt}\left(\frac{\partial U}{\partial \dot{x}_j}\right)$$

we can still construct a Lagrange equation of the form

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_j}\right) - \frac{\partial L}{\partial x_j} = 0 \text{ where } L = T - U = \text{ Lagrangian}$$

We can get the Lorentz force law into this form by using a mathematical trick

$$\frac{dA_j}{dt} = \frac{d}{dt}\left(\frac{\partial}{\partial v_j}(\vec{v}\cdot\vec{A})\right) = \frac{d}{dt}\left(\frac{\partial}{\partial v_j}(\vec{v}\cdot\vec{A} - q\phi)\right)$$

where we have used the fact that the potential ϕ is independent of the velocity, to obtain

$$F_x = -\frac{\partial}{\partial x}\left(q\phi - \frac{q}{c}\vec{v}\cdot\vec{A}\right) + \frac{d}{dt}\left(\frac{\partial}{\partial v_x}\left(q\phi - \frac{q}{c}\vec{v}\cdot\vec{A}\right)\right)$$

This says that we need to choose the generalized potential U as

$$U = q\phi - \frac{q}{c}\vec{v}\cdot\vec{A}$$

and get the Lagrangian

$$L = T - U = \frac{1}{2}m\vec{v}^2 - q\phi + \frac{q}{c}\vec{v}\cdot\vec{A}$$

This gives the associated canonical momentum

$$\vec{p} = \frac{\partial L}{\partial \vec{v}} = m\vec{v} + \frac{q}{c}\vec{A}$$

The canonical momentum is **NOT** the simply the mechanical momentum but now includes an **extra** term proportional to the vector potential(the momentum of the field!).

The Hamiltonian is derived from the Lagrangian using

$$H = \vec{p} \cdot \vec{v} - L = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\varphi$$

This says that the simplest way of coupling the electromagnetic field to the motion of the particle is to replace the momentum by the quantity

$$\vec{p} - \frac{q}{c}\vec{A}$$

which **includes** the momentum associated with the electromagnetic field.

This method of introducing the electromagnetic field into the equations of motion of a particle is called **minimal coupling**.

We will see its relationship to the important concept of **gauge invariance** shortly.

The transition to quantum mechanics is now done in the standard manner.

$$\hat{H}\,|\psi(t)\rangle = E\,|\psi(t)\rangle = ih\frac{\partial}{\partial t}\,|\psi(t)\rangle$$

$$\langle\vec{r}|\,\hat{H}\,|\psi(t)\rangle = E\,\langle\vec{r}\mid\psi(t)\rangle = ih\frac{\partial}{\partial t}\,\langle\vec{r}\mid\psi(t)\rangle$$

$$\langle\vec{r}|\,\hat{H}\,|\psi(t)\rangle = E\psi(\vec{r},t) = ih\frac{\partial\psi(\vec{r},t)}{\partial t}$$

where now we have

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\vec{A}(\hat{\mathbf{r}},t)\right)^2 + q\phi(\hat{\mathbf{r}},t)$$

Using

$$\hat{\mathbf{p}} = \frac{\hbar}{i}\nabla$$

we then get the Schrodinger equation

$$\langle \vec{r}| \left[\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\vec{A}(\hat{\mathbf{r}},t)\right)^2 + q\phi(\hat{\mathbf{r}},t)\right] |\psi(t)\rangle = E\psi(\vec{r},t) = ih\frac{\partial\psi(\vec{r},t)}{\partial t}$$

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}(\vec{r},t)\right)^2 + q\phi(\vec{r},t)\right] \langle \vec{r} \mid \psi(t)\rangle = E\psi(\vec{r},t) = ih\frac{\partial\psi(\vec{r},t)}{\partial t}$$

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}(\vec{r},t)\right)^2 \psi(\vec{r},t) + q\phi(\vec{r},t)\psi(\vec{r},t) = E\psi(\vec{r},t) = ih\frac{\partial\psi(\vec{r},t)}{\partial t}$$

the change

The Schrodinger equation for a charged particle in an electromagnetic field must be invariant under a *gauge transformation* (since Maxwell's equations are so invariant), which is represented by the relations

$$\vec{A} \rightarrow \vec{A}' = \vec{A} + \nabla S(\vec{r},t)$$

$$\phi \rightarrow \phi' = \phi - \frac{1}{c}\frac{\partial S(\vec{r},t)}{\partial t}$$

where $S(\vec{r},t)$ is any arbitrary function.

In order for the Schrodinger equation to be invariant it must be transformed to

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}'(\vec{r},t)\right)^2 \psi'(\vec{r},t) + q\phi'(\vec{r},t)\psi'(\vec{r},t) = ih\frac{\partial\psi'(\vec{r},t)}{\partial t}$$

same form!

where the wave function is at most only changed by an overall phase factor, i.e.,

$$\psi'(\vec{r},t) = \psi(\vec{r},t)e^{\frac{iq}{\hbar c}S(\vec{r},t)}$$

Proof:

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}'(\vec{r},t)\right)^2 \psi'(\vec{r},t) + q\phi'(\vec{r},t)\psi'(\vec{r},t) = ih\frac{\partial\psi'(\vec{r},t)}{\partial t}$$

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla S\right)^2 \psi e^{\frac{iq}{\hbar c}S} + (q\phi - \frac{q}{c}\frac{\partial S}{\partial t})\psi e^{\frac{iq}{\hbar c}S} = ih\frac{\partial\psi e^{\frac{iq}{\hbar c}S}}{\partial t}$$

Finally, using the identities

$$\frac{\partial\psi e^{\frac{iq}{\hbar c}S}}{\partial t} = \frac{\partial\psi}{\partial t}e^{\frac{iq}{\hbar c}S} + \frac{iq}{\hbar c}\frac{\partial S}{\partial t}\psi e^{\frac{iq}{\hbar c}S}$$

$$\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla S\right)\left(\psi e^{\frac{iq}{\hbar c}S}\right) = e^{\frac{iq}{\hbar c}S}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}\right)\psi$$

we get the original Schrodinger equation back.

This result shows that the solutions of the gauge-transformed Schrodinger equation still describes the same physical states.

The wave functions or state vectors differ by a phase factor that depends on space and time and thus, the invariance is LOCAL rather than GLOBAL (a phase factor independent of space and time).

It is then clear that it is NOT the canonical momentum $\hat{\mathbf{p}} = -i\hbar\nabla$ (whose expectation value is *NOT gauge invariant*), but the genuine kinetic momentum

$$\hat{p} - \frac{q}{c}\vec{A}(\hat{r},t)$$

(whose expectation value IS gauge invariant), that represents a ***measurable*** quantity.

In any physical system, if the momentum operator $\hat{p}$ appears, then it must always be replaced by

$$\hat{p} - \frac{q}{c}\vec{A}(\hat{r}, t)$$

if we turn on an electromagnetic field.

This is the only way to guarantee gauge invariance in quantum mechanics.

Quantum mechanics + electromagnetism requires this *minimal coupling* for gauge invariance to be valid.

It is important to remember that local gauge transformations of the electromagnetic potentials requires that wave functions or state vectors transform via local phase changes, which means a phase factor that depends on space and time.

Feynman showed that the effect of turning on a magnetic field is to multiply the wave functions or probability amplitudes by the phase factor

$$\exp\left[\frac{iq}{\hbar c}\int_{path} d\vec{\ell}\cdot\vec{A}(\vec{r}, t)\right]$$

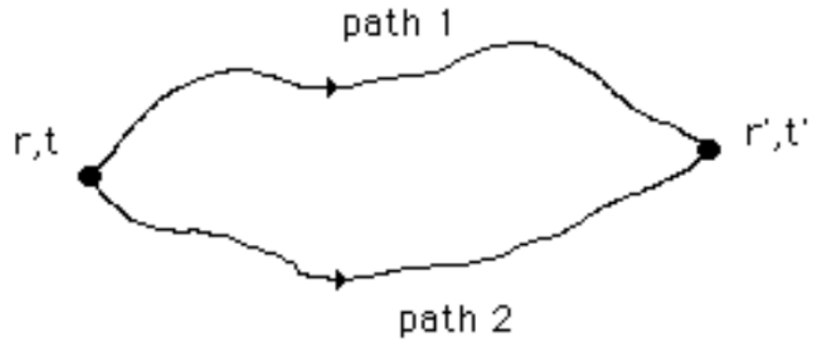
this is the important result!!

Remember two earlier Feynman lectures

The Aharonov-Bohm Effect

The extra phase factor has a rather striking and unexpected consequence.

Let $\vec{A}$ be independent of *t* and consider the possible interference between the motions along two different paths as shown in the Figure.



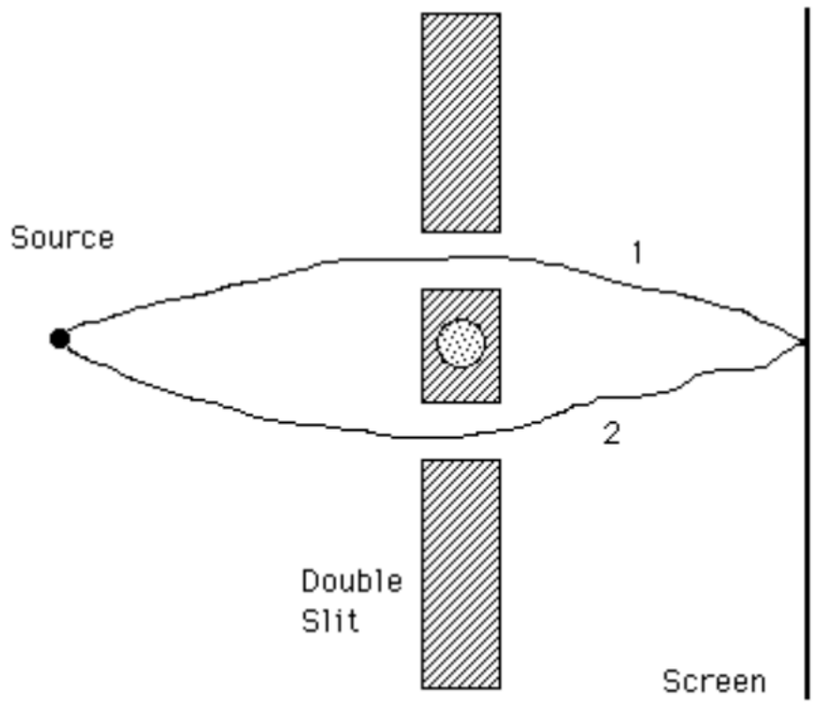
2-Path Experiment

When a magnetic field is turned on, the relative phase for the two paths (1 and 2) is changed by a factor

$$\frac{q}{\hbar c}\left[\int_{path1} d\vec{\ell}\cdot\vec{A} - \int_{path2} d\vec{\ell}\cdot\vec{A}\right] = \frac{q\Phi}{\hbar c}$$

where Φ = the total magnetic flux passing through the loop formed by the two paths or the flux enclosed by the loop (this is just using Ampere's law from Electromagnetic Theory).

Now consider the actual experimental setup shown in the next Figure.



Aharonov-Bohm Experiment

The cylindrical solenoid between the two slits generates a magnetic field out of the page and **confined** to the region of the solenoid.

This implies that the particles are traveling in regions *free* of any magnetic fields.

The *enclosed flux is NOT zero*, however.

As the flux is increased, the relative phase between the two paths changes as described above and the diffraction pattern on the screen changes.

This occurs even though there are no magnetic fields present along the paths.

There does exist, however, a nonzero vector potential in these regions and the relative phase is changing because the vector potential is changing.

This illustrates most powerfully that it is the electromagnetic potential, rather than the electromagnetic fields, as one might assume from Maxwell's equations, that are the fundamental physical quantities in quantum mechanics. This is called the *Aharonov-Bohm effect*.

Classically, the electric and magnetic fields, $\vec{E}$ and $\vec{B}$ are the physically relevant quantities, since they determine the Lorentz force.

In regions where the electric and magnetic fields are zero, a charged particle feels no force.

The vector and scalar potentials $\vec{A}$ and ϕ serve in classical physics only as auxiliary quantities.

In quantum mechanics, the vector potential $\vec{A}(\vec{r})$ is the fundamental physical field.

The wave function, however, always has the property that physical variables and physical effects only depend on gauge-invariant quantities.

Time Evolution of Probabilities

Now that we have solved for the eigenvectors and eigenvalues of several systems we will return to a discussion of the time evolution of probability amplitudes.

Along the way we will reinforce the details about the most fundamental procedure in quantum mechanics.

Suppose we have some physical system that is describable by quantum mechanics.

We would like to be able to answer the following fundamental question?

> If the system is in the state $|\alpha\rangle$ at time $t = 0$,
> what is the probability that it will be in the
> state $|\beta\rangle$ at time t?

These two states are usually defined as follows:

$$|\alpha\rangle = \text{initial state} = \text{state prepared by experimenter}$$
$$|\beta\rangle = \text{final state} = \text{state defined by measuring device}$$

The formal answer to the question is

$$P_{\beta\alpha}(t) = |Amplitude_{\beta\alpha}(t)|^2 = |A_{\beta\alpha}(t)|^2 = \left|\langle\beta|\,\hat{U}(t)\,|\alpha\rangle\right|^2$$

where $\hat{U}(t)$ is the time evolution operator.

Let us assume for simplicity at this stage that the Hamiltonian $\hat{H}$ does not explicitly dependent on time t.

From our earlier discussions, we then have

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

so that the probability amplitude becomes

$$A_{\beta\alpha}(t) = \langle\beta|\,\hat{U}(t)\,|\alpha\rangle = \langle\beta|\,e^{-\frac{i}{\hbar}\hat{H}t}\,|\alpha\rangle$$

The most important rule in quantum mechanics is the following:

> If you are evaluating an amplitude involving a particular operator, $\hat{H}$ in this case, then switch to a basis for the space corresponding to the eigenvectors of the that operator.

This basis is called the *HOME* space.

This is carried out by inserting identity operators as sums of *projection* operators written in the energy eigenvector basis:

$$\begin{aligned} A_{\beta\alpha}(t) &= \langle\beta|\,e^{-\frac{i}{\hbar}\hat{H}t}\,|\alpha\rangle = \langle\beta|\,\hat{I}e^{-\frac{i}{\hbar}\hat{H}t}\hat{I}\,|\alpha\rangle \\ &= \sum_{E}\sum_{E'}\langle\beta\mid E\rangle\langle E|\,e^{-\frac{i}{\hbar}\hat{H}t}\,|E'\rangle\langle E'\mid\alpha\rangle \end{aligned}$$

where

$$\begin{aligned} &\hat{H}\,|E\rangle = E\,|E\rangle \ \text{ and } \ \hat{H}\,|E'\rangle = E'\,|E'\rangle \\ &\langle E\mid E'\rangle = \delta_{EE'} \\ &\sum_{E}|E\rangle\langle E| = \hat{I} = \sum_{E'}|E'\rangle\langle E'| \end{aligned}$$

It is clear that the time evolution calculation is most easily done in this basis.

We then have

$$
\begin{aligned}
A_{\beta\alpha}(t) &= \sum_E \sum_{E'} \langle \beta \mid E \rangle \langle E | e^{-\frac{i}{\hbar}E't} | E' \rangle \langle E' \mid \alpha \rangle \\
&= \sum_E \sum_{E'} e^{-\frac{i}{\hbar}E't} \langle \beta \mid E \rangle \langle E \mid E' \rangle \langle E' \mid \alpha \rangle \\
&= \sum_E \sum_{E'} e^{-\frac{i}{\hbar}E't} \langle \beta \mid E \rangle \delta_{EE'} \langle E' \mid \alpha \rangle \\
&= \sum_E e^{-\frac{i}{\hbar}E't} \langle \beta \mid E \rangle \langle E \mid \alpha \rangle
\end{aligned}
$$

Let us now describe a typical procedure:

1. Determine the initial state of the system $= |\alpha\rangle$
2. Expand the initial state in terms of the energy basis

$$|\alpha\rangle = \sum_{E''} |E''\rangle \langle E'' \mid \alpha\rangle$$

   which means we know the coefficients $\langle E'' \mid \alpha \rangle$
3. Expand the final state in terms of the energy basis

$$|\beta\rangle = \sum_{E''} |E''\rangle \langle E'' \mid \beta\rangle$$

   which means we know the coefficients $\langle E'' \mid \beta \rangle$
4. Calculate the amplitude and probability.

Example - Infinite Square Well System

Suppose that a particle in an infinite square well $[-a/2, +a/2]$ is initially in the state $|\alpha\rangle$, such that

$$\langle x \mid \alpha \rangle = \begin{cases} 0 & x < 0 \\ \frac{2}{\sqrt{a}} & 0 \le x \le \frac{a}{4} \\ 0 & x > \frac{a}{4} \end{cases}$$

Now we have found that

$$\langle x \mid E \rangle = \begin{cases} \frac{2}{\sqrt{a}} \cos \frac{n\pi x}{a} & n \text{ odd} \\ \frac{2}{\sqrt{a}} \sin \frac{n\pi x}{a} & n \text{ even} \end{cases}$$

"wave functions"

where

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \qquad n = 1, 2, 3, 4, \ldots$$

Therefore, we get

$$\langle E_n \mid \alpha \rangle = \int_{-\frac{a}{2}}^{\frac{a}{2}} \langle E_n \mid x \rangle \langle x \mid \alpha \rangle \, dx = \frac{2}{\sqrt{a}} \int_0^{\frac{a}{4}} \langle E_n \mid x \rangle \, dx$$

$$= \frac{2\sqrt{2}}{n\pi} \begin{cases} \sin \frac{n\pi}{4} & n \text{ odd} \\ -\cos \frac{n\pi}{4} & n \text{ even} \end{cases}$$

or

$$|\alpha\rangle = \langle E_1 \mid \alpha \rangle |E_1\rangle + \langle E_2 \mid \alpha \rangle |E_2\rangle + \langle E_3 \mid \alpha \rangle |E_3\rangle + \ldots$$

$$= \frac{2}{\pi} |E_1\rangle + \frac{2}{3\pi} |E_3\rangle + \frac{2\sqrt{2}}{4\pi} |E_4\rangle + \frac{2}{5\pi} |E_5\rangle - \frac{2}{7\pi} |E_7\rangle - \frac{2\sqrt{2}}{8\pi} |E_8\rangle + \ldots$$

If we assume that the final state $|\beta\rangle$ is an energy eigenstate, say $|E_n\rangle$, we then have the probability amplitude that the particle started out in state $|\alpha\rangle$ at $t = 0$ is found in the state $|E_n\rangle$ at time t is

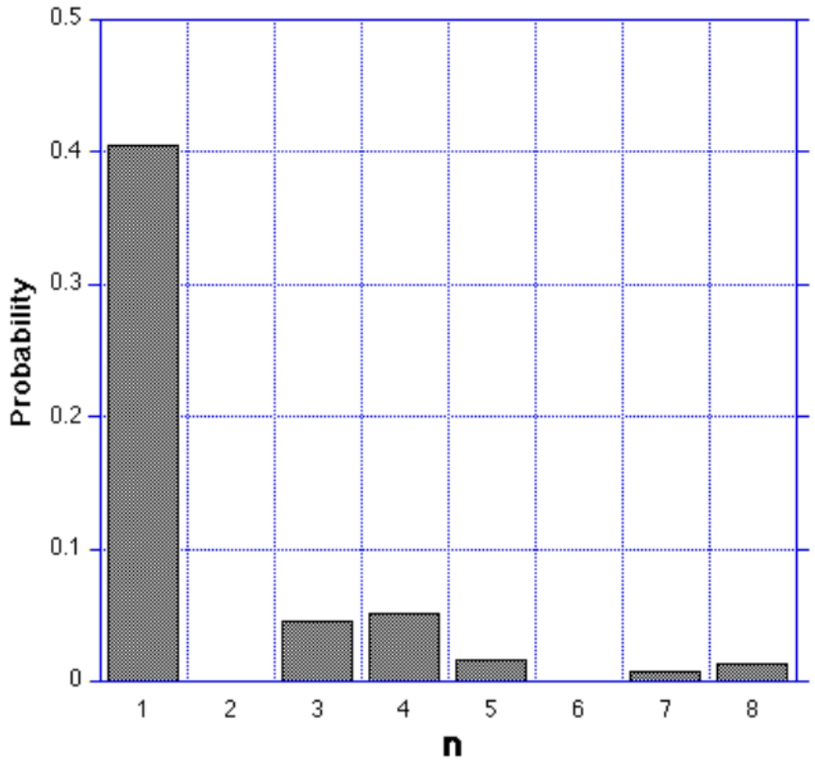
$$A_{n\alpha}(t) = \sum_E e^{-\frac{i}{\hbar} Et} \langle E_n \mid E \rangle \langle E \mid \alpha \rangle = e^{-\frac{i}{\hbar} E_n t} \langle E_n \mid \alpha \rangle$$

and the corresponding probabilities are

$$P_{n\alpha}(t) = |\langle E_n \mid \alpha \rangle|^2$$

which is independent of time.

A plot of these fixed probabilities versus n is shown in the Figure below.



Probabilities

If, on the other hand, we assume that the final state is a linear combination of two energy eigenstates, say,

$$|\beta\rangle = \frac{1}{\sqrt{2}}|E_1\rangle + \frac{1}{\sqrt{2}}|E_3\rangle$$

then we have the probability amplitude that the particle started out in state $|\alpha\rangle$ at $t = 0$ is found in the state $|\beta\rangle$ at time t is

$$\begin{aligned} A_{\beta\alpha}(t) &= \sum_E e^{-\frac{i}{\hbar}Et}\langle\beta \mid E\rangle\langle E \mid \alpha\rangle \\ &= \frac{1}{\sqrt{2}}\left(e^{-\frac{i}{\hbar}E_1 t}\langle E_1 \mid \alpha\rangle + e^{-\frac{i}{\hbar}E_3 t}\langle E_3 \mid \alpha\rangle\right) \end{aligned}$$

and the corresponding probability is

$$
\begin{aligned}
P_{\beta\alpha}(t) = |\langle\beta \mid \alpha\rangle|^2 &= \frac{1}{2}\left|e^{-\frac{i}{\hbar}E_1 t}\langle E_1 \mid \alpha\rangle + e^{-\frac{i}{\hbar}E_3 t}\langle E_3 \mid \alpha\rangle\right|^2 \\
&= \frac{1}{2}\left|e^{-\frac{i}{\hbar}E_1 t}\frac{2}{\pi} + e^{-\frac{i}{\hbar}E_3 t}\frac{2}{3\pi}\right|^2 = \frac{2}{\pi^2}\left|\frac{1}{3} + e^{\frac{i}{\hbar}(E_3 - E_1)t}\right|^2 \\
&= \frac{2}{\pi^2}\left(\frac{1}{9} + \frac{2}{3}\cos\left[\frac{1}{\hbar}(E_3 - E_1)t\right] + 1\right) \\
&= \frac{20}{9\pi^2}\left(1 + \frac{3}{5}\cos\left[\frac{1}{\hbar}(E_3 - E_1)t\right]\right)
\end{aligned}
$$

which is dependent on time.

In this case the probability of observing this final state oscillates between 0.18 and 0.72.

Translation Invariant Potential - Band Structure

We now consider a potential that is *periodic in space*, which means that it is *translationally invariant*, i.e.,

$$V(x) = V(x + a) \text{ where } a = \text{ some fixed distance}$$

This might represent an electron in a 1-dimensional crystal lattice, where a is the distance between atoms.

The change in the allowed energy spectrum caused by the periodicity of the lattice is rather striking.

The Hamiltonian of the system is

$$\hat{H}(x,p) = \frac{p^2}{2m} + V(x)$$

This Hamiltonian is invariant if we translate a fixed distance a

$$\hat{H}(x + a, p) = \frac{p^2}{2m} + V(x + a) = \frac{p^2}{2m} + V(x) = \hat{H}(x,p)$$

This means that the transformation operator $\hat{T}(a)$ that corresponds to a translation by a distance a *commutes* with the Hamiltonian

$$\left[\hat{H}, \hat{T}(a)\right] = 0$$

and thus they must *share a set of eigenfunctions*.

From our earlier discussion, the translation operator has the defining property that, if the state $|\psi\rangle$ has the wave function $\langle x|\psi\rangle$ in the position representation, then the state $\hat{T}(a)|\psi\rangle$ has the wave function

$$\langle x|\hat{T}(a)|\psi\rangle = \langle x + a \mid \psi\rangle$$

Let us re—derive the eigenfunctions of $\hat{T}(a)$.

If $|\psi\rangle$ is an eigenstate of the $\hat{T}(a)$ operator, then we must have

$$\hat{T}(a)|\psi\rangle = \lambda|\psi\rangle \text{ where } \lambda = \text{ the eigenvalue}$$

and thus

$$\psi(x + a) = \langle x|\hat{T}(a)|\psi\rangle = \lambda\langle x \mid \psi\rangle = \lambda\psi(x)$$

With hindsight, we write λ in the form e^{ika} which defines k.

We then have

$$\psi(x + a) = e^{ika}\psi(x)$$

If we define

$$u_k(x) = e^{-ikx}\psi(x)$$

we then have that

$$\psi(x + a) = e^{ik(x+a)}u_k(x + a) = e^{ika}\psi(x) = e^{ika}e^{ikx}u_k(x)$$
$$u_k(x + a) = u_k(x)$$

which says that $u_k(x)$ is also periodic in space with period a.

The eigenfunctions of $\hat{T}$ (a) are then given by

$$\psi(x) = e^{ikx} u_k(x)$$

which is a *plane wave modulated by a function with the periodicity of the lattice* (potential).

This type of wave function is called a *Bloch wave*.

We note that k must be real since if k were not real, then the eigenfunction would diverge as x gets large and thus be unrenormalizable, which is not allowed.

Since $\hat{H}$ and $\hat{T}$(a) must share a set of eigenfunctions, we can construct a complete set of energy eigenstates in the form of Bloch waves.

This means that we can find at least one energy eigenstate for each possible $\lambda = e^{ika}$, since all λ are eigenvalues of $\hat{T}$ (a).

Note also that the values k and $k + 2\pi\, n/a$ give the same eigenvalue and thus we can restrict our attention to k values in the interval

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

and we will be including all possible eigenvalues of $\hat{T}$ (a).

Example

Let us now consider the specific example of a 1-dimensional periodic array of delta functions

$$V(x) = \sum_{n=-\infty}^{\infty} v_0 \delta(x - na)$$

which corresponds to the so-called *Kronig-Penney model*.

In the interval $0 < x < a$ the potential vanishes and the solution to the Schrodinger equation is of the form

$$\psi(x) = Ae^{iqx} + Be^{-iqx} \text{ where } E = \frac{\hbar^2 q^2}{2m}$$

Therefore, in the interval $0 < x < a$, we must have

$$u_k(x) = Ae^{i(q-k)x} + Be^{-i(q+k)x}$$

The coefficients A and B are fully determined by two conditions:

1. $\psi(x)$ and hence $u_k(x)$ must be continuous at the lattices sites

$$\lim_{\eta \to 0}(u_k(\eta) - u_k(-\eta)) \to 0$$

Periodicity then says that $u_k(-\eta) = u_k(a-\eta)$ and hence we must also have

$$\lim_{\eta \to 0}(u_k(\eta) - u_k(a-\eta)) \to 0$$

which gives

$$A + B = Ae^{i(q-k)a} + Be^{-i(q+k)a} \qquad \text{(condition 1)}$$

2. $d\psi(x)/dx$ is discontinuous at the lattice points, as we showed earlier, as follows:

$$\lim_{\eta \to 0} \frac{\hbar^2}{2m} \left(\left.\frac{d\psi(x)}{dx}\right|_{x=\eta} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\eta} \right) = v_0 \psi(0)$$

We have

$$\lim_{\eta\to 0}\left(\left.\frac{d\psi(x)}{dx}\right|_{x=\eta}\right) = iq(A-B)$$

$$\lim_{\eta\to 0}\left(\left.\frac{d\psi(x)}{dx}\right|_{x=-\eta}\right) = e^{-ika}\lim_{\eta\to 0}\left(\left.\frac{d\psi(x)}{dx}\right|_{x=a-\eta}\right)$$

$$= e^{-ika}iq\left(Ae^{iqa} - Be^{-iqa}\right)$$

$$\psi(0) = A + B$$

which gives

$$\frac{\hbar^2}{2m}iq\left(A - B - Ae^{i(q-k)a} + Be^{-i(q+k)a}\right)$$

$$= v_0(A+B) \qquad \text{(condition 2)}$$

We only need these two conditions and do not need to worry about all of the rest of the potential because of the periodicity.

We solve for the ratio A/B in each equation and equate the two results to get a transcendental equation for q in terms of k (which then gives us the allowed energy values).

We get the equation

$$\cos ka = \cos qa + \frac{mv_0}{q\hbar^2}\sin qa$$

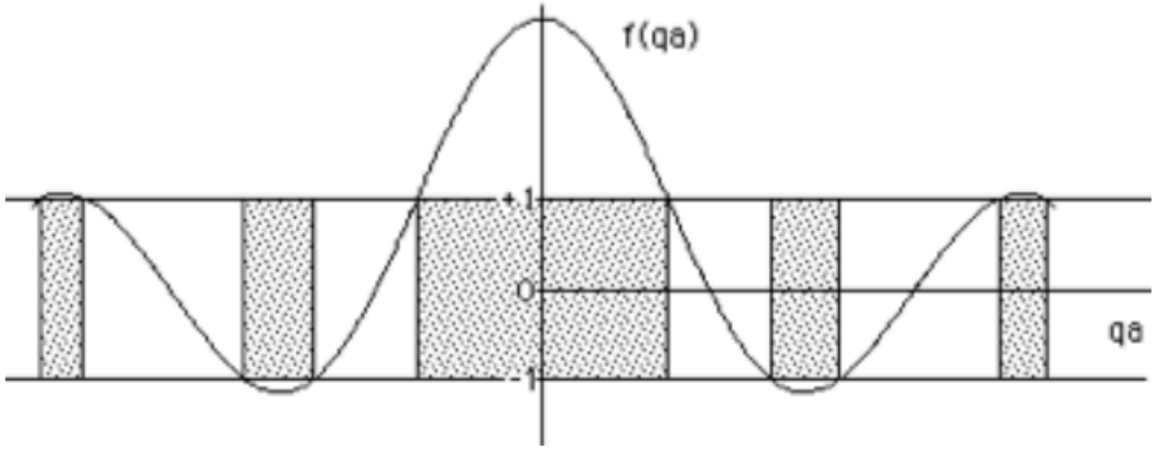
Now for any given value of k we must have

$$-1 \le \cos ka \le +1$$

Therefore, if we plot

$$\cos ka = \cos qa + \frac{mv_0 a}{\hbar^2}\frac{\sin qa}{qa} \quad \text{versus} \quad qa$$

the only allowed q values are between the two lines representing ±1 as shown in the Figure below.



Allowed q values

i.e., q must always lie in the unshaded areas.

For each value of cos ka there are an infinite number of solutions.

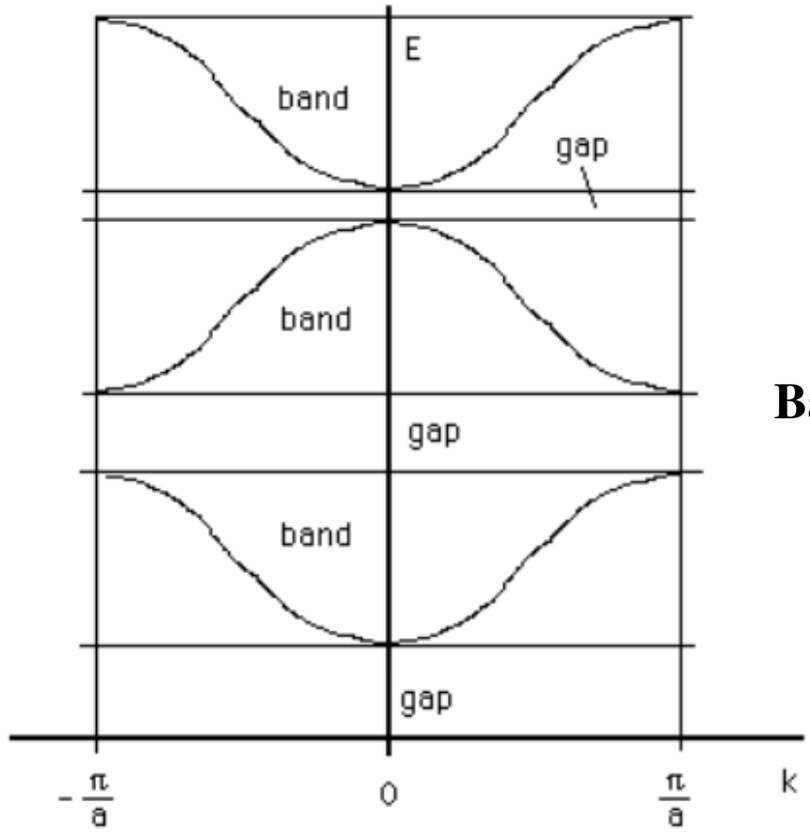
Taking k in the range $-\pi/a \le k \le \pi/a$, we can plot

$$E = \frac{\hbar^2 q^2}{2m} \quad \text{versus} \quad ka$$

as shown in the Figure.

The possible energy values lie in bands, with gaps between them.

This structure of the energy spectrum with bands and gaps occurs for all periodic potentials, which is the dominant feature in Solid State Physics.



Bands and Gaps

Chapter 7 - Angular Momentum; 2- and 3-Dimensions

Angular Momentum Eigenvalues and Eigenvectors

Earlier, we derived the commutation relations that define angular momentum operators

the Hermitian generator of rotations

$$\left[\hat{J}_i, \hat{J}_j\right] = i\hbar\varepsilon_{ijk}\hat{J}_k \equiv i\hbar\sum_k \varepsilon_{ijk}\hat{J}_k$$

where

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } ijk = \text{even permutation of } 123 \\ -1 & \text{if } ijk = \text{odd permutation of } 123 \\ 0 & \text{if any two indices are identical} \end{cases}$$

and the *Einstein summation convention over repeated indices* is understood if the summation sign is left out (unless an explicit override is given).

In addition, these are all Hermitian operators, i.e., $(\hat{J}_i)^\dagger = \hat{J}_i^\dagger = \hat{J}_i$.

Since these three operators form a *closed commutator algebra* (no other operators are involved), we can solve for the eigenvectors and eigenvalues using only the commutators.

The three operators $\hat{J}_1$, $\hat{J}_2$ and $\hat{J}_3$ do not commute with each other and hence do not share a common set of eigenvectors (called a *representation*).

However, there exists another operator that commutes with each of the angular momentum components separately.

If we define

$$\hat{J}^2 = \sum_{i=1}^{3} \hat{J}_i^2$$

which is the square of the total angular momentum vector, we have

$$\left[\hat{J}^2, \hat{J}_i\right] = 0 \text{ for } i = 1, 2, 3$$

In addition, we have $(\hat{J}^2)^\dagger = \hat{J}^2$, so that $\hat{J}^2$ is Hermitian also.

The commutation relations and the Hermitian property say that $\hat{J}^2$ and any one of the components *share a complete set of common eigenvectors*.

By convention, we choose to use $\hat{J}^2$ and $\hat{J}_3$ as the two operators, whose eigenvalues(good quantum numbers) will characterize the set of common eigenvectors.

As we shall see, $\hat{J}^2$ is a so-called *Casimir invariant operator* that characterizes(labels) the representations(set of eigenvectors).

In particular, the eigenvalue of $\hat{J}^2$ characterizes the representation and the eigenvalues of one of the components of the angular momentum (usually $\hat{J}_3$) will *characterize the eigenvectors within a representation*.

We define the eigenvector/eigenvalue relations by the equations

$$\hat{J}^2 |\lambda m\rangle = \lambda \hbar^2 |\lambda m\rangle$$
$$\hat{J}_3 |\lambda m\rangle = m\hbar |\lambda m\rangle$$

where the appropriate factors of $\hbar$ that have been explicitly put into the relations make m and λ dimensionless numbers.

We now define some other operators and their associated commutators so that we can use them in our derivations.

$$\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2$$
$$\hat{J}_- = \left(\hat{J}_+\right)^+ \rightarrow \text{ they are not Hermitian operators}$$

We then have

$$\left[\hat{J}^2, \hat{J}_\pm\right] = \left[\hat{J}^2, \hat{J}_1\right] \pm i\left[\hat{J}^2, \hat{J}_2\right] = 0$$

$$\left[\hat{J}_3, \hat{J}_\pm\right] = \left[\hat{J}_3, \hat{J}_1\right] \pm i\left[\hat{J}_3, \hat{J}_2\right]$$

$$= i\hbar\hat{J}_2 \mp i\left(i\hbar\hat{J}_1\right) = \pm\hbar\hat{J}_\pm$$

and

$$\left[\hat{J}_+, \hat{J}_-\right] = \left[\hat{J}_1, \hat{J}_1\right] + i\left[\hat{J}_2, \hat{J}_1\right] - i\left[\hat{J}_1, \hat{J}_2\right] - \left[\hat{J}_2, \hat{J}_2\right]$$

$$= -2i\left[\hat{J}_1, \hat{J}_2\right] = 2\hbar\hat{J}_3$$

and

$$\hat{J}_+\hat{J}_- = \left(\hat{J}_1 + i\hat{J}_2\right)\left(\hat{J}_1 - i\hat{J}_2\right)$$

$$= \hat{J}_1^2 + \hat{J}_2^2 - i\left[\hat{J}_1, \hat{J}_2\right] = \hat{J}^2 - \hat{J}_3^2 + \hbar\hat{J}_3$$

and

$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3$$

Finally, we have

$$\hat{J}^2 = \frac{\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+}{2} + \hat{J}_3^2$$

Derivation of Eigenvalues

Now the definitions above tell us that

$$\langle \lambda m | \hat{J}^2 | \lambda m \rangle = \lambda\hbar^2 \langle \lambda m \mid \lambda m \rangle = \sum_i \langle \lambda m | \hat{J}_i^2 | \lambda m \rangle$$

$$\lambda\hbar^2 \langle \lambda m \mid \lambda m \rangle = \sum_i \langle \lambda m | \hat{J}_i\hat{J}_i | \lambda m \rangle = \sum_i \langle \lambda m | \hat{J}_i^+\hat{J}_i | \lambda m \rangle$$

Let us define the new vector $|\alpha_i\rangle = \hat{J}_i |\lambda m\rangle$.

Remember that the norm of any vector is non-negative, i.e., $\langle a \mid a\rangle \geq 0$.

Therefore

$$\langle \lambda m \mid \lambda m\rangle \geq 0 \text{ and } \langle \alpha_i \mid \alpha_i\rangle \geq 0$$

Now since $\langle\alpha_i| = \langle\lambda m| \hat{J}^{\dagger}_i$ we have

$$\lambda\hbar^2 \langle \lambda m \mid \lambda m\rangle = \sum_i \langle \lambda m| \hat{J}_i^{+} \hat{J}_i |\lambda m\rangle = \sum_i \langle \alpha_i \mid \alpha_i\rangle \geq 0$$

or we have

$$\lambda \geq 0 \text{ or the eigenvalues of } \geq 0$$

This says that for a fixed value of λ (the eigenvalue of $\hat{J}^2$), which characterizes the representation, there must be maximum and minimum values of m (the eigenvalue of $\hat{J}_3$), which characterizes the eigenvectors within a representation.

Now we have

$$\begin{aligned}\hat{J}_3\hat{J}_+ |\lambda m\rangle &= \hat{J}_3(\hat{J}_+ |\lambda m\rangle) \\ &= (\hat{J}_+\hat{J}_3 + [\hat{J}_3, \hat{J}_+]) |\lambda m\rangle = (\hat{J}_+\hat{J}_3 + \hbar\hat{J}_+) |\lambda m\rangle \\ &= \hbar(m+1)\hat{J}_+ |\lambda m\rangle = \hbar(m+1)(\hat{J}_+ |\lambda m\rangle)\end{aligned}$$

which says that $\hat{J}_+ |\lambda m\rangle$ is an eigenvector of $\hat{J}_3$ with the *raised* eigenvalue $\hbar$ (m+1), i.e., $\hat{J}_+ |\lambda m\rangle \propto |\lambda, m+1\rangle$ (remember the harmonic oscillator discussion).

Since we already showed that for fixed λ, there must be a maximum value of m, say $m_{\max}$, then it must be the case that for that particular m-value we have

$$\hat{J}_+ |\lambda m_{\max}\rangle = 0$$

If this were not true, then we would have

$$\hat{J}_+ |\lambda m_{\max}\rangle \propto |\lambda, m_{\max}+1\rangle$$

but this violates the statement that $m_{\max}$ was was the maximum m-value.

Using this result we find

$$\hat{J}_-\hat{J}_+ |\lambda m_{\max}\rangle = 0 = \left(\hat{J}^2 - \hat{J}_3^2 - \hbar\hat{J}_3\right)|\lambda m_{\max}\rangle$$
$$\hbar^2\left(\lambda - m_{\max}^2 - m_{\max}\right)|\lambda m_{\max}\rangle = 0$$
$$\lambda - m_{\max}^2 - m_{\max} = 0 \rightarrow \lambda = m_{\max}^2 + m_{\max}$$
$$\lambda = m_{\max}(m_{\max}+1)$$

It is convention to define

$$m_{\max} = j \text{ and hence } \lambda = j(j+1)$$

In the same way we can show

$$\hat{J}_3\hat{J}_- |\lambda m\rangle = \hat{J}_3(\hat{J}_- |\lambda m\rangle)$$
$$= (\hat{J}_-\hat{J}_3 + [\hat{J}_3, \hat{J}_-])|\lambda m\rangle = (\hat{J}_-\hat{J}_3 - \hbar\hat{J}_+)|\lambda m\rangle$$
$$= \hbar(m-1)\hat{J}_- |\lambda m\rangle = \hbar(m-1)(\hat{J}_- |\lambda m\rangle)$$

which says that $\hat{J}_-|\lambda m\rangle$ is an eigenvector of $\hat{J}_3$ with the *lowered* eigenvalue $\hbar(m-1)$, i.e., $\hat{J}_-|\lambda m\rangle \propto |\lambda, m-1\rangle$.

If we let the minimum value of m be $m_{\min}$, then as before we must have

$$\hat{J}_- |\lambda m_{\min}\rangle = 0$$

or $m_{\min}$ is not the minimum value of m.

This says that

$$\hat{J}_+\hat{J}_-\left|\lambda m_{\min}\right\rangle = 0 = \left(\hat{J}^2 - \hat{J}_3^2 + \hbar\hat{J}_3\right)\left|\lambda m_{\min}\right\rangle$$

$$\hbar^2\left(\lambda - m_{\min}^2 + m_{\min}\right)\left|\lambda m_{\min}\right\rangle = 0$$

$$\lambda - m_{\min}^2 + m_{\min} = 0 \rightarrow \lambda = m_{\min}^2 - m_{\min}$$

$$\lambda = m_{\min}(m_{\min} - 1) = j(j+1)$$

which says that

$$m_{\min} = -j$$

We have thus shown that the pair of operators $\hat{J}^2$ and $\hat{J}_3$ have a common set of eigenvectors $|jm\rangle$ (we now use the labels j and m), where we have found that

$$-j \le m \le j$$

and the allowed m-values change by steps of one, i.e., for a given j-value, the allowed m-values are

$$-j, -j+1, -j+2, \ldots\ldots, j-2, j-1, j$$

which implies that

$$2j = \text{ integer}$$

or

$$j = \frac{\text{integer}}{2} \ge 0 \quad \text{the allowed values}$$

Thus, we have the *allowed sets or representations of the angular momentum commutation relations* given by

$$j = 0 \quad , \quad m = 0$$

$$j = \frac{1}{2} \quad , \quad m = \frac{1}{2}, -\frac{1}{2}$$

$$j = 1 \quad , \quad m = 1, 0, -1$$

$$j = \frac{3}{2} \quad , \quad m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$$

and so on.

For each value of j, there are $2j + 1$ allowed m-values in the eigenvalue spectrum(representation) and

$$\hat{J}^2 |jm\rangle = \hbar^2 j(j+1) |jm\rangle$$

$$\hat{J}_3 |jm\rangle = m\hbar |jm\rangle$$

Before proceeding, we need a few more relations.

We found earlier that

$$\hat{J}_+ |jm\rangle = C_+ |j, m+1\rangle = |\alpha_+\rangle$$

$$\hat{J}_- |jm\rangle = C_- |j, m-1\rangle = |\alpha_-\rangle$$

and from these we have

$$\langle\alpha_+| = C_+^* \langle j, m+1|$$

$$\langle\alpha_-| = C_-^* \langle j, m-1|$$

We can then say that

$$
\begin{aligned}
\langle \alpha_+ \mid \alpha_+ \rangle &= |C_+|^2 \langle j, m+1 \mid j, m+1 \rangle = |C_+|^2 \\
&= (\langle jm| (\hat{J}_+)^+)(\hat{J}_+ |jm\rangle) \\
&= \langle jm| \hat{J}_- \hat{J}_+ |jm\rangle \\
&= \langle jm| \left(\hat{J}^2 - \hat{J}_3^2 - \hbar \hat{J}_3\right) |jm\rangle \\
&= \langle jm| \hbar^2 (j(j+1) - m^2 - m) |jm\rangle \\
&= \hbar^2 (j(j+1) - m^2 - m) \langle jm \mid jm \rangle \\
&= \hbar^2 (j(j+1) - m^2 - m)
\end{aligned}
$$

or

$$
C_+ = \hbar \sqrt{j(j+1) - m(m+1)}
$$

and similarly

$$
\begin{aligned}
\langle \alpha_- \mid \alpha_- \rangle &= |C_-|^2 \langle j, m-1 \mid j, m-1 \rangle = |C_-|^2 \\
&= (\langle jm| (\hat{J}_-)^+)(\hat{J}_- |jm\rangle) \\
&= \langle jm| \hat{J}_+ \hat{J}_- |jm\rangle \\
&= \langle jm| \left(\hat{J}^2 - \hat{J}_3^2 + \hbar \hat{J}_3\right) |jm\rangle \\
&= \langle jm| \hbar^2 (j(j+1) - m^2 + m) |jm\rangle \\
&= \hbar^2 (j(j+1) - m^2 + m) \langle jm \mid jm \rangle \\
&= \hbar^2 (j(j+1) - m^2 + m)
\end{aligned}
$$

or

$$C_- = \hbar\sqrt{j(j+1) - m(m-1)}$$

Therefore, we have the very important relations for the raising/lowering or ladder operators

$$\hat{J}_\pm |jm\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\,|j, m\pm 1\rangle$$
$$= \hbar\sqrt{(j\pm m+1)(j\mp m)}\,|j, m\pm 1\rangle$$

stop

Transformations and Generators; Spherical Harmonics (now we see how messy 3-dimensions gets)

There are many vector operators and vector component operators in the following discussions.

To avoid confusing notation, we will adopt the following conventions:

$\vec{A}_{op}$ = a vector operator

A_j = a vector component operator

$\hat{B}$ = any non - vector operator or it might be a unit vector (context will decide)

$\vec{q}$ = an ordinary vector

As we showed earlier, the angular momentum operators are the generators of rotations.

The unitary transformation operator for a rotation through an angle θ about an axis along the direction specified by the unit vector $\hat{n}$ is given by

$$\hat{U}_{\hat{n}}(\theta) = e^{-\frac{i}{\hbar}\theta\hat{n}\cdot\vec{J}_{op}}$$

where $\vec{J}_{op}$ is the angular momentum operator = generator of rotations.

What does the $\hat{J}_3$ operator look like in the position representation?

We will quickly get an idea of the answer and then step back and do things in more detail.

Suppose that we have a position representation wave function $\psi(\vec{r})$.

For a rotation about the 3-axis, we showed earlier that for an infinitesimal angle ε

$$\hat{U}_3(\varepsilon)\psi(x_1, x_2, x_3) = \psi(x_1 \cos\varepsilon + x_2 \sin\varepsilon, -x_1 \sin\varepsilon + x_2 \cos\varepsilon, x_3)$$

In general, for infinitesimal shifts(a in the case below) in the coordinates, we have, to lowest order in the infinitesimals, for a function of one variable

$$f(x + a) = f(x) + a\frac{\partial f}{\partial x}$$

Extending this to two variables, we have, to first order in infinitesimals a and b,

$$f(x + a, y + b) = f(x, y) + a\frac{\partial f}{\partial x} + b\frac{\partial f}{\partial y}$$

Therefore, for an infinitesimal angle of rotation ε,

$$\begin{aligned}\hat{U}_3(\varepsilon)\psi(x_1, x_2, x_3) &= \psi(x_1 \cos\varepsilon + x_2 \sin\varepsilon, -x_1 \sin\varepsilon + x_2 \cos\varepsilon, x_3) \\ &= \psi(x_1, x_2, x_3) + \varepsilon x_2 \frac{\partial\psi}{\partial x_1} - \varepsilon x_1 \frac{\partial\psi}{\partial x_2} \\ &= \left(1 + \varepsilon\left(x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2}\right)\right)\psi(x_1, x_2, x_3)\end{aligned}$$

But we also have (to first order)

$$\hat{U}_3(\varepsilon)\psi(x_1, x_2, x_3) = (1 - \frac{i}{\hbar}\varepsilon\hat{J}_3)\psi(x_1, x_2, x_3)$$

Putting these two equations together we have

$$\hat{J}_3 = -i\hbar\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right) = (\vec{r}_{op}\times(-i\hbar\nabla))_3$$

$$= (\vec{r}_{op}\times\vec{p}_{op})_3 = \left(\vec{L}_{op}\right)_3 = \hat{L}_3$$

the normal cross product rule but now between operators!

where

$\vec{L}_{op}$ = orbital angular momentum operator

$\vec{r}_{op} = (\hat{x},\hat{y},\hat{z}) = (\hat{x}_1,\hat{x}_2,\hat{x}_3)$

$\vec{p}_{op} = (\hat{p}_x,\hat{p}_y,\hat{p}_z) = (\hat{p}_1,\hat{p}_2,\hat{p}_3)$

Since $\vec{L}_{\text{op}}$ is an angular momentum, it must have the commutation relations

$$\left[\hat{L}_i,\hat{L}_j\right] = i\hbar\varepsilon_{ijk}\hat{L}_k$$

where as we indicated above

$$\hat{L}_1 = \hat{x}_2\hat{p}_3 - \hat{x}_3\hat{p}_2$$

$$\hat{L}_2 = \hat{x}_3\hat{p}_1 - \hat{x}_1\hat{p}_3$$

$$\hat{L}_3 = \hat{x}_1\hat{p}_2 - \hat{x}_2\hat{p}_1$$

and

$$\vec{L}^{+}_{op} = \vec{L}_{op}$$

Using

$$\left[\hat{x}_i,\hat{p}_j\right] = i\hbar\delta_{ij}$$

we get

$$\left[\hat{L}_i,x_j\right] = i\hbar\varepsilon_{ijk}x_k$$

and for $\hat{n}$ = a unit vector

$$\sum_i \hat{n}_i \left[\hat{L}_i, x_j\right] = i\hbar \sum_i \hat{n}_i \varepsilon_{ijk} x_k$$

$$\left[\hat{n}\cdot\vec{L}_{op}, x_j\right] = i\hbar \left(\vec{r}_{op}\times\hat{n}\right)_j$$

$$\left[\hat{n}\cdot\vec{L}_{op}, \vec{r}_{op}\right] = \sum_j \left[\hat{n}\cdot\vec{L}_{op}, x_j\right]\hat{e}_j$$

$$= i\hbar \sum_j \left(\vec{r}_{op}\times\hat{n}\right)_j \hat{e}_j = i\hbar \left(\vec{r}_{op}\times\hat{n}\right)$$

where we have used

$$\vec{A}\times\vec{B} = \sum_{ijk} \varepsilon_{ijk} A_j B_k \hat{e}_i$$

Similarly, we get

$$\left[\hat{n}\cdot\vec{L}_{op}, \vec{p}_{op}\right] = i\hbar \left(\vec{p}_{op}\times\hat{n}\right)$$

Now let us step back and consider rotations in 3-dimensional space and try to get a better physical understanding of what is happening.

Consider the operator

$$\vec{r}\,'_{op} = \vec{r}_{op} + \vec{\alpha}\times\vec{r}_{op}$$

where $\vec{\alpha}$ = ordinary **infinitesimal** vector.

Now let $|\vec{r}_0\rangle$ = an eigenstate of $\vec{r}_{op}$ with eigenvalue $\vec{r}_0$, i.e.,

$$\vec{r}_{op}\,|\vec{r}_0\rangle = \vec{r}_0\,|\vec{r}_0\rangle$$

We then have

$$\vec{r}\,'_{op}\,|\vec{r}_0\rangle = \vec{r}\,'_0\,|\vec{r}_0\rangle = \left(\vec{r}_0 + \vec{\alpha}\times\vec{r}_0\right)|\vec{r}_0\rangle$$

which says that $|\vec{r}_0\rangle$ is also an eigenstate of $\vec{r}\,'_{op}$ (different eigenvalues).

Now, for simplicity, let $\vec{\alpha} = \alpha\,\hat{e}_3$ (rotation about z-axis), which says that

$$\vec{\alpha} \times \vec{r}_0 = \alpha\hat{e}_3 \times (x_{01}\hat{e}_1 + x_{02}\hat{e}_2 + x_{03}\hat{e}_3) = \alpha x_{01}\hat{e}_2 - \alpha x_{02}\hat{e}_1$$

$$\vec{r}_0 + \vec{\alpha} \times \vec{r}_0 = (x_{01} - \alpha x_{02})\hat{e}_1 + (x_{02} + \alpha x_{01})\hat{e}_2 + x_{03}\hat{e}_3$$

This last expression is the vector we get if we rotate $\vec{r}_0$ about $\hat{\alpha} = \vec{\alpha}/|\vec{\alpha}|$ ($\hat{e}_3$ in this case) by an infinitesimal angle $\hat{\alpha} = |\vec{\alpha}|$.

This result generalizes for $\vec{\alpha}$ in any direction.

Since the eigenvalues of $\vec{r}'_{op}$ are those of $\vec{r}_{op}$ rotated by $|\vec{\alpha}|$ about $\vec{\alpha}$, we conclude that $\vec{r}'_{op}$ is the position operator rotated by rotated by $|\vec{\alpha}|$ about $\vec{\alpha}$.

Alternatively, $\vec{r}'_{op}$ is the position operator in a coordinate frame rotated by $|\vec{\alpha}|$ about $\vec{\alpha}$ (corresponds to active/passive views).

To connect this to generators, unitary transformations, and angular momentum, we proceed as follows. We can rewrite $\vec{r}'_{op}$ as

$$\vec{r}\,'_{op} = \vec{r}_{op} + \frac{i}{\hbar}\left[\vec{\alpha}\cdot\vec{L}_{op}, \vec{r}_{op}\right]$$

which is equivalent (to first order in α) to

$$\vec{r}\,'_{op} = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\vec{r}_{op}e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}} \qquad \text{i.e.,} \quad \vec{r}\,'_{op} = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\vec{r}_{op}e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}$$

$$= (\hat{I} + \frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op})\vec{r}_{op}(\hat{I} - \frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}) + O(\alpha^2)$$

$$= \vec{r}_{op} + \frac{i}{\hbar}\left[\vec{\alpha}\cdot\vec{L}_{op}, \vec{r}_{op}\right] + O(\alpha^2)$$

Earlier, however, we showed that, if the state vector transforms as

$$|\psi'\rangle = \hat{U}\,|\psi\rangle$$

then the operators transform as

$$\hat{U}^{-1}\hat{O}\hat{U}$$

which then implies that the rotation operator is

$$\hat{U}(\vec{\alpha}) = e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}$$

as we expect.

This result derived for infinitesimal rotation angles holds for finite rotation angles also.

Let us look at the effect on state vectors

$$\vec{r}\,'_{op}\,|\vec{r}_0\rangle = \vec{r}\,'_0\,|\vec{r}_0\rangle = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\vec{r}_{op}e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\,|\vec{r}_0\rangle$$

$$\vec{r}_{op}e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\,|\vec{r}_0\rangle = \vec{r}\,'_0e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\,|\vec{r}_0\rangle$$

or

$$e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\,|\vec{r}_0\rangle$$

is an eigenstate of $\vec{r}_{op}$ with eigenvalue $\vec{r}\,'_0$ or

$$|\vec{r}\,'_0\rangle = e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}\,|\vec{r}_0\rangle \text{ and } \langle\vec{r}\,'_0| = \langle\vec{r}_0|\,e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}}$$

and thus $\vec{L}_{op}$ is the generator of **ordinary** rotations in 3-dimensional space.

For wave functions we have $\psi(\vec{r}_0) = \langle\vec{r}_0 \mid \psi\rangle$.

Using this result, the wave function transforms as

$$\psi(\vec{r}\,'_0) = \langle \vec{r}\,'_0 \mid \psi \rangle = \langle \vec{r}_0 | \, e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}} \, | \psi \rangle$$
$$= \langle \vec{r}_0 \mid \psi' \rangle = \psi'(\vec{r}_0) = \text{ wave function at rotated point } \vec{r}\,'_0$$

Now, we have seen that

$$\vec{L}_{op} = \vec{r}_{op} \times \vec{p}_{op} = -i\hbar \vec{r}_{op} \times \nabla$$

This can easily be evaluated in different coordinate systems.

Cartesian Coordinates

$$\vec{L}_{op} = -i\hbar \sum_{ijk} \varepsilon_{ijk} x_j \frac{\partial}{\partial x_k} \hat{e}_i$$

$$\hat{L}_1 = -i\hbar \left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right)$$

$$\hat{L}_2 = -i\hbar \left(x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right) \quad , \quad \hat{L}_3 = -i\hbar \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right)$$

as we saw at the beginning of this discussion.

Spherical-Polar Coordinates

We have $$\vec{r} = r\hat{e}_r \text{ and } \nabla = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi}$$

where

$$\hat{e}_r = \sin\theta \cos\varphi \hat{e}_1 + \sin\theta \sin\varphi \hat{e}_2 + \cos\theta \hat{e}_3$$
$$\hat{e}_\theta = \cos\theta \cos\varphi \hat{e}_1 + \cos\theta \sin\varphi \hat{e}_2 + \sin s\theta \hat{e}_3$$
$$\hat{e}_\varphi = -\sin\theta \hat{e}_1 + \cos\theta \hat{e}_2$$

which gives

$$\vec{L}_{op} = -i\hbar\left[\hat{e}_\varphi \frac{\partial}{\partial\theta} - \hat{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right]$$

and

$$\hat{L}_3 = \hat{L}_z = \hat{e}_z \cdot \vec{L}_{op} = -i\hbar\frac{\partial}{\partial\varphi}$$

$$\vec{L}_{op}^2 = \vec{L}_{op} \cdot \vec{L}_{op} = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

Similarly, we have

$$\hat{L}_1 = \hat{L}_x = i\hbar\left[\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right]$$

$$\hat{L}_2 = \hat{L}_y = -i\hbar\left[\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right]$$

3 dimensions is significantly more complicated than 1 dimension

and

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\vec{L}_{op}^2}{\hbar^2 r^2}$$

Eigenfunctions; Eigenvalues; Position Representation

Since $\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\varepsilon_{ijk}\hat{L}_k$ and $\left[\hat{L}_{op}^2, \hat{L}_j\right] = 0$

the derivation of the eigenvalues and eigenvectors follows from our earlier work, i.e., the equations

$$\hat{L}_{op}^2 |\ell m\rangle = \hbar^2\ell(\ell+1)|\ell m\rangle \text{ and } \hat{L}_3|\ell m\rangle = \hbar m|\ell m\rangle$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

imply

$$\ell = \frac{\text{integer}}{2} \geq 0$$

and for a given value of ℓ , m takes on the $2\ell+1$ values

$$m = -\ell, -\ell+1, -\ell+2, \ldots\ldots\ldots, \ell-2, \ell-1, \ell$$

If we move back into 3-dimensional space and define

$$Y_{\ell m}(\theta,\varphi) = \langle \theta\varphi \mid \ell m \rangle = \text{ spherical harmonic}$$

then we have the defining equations for the $Y_{\ell m}(\theta,\phi)$ given by

$$\begin{aligned}
\langle \theta\varphi | \vec{L}^2_{op} | \ell m \rangle &= \vec{L}^2_{op} \langle \theta\varphi \mid \ell m \rangle = \vec{L}^2_{op} Y_{\ell m}(\theta,\varphi) \\
&= \hbar^2 \ell(\ell+1) \langle \theta\varphi \mid \ell m \rangle = \hbar^2 \ell(\ell+1) Y_{\ell m}(\theta,\varphi) \\
\langle \theta\varphi | \hat{L}_3 | \ell m \rangle &= \hat{L}_3 \langle \theta\varphi \mid \ell m \rangle = \hat{L}_3 Y_{\ell m}(\theta,\varphi) \\
&= \hbar m \langle \theta\varphi \mid \ell m \rangle = \hbar m Y_{\ell m}(\theta,\varphi)
\end{aligned}$$

Before determining the functional form of the $Y_{\ell m}$'s, we must step back and see if there are any restrictions that need to be imposed on the possible eigenvalues ℓ and m due to the fact that we are in a real 3-dimensional space - we are physicists after all!

In general, eigenvalue restrictions come about only from the imposition of physical boundary conditions.

A standard boundary condition that is usually imposed is the following:

In real 3-dimensional space, if we rotate the system (or the axes by 2π, then we get back the same world.

This means that the $Y_{\ell m}(\theta,\phi)$ should be single-valued under such rotations or that

$$Y_{\ell m}(\theta,\varphi+2\pi) = Y_{\ell m}(\theta,\varphi)$$

Now from the general rules we have developed, this gives

$$\langle \theta, \varphi + 2\pi \mid \ell m \rangle = \langle \theta\varphi | \, e^{2\pi i \hat{L}_3/\hbar} \, | \ell m \rangle = e^{2\pi m i} \langle \theta, \varphi \mid \ell m \rangle$$

or that single-valuedness of the wave function requires that

$$\langle \theta, \varphi + 2\pi \mid \ell m \rangle = \langle \theta\varphi | \, e^{2\pi i \hat{L}_3/\hbar} \, | \ell m \rangle = e^{2\pi m i} \langle \theta, \varphi \mid \ell m \rangle$$

This says, that for orbital angular momentum in real 3-dimensional space, no 1/2-integer values are allowed for *m* and hence that ℓ must be an integer.

The allowed sets are:

$$\ell = 0 \quad , \quad m = 0$$
$$\ell = 1 \quad , \quad m = -1, 0, 1$$
$$\ell = 2 \quad , \quad m = -2, -1, 0, 1, 2$$

and so on.

It is important to note that we are imposing a much stronger condition than is necessary.

In general, as we have stated several times, it is not the state vectors, operators or wave functions that have any physical meaning in quantum mechanics.

The only quantities that have physical meaning are those directly related to measurable quantities, namely, the probabilities, and the expectation values.

This single-valued condition on m is not needed for the single-valuedness of the expectation values, since the extra phase factors involving *m* will cancel out during the calculation of the expectation value.

Experiment, however, says that ℓ is an integer only, so it seems that the strong condition is valid.

We cannot prove that this is so, however.

Let us now figure out the $Y_{\ell m}(\theta,\phi)$.

We have

$$\hat{L}_3 Y_{\ell m}(\theta,\varphi) = \frac{\hbar}{i}\frac{\partial}{\partial\varphi} Y_{\ell m}(\theta,\varphi) = \hbar m Y_{\ell m}(\theta,\varphi)$$

which tells us the ϕ-dependence.

$$Y_{\ell m}(\theta,\varphi) = e^{im\varphi} P_{\ell m}(\theta)$$

Now we also must have, since ℓ = maximum value of m

$$\langle\theta\varphi|\,\hat{L}_+\,|\ell\ell\rangle = 0 = \hat{L}_+\,\langle\theta\varphi\,|\,\ell\ell\rangle = \hat{L}_+ Y_{\ell\ell}(\theta,\varphi)$$

Using the expressions for $\hat{L}_x, \hat{L}_y, \hat{L}_+$ and $\hat{L}_-$ we have

$$\frac{\hbar}{i} e^{i\varphi}\left[i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\varphi}\right] Y_{\ell\ell}(\theta,\varphi) = 0$$

Using

$$\frac{\hbar}{i}\frac{\partial}{\partial\varphi} Y_{\ell\ell}(\theta,\varphi) = \ell\hbar Y_{\ell\ell}(\theta,\varphi)$$

we get

$$\left[\frac{\partial}{\partial\theta} - \ell\cot\theta\right] P_{\ell\ell}(\theta) = 0$$

or

$$P_{\ell\ell}(\theta) = (\sin\theta)^\ell$$

Therefore, the final expression is

$$Y_{\ell\ell}(\theta,\varphi) = A_{\ell m} e^{i\ell\varphi}(\sin\theta)^\ell$$

Now that we have generated the topmost spherical harmonic.

We can generate all the others for a given ℓ using the lowering operators, i.e.,

$$\hat{L}_- Y_{\ell m}(\theta,\varphi) = \hbar\sqrt{\ell(\ell+1)-m(m-1)}\,Y_{\ell m-1}(\theta,\varphi)$$

where

$$\hat{L}_- = \frac{\hbar}{i}e^{-i\varphi}\left[i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\varphi}\right]$$

In general, we choose the $A_{\ell m}$ so that the $Y_{\ell m}$ (θ,ϕ) are normalized, i.e.,

$$1 = \int d\Omega\,|Y_{\ell m}(\theta,\varphi)|^2 = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta\,|Y_{\ell m}(\theta,\varphi)|^2$$

Since the $Y_{\ell m}$ (θ,ϕ) are eigenfunctions of a Hermitian operators, they form a compete set which we can always make orthogonal so that we also assume that we have

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta Y^*_{\ell' m'}(\theta,\varphi)Y_{\ell m}(\theta,\varphi) = \delta_{\ell'\ell}\delta_{m'm}$$

The algebra is complicated.

The general result is

$$Y_{\ell m}(\theta,\varphi) - \frac{(-1)\ell}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}\frac{e^{im\varphi}}{(\sin\theta)^m}\left(\frac{d}{d\cos\theta}\right)^{\ell-m}(\sin\theta)^{2\ell}$$

Some examples are:

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \quad , \quad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin\theta \quad , \quad Y_{20} = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$$

$$Y_{2,\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\varphi} \quad , \quad Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\varphi}$$

Some Properties

$$Y_{\ell,-m}(\theta,\varphi) = (-1)^m Y^*_{\ell,m}(\theta,\varphi)$$

Under the parity operation

$$\vec{r} \to -\vec{r} \text{ or } r \to r, \theta \to \pi - \theta, \varphi \to \varphi + \pi$$

This says that

$$e^{im\varphi} \to e^{im\varphi} e^{im\pi} = (-1)^m e^{im\varphi}$$

$$\sin\theta \to \sin(\pi - \theta) \to \sin\theta$$

$$\cos\theta \to \cos(\pi - \theta) \to -\cos\theta$$

which imply that

$$Y_{\ell,m}(\theta,\varphi) \to (-1)^\ell Y_{\ell,m}(\theta,\varphi)$$

Therefore

if ℓ is even, then we have an even parity state

if ℓ is odd, then we have an odd parity state

Since they form a complete set, any function of (θ, ϕ) can be expanded in terms of the $Y_{\ell m}(\theta,\phi)$ (the $Y_{\ell m}(\theta,\phi)$ are a basis), i.e., we can write

$$f(\theta,\varphi) = \sum_{\ell,m} f_{\ell m} Y_{\ell,m}(\theta,\varphi)$$

where

$$f_{\ell m} = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta Y^*_{\ell' m'}(\theta,\varphi) f(\theta,\varphi)$$

Spin

As we discussed earlier, a second kind of angular momentum exists in quantum mechanics.

It is related to internal degrees of freedom of particles and is not related in any way to ordinary 3-dimensional space properties.

We designate this new angular momentum by spin and represent it by the operator $\vec{S}_{op}$, where since it is an angular momentum, its components must satisfy the commutators

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\varepsilon_{ijk}\hat{S}_k$$

where we have used the Einstein summation convention over repeated indices.

The analysis for the eigenvalues and eigenvectors follows the same path as for earlier discussions.

We have

$$\vec{S}^2_{op}\left|s, m_s\right\rangle = \hbar^2 s(s+1)\left|s, m_s\right\rangle$$
$$\hat{S}_3\left|s, m_s\right\rangle = \hbar m_s\left|s, m_s\right\rangle$$

which, together with the commutators, gives the following results.

For a given value of s, we have $2s + 1$ m_s-values

$$m_s = -s, -s+1, -s+2, \ldots\ldots, s-2, s-1, s$$

where

$$s = \frac{\text{integer}}{2} \geq 0$$

There are no boundary conditions restricting the value of s, so we can have both integer and half-integer values.

We now turn our attention to a most important special case and then generalize the details.

Spin 1/2

We define a new operator $\vec{\sigma}_{op}$ such that

$$\vec{S}_{op} = \frac{1}{2}\hbar\vec{\sigma}_{op}$$

where $\vec{\sigma}_{op} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$ are called the Pauli spin operators.

It is experimentally observed that if one measures the component of this spin angular momentum along any direction, one always obtains either $\pm\hbar/2$.

If we designate the state with spin = $+\hbar/2$ or spin up in the $\hat{n}$ direction by the ket vectors $|\hat{n}\uparrow\rangle$ or $|\hat{n}\ +\rangle$, we then have

$$\vec{S}_{op}\cdot\hat{n}\,|\hat{n}\uparrow\rangle = \frac{\hbar}{2}|\hat{n}\uparrow\rangle \text{ and } \vec{S}_{op}\cdot\hat{n}\,|\hat{n}\downarrow\rangle = -\frac{\hbar}{2}|\hat{n}\downarrow\rangle$$

Any pair of eigenvectors $|\hat{n}\uparrow\rangle$ or $|\hat{n}\downarrow\rangle$ for a given direction $\hat{n}$ form a basis for the vector space associated with spin = 1/2 and we have

$\langle \hat{n} \uparrow | \psi \rangle =$ amplitude for finding spin "up" along $\hat{n}$ if we are in the state $|\psi\rangle$

$\langle \hat{n} \downarrow | \psi \rangle =$ amplitude for finding spin "down" along $\hat{n}$ if we are in the state $|\psi\rangle$

These two amplitudes exhaust all possible measurements for spin = 1/2 in the $\hat{n}$ direction and therefore completely specify the state $|\psi\rangle$.

That is what we mean physically when we say they form a basis set or representation.

When we build the standard basis from these amplitudes, we choose it to be an eigenstate of the $\hat{S}_3$ or $\hat{S}_z$ operator, i.e., if we write

$$|\psi\rangle = \begin{pmatrix} \langle z \uparrow | \psi \rangle \\ \langle z \downarrow | \psi \rangle \end{pmatrix} = \text{a 2 - component vector}$$

then the appropriate basis is

$$|z \uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \text{spin up in z - direction}$$

$$|z \downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \text{spin down in z - direction}$$

Matrix Representations

Using this basis, the matrix representation of $\hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$ is

$$S_z = \begin{pmatrix} \langle z \uparrow | \hat{S}_z | z \uparrow \rangle & \langle z \uparrow | \hat{S}_z | z \downarrow \rangle \\ \langle z \downarrow | \hat{S}_z | z \uparrow \rangle & \langle z \downarrow | \hat{S}_z | z \downarrow \rangle \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

$$\rightarrow \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Now

$$\hat{S}_{\pm} = \hat{S}_x \pm i\hat{S}_y$$

$$\rightarrow \hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} \text{ and } \hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i}$$

Therefore, using

$$S_x = \begin{pmatrix} \langle z\uparrow|\hat{S}_x|z\uparrow\rangle & \langle z\uparrow|\hat{S}_x|z\downarrow\rangle \\ \langle z\downarrow|\hat{S}_x|z\uparrow\rangle & \langle z\downarrow|\hat{S}_x|z\downarrow\rangle \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x$$

$$\rightarrow \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and in a similar way

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Properties of the $\hat{\sigma}_i$

From

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\varepsilon_{ijk}\hat{S}_k$$

and

$$\vec{S}_{op} = \frac{1}{2}\hbar\vec{\sigma}_{op}$$

we get the commutation relations

$$\left[\hat{\sigma}_i, \hat{\sigma}_j\right] = 2i\varepsilon_{ijk}\hat{\sigma}_k$$

In addition, we have

$$\hat{\sigma}_i\hat{\sigma}_j = i\varepsilon_{ijk}\hat{\sigma}_k \quad i \neq j$$

$$\hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i = \{\hat{\sigma}_i, \hat{\sigma}_j\} = 0 \text{ (called the anticommutator)}$$

$$\hat{\sigma}_{\mathrm{i}}^2 = \hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The fact that the spin = 1/2 operators anticommute is directly linked to the existence of fermions as one sees when the relativistic equation for the electron is studied.

Put all together, these relations give

$$\hat{\sigma}_i\hat{\sigma}_j = \delta_{ij} + i\varepsilon_{ijk}\hat{\sigma}_k$$

or going back to the $\hat{S}_i$

$$\hat{S}_i\hat{S}_j = \frac{\hbar^2}{4}\delta_{ij} + i\varepsilon_{ijk}\frac{\hbar}{2}\hat{S}_k$$

In the special case of spin = 1/2, we have

$$\vec{S}_{op}^2 = \frac{\hbar^2}{4}\left(\hat{\sigma}_x^2 + \hat{\sigma}_y^2 + \hat{\sigma}_z^2\right) = \frac{\hbar^2}{4}\left(\hat{I} + \hat{I} + \hat{I}\right)$$

$$= \frac{3\hbar^2}{4}\hat{I} = \hbar^2 s(s+1)\hat{I} \text{ with } s = \frac{1}{2}$$

A very useful property that we will employ many time later on is

$$\begin{aligned}(\vec{a}\cdot\vec{\sigma}_{op})\left(\vec{b}\cdot\vec{\sigma}_{op}\right) &= a_i\hat{\sigma}_i b_j\hat{\sigma}_j \\ &= \delta_{ij}a_ib_j + i\varepsilon_{ijk}a_ib_j\hat{\sigma}_k = a_ib_i + i\varepsilon_{ijk}a_ib_j\hat{\sigma}_k \\ &= \vec{a}\cdot\vec{b} + i(\vec{a}\times\vec{b})\cdot\vec{\sigma}_{op}\end{aligned}$$

Rotations in Spin Space

We have said that

$$\vec{S}_{op}\cdot\hat{n}\,|\hat{n}\pm\rangle = \pm\frac{\hbar}{2}\,|\hat{n}\pm\rangle$$

What do the states $|\,\hat{n}\,\pm\rangle$ look like in the $|\,\hat{z}\,\pm\rangle$ basis?

One way to find out is the direct approach.

Let us choose a Cartesian basis for the unit vector (we will look at other choices afterwards)

$$\hat{n} = (n_x, n_y, n_z) \quad , \qquad \text{all real}$$

We then have

$$\vec{S}_{op}\cdot\hat{n} = \frac{\hbar}{2}\vec{\sigma}_{op}\cdot\hat{n} = \frac{\hbar}{2}(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z)$$

$$= \frac{\hbar}{2}\left(n_x\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + n_y\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + n_z\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right)$$

$$= \frac{\hbar}{2}\begin{pmatrix} n_z & n_x - in_y\\ n_x + in_y & -n_z\end{pmatrix}$$

and

$$\vec{S}_{op}\cdot\hat{n}\,|\hat{n}+\rangle = +\frac{\hbar}{2}\,|\hat{n}+\rangle$$

$$\frac{\hbar}{2}\begin{pmatrix} n_z & n_x - in_y\\ n_x + in_y & -n_z\end{pmatrix}\begin{pmatrix} a\\ b\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a\\ b\end{pmatrix}$$

where we have represented

$$|\hat{n}+\rangle = \begin{pmatrix} a\\ b\end{pmatrix}$$

This matrix equation gives two homogeneous equations for a and b

$$(n_z - 1)a + (n_x - in_y)b = 0$$
$$(n_x + in_y)a - (n_z + 1)b = 0$$

or

$$\frac{a}{b} = -\frac{n_x - in_y}{n_z - 1} = \frac{n_z + 1}{n_x + in_y}$$

The homogeneous equations have a non-trivial solution only if the determinant of the coefficients of a and b equals zero or $(n_z + 1)(n_z - 1) + (n_x - in_y)(n_x + in_y) = 0$

We assume that the vector $|\ \hat{n}\ +\rangle$ is normalized to one or

$$|a|^2 + |b|^2 = 1$$

Putting all this together we get $a = \frac{1}{\sqrt{2}}\sqrt{1 + n_z}$ and $b = \frac{1}{\sqrt{2}}\sqrt{1 - n_z}$

$$|\hat{n}+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1 + n_z} \\ \sqrt{1 - n_z} \end{pmatrix}$$

We can easily check this by letting $|\hat{n}+\rangle = |\ \hat{z}+\rangle$ or $n_z = 1, n_x = n_y = 0$ which gives

$$|\hat{z}+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

as expected.

In a similar manner

$$|\hat{n}-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -\sqrt{1 - n_z} \\ \sqrt{1 + n_z} \end{pmatrix}$$

Note that the two vectors $|\ \hat{n}\ +\rangle$ and $|\ \hat{n}\ -\rangle$ are orthonormal as we expect.

This calculation can also be carried out in other coordinate bases.

For the spherical-polar basis we get

$$\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$

$$\vec{S}_{op}\cdot\hat{n} = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}$$

$$|\hat{n}+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} \text{ and } |\hat{n}-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}$$

What can we say about operators in the spin = 1/2 vector space?

Any such operator $\hat{B}$ can be expressed as a linear combination of the four linearly independent matrices $\{\hat{I}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$ (they are, in fact, a basis for all 2 × 2 matrices)

$$\hat{B} = a_0\hat{I} + a_x\hat{\sigma}_x + a_y\hat{\sigma}_y + a_z\hat{\sigma}_z = a_0\hat{I} + a\cdot\vec{\sigma}_{op} = \begin{pmatrix} a_0 + a_z & a_x - ia_y \\ a_x + ia_y & a_0 - a_z \end{pmatrix}$$

In particular, the density operator or the state operator $\hat{W}$ which is the same as any other operator can be written as

$$\hat{W} = \frac{1}{2}(\hat{I} + \vec{a}\cdot\vec{\sigma}_{op})$$

where the factor of 1/2 has been chosen so that we have the required property

$$Tr\hat{W} = \frac{1}{2}Tr\hat{I} + a_i Tr\sigma_i = 1 \text{ since } Tr\sigma_i = 0$$

Since $\hat{W} = \hat{W}^{\dagger}$ we must also have all the a_i real.

What is the physical meaning of the vector $\vec{a}$?

Consider the following

$$\begin{aligned}\langle\hat{\sigma}_x\rangle &= Tr(\hat{W}\hat{\sigma}_x) = \frac{1}{2}Tr((\hat{I} + a_x\hat{\sigma}_x + a_y\hat{\sigma}_y + a_z\hat{\sigma}_z)\hat{\sigma}_x) \\ &= \frac{1}{2}Tr(\hat{\sigma}_x + a_x\hat{\sigma}_x^2 + a_y\hat{\sigma}_y\hat{\sigma}_x + a_z\hat{\sigma}_z\hat{\sigma}_x) \\ &= \frac{1}{2}Tr(\hat{\sigma}_x + a_x\hat{I} - ia_y\hat{\sigma}_z + ia_z\hat{\sigma}_y) \\ &= \frac{a_x}{2}Tr(\hat{I}) = a_x\end{aligned}$$

or, in general,

$$\langle\vec{\sigma}_{op}\rangle = Tr\left(\hat{W}\vec{\sigma}_{op}\right) = \vec{a} = \text{ polarization vector}$$

Now the eigenvalues of $\hat{W}$ are equal to

$$\frac{1}{2} + \text{ eigenvalues of } \vec{a}\cdot\vec{\sigma}_{op}$$

and from our earlier work the eigenvalues are $\vec{a} \cdot \vec{\sigma}_{op} = \pm 1$.

Therefore the eigenvalues of $\hat{W}$ are

$$\frac{1}{2}(1 \pm |\vec{a}|)$$

But, as we showed earlier, all eigenvalues of $\hat{W}$ are ≥ 0, which says that then polarization vectors have a length $|\vec{a}|$ restricted to $0 \leq |\vec{a}| \leq 1$.

Pure states have $|\vec{a}| = 1$ and this gives eigenvalues 1 and 0 for $\hat{W}$, which corresponds to *maximum* polarization.

Note that for $\vec{a} = \hat{e}_3$ a $= \hat{e}_3$, we have

$$\hat{W} = \frac{1}{2}(\hat{I}+\hat{\sigma}_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |z+\rangle\langle z+|$$

as it should for a pure state.

An unpolarized state has $|\vec{a}| = 0$ and this gives eigenvalues (1/2, 1/2) for $\hat{W}$.

This represents an *isotropic* state where $\langle \hat{S}_i \rangle = 0$.

In this case we have

$$\hat{W} = \frac{1}{2}\hat{I} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}|z+\rangle\langle z+| + \frac{1}{2}|z-\rangle\langle z-|$$

as we expect for a nonpure state or a mixture.

Let us now connect all of this stuff to rotations in spin space.

For an infinitesimal rotation through angle $\alpha = |\vec{\alpha}|$ about an axis along $\alpha\hat{} = \vec{\alpha}/\alpha$, a unit vector $\hat{m}$ becomes

$$\hat{n} = \hat{m} + \vec{\alpha} \times \hat{m}$$

Following the same steps as earlier, this implies

$$\vec{S}_{op} \cdot \hat{n} = \vec{S}_{op} \cdot \hat{m} + \vec{S}_{op} \cdot (\vec{\alpha} \times \hat{m}) = \vec{S}_{op} \cdot \hat{m} + \varepsilon_{ijk}\alpha_i \hat{m}_j \hat{S}_k$$

But we have

$$\varepsilon_{ijk}\hat{S}_k = \frac{1}{i\hbar}\left[\hat{S}_i, \hat{S}_j\right]$$

which implies that

$$\vec{S}_{op}\cdot\hat{n} = \vec{S}_{op}\cdot\hat{m} + \frac{1}{i\hbar}\left[\hat{S}_i, \hat{S}_j\right]\alpha_i\hat{m}_j$$

$$= \vec{S}_{op}\cdot\hat{m} + \frac{1}{i\hbar}[\vec{S}_{op}\cdot\vec{\alpha}, \vec{S}_{op}\cdot\hat{m}]$$

Using the same approximations as we did earlier, we can see that this expression, to first order in α, is equivalent to

$$\vec{S}_{op}\cdot\hat{n} = e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}\vec{S}_{op}\cdot\hat{m}e^{\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}$$

This result holds for finite rotation angles also.

Now using this result, we have

$$\vec{S}_{op}\cdot\hat{n}\left[e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}|\hat{m}+\rangle\right] = \left[e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}\vec{S}_{op}\cdot\hat{m}\right]|\hat{m}+\rangle$$

$$= \frac{\hbar}{2}\left[e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}|\hat{m}+\rangle\right]$$

This says that

$$e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}|\hat{m}+\rangle = |\hat{n}+\rangle \text{ and similarly } e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}|\hat{m}-\rangle = |\hat{n}-\rangle$$

The rotation that takes $\hat{m}\rightarrow\hat{n}$ is not unique, however.

We are free to rotate by an arbitrary amount about $\hat{n}$ after rotating $\hat{m}$ into $\hat{n}$.

This freedom corresponds to adding a phase factor.

We say that the unitary operator

$$e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}}$$

has the effect of rotating the eigenstate of $\vec{S}_{op}\cdot\hat{m}$ into the eigenstate of $\vec{S}_{op}\cdot\hat{n}$.

The operator performs rotations on the spin degrees of freedom.

The equations are analogous to those for real rotations in space generated by $\vec{L}_{op}$.

Let us now work out a very useful identity.

We can write

$$e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}} = e^{-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}} = \sum_{n=0}^{\infty} \frac{\left(-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}\right)^n}{n!}$$

Now we have

$$\left(\vec{\sigma}_{op}\cdot\vec{\alpha}\right)^2 = \vec{\alpha}\cdot\vec{\alpha} + i(\vec{\alpha}\times\vec{\alpha})\cdot\vec{\sigma}_{op} = \vec{\alpha}^2 = \alpha^2$$

Therefore

$$e^{-\frac{i}{\hbar}\vec{S}_{op}\cdot\vec{\alpha}} = \hat{I} + \frac{1}{1!}\left(-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}\right) + \frac{1}{2!}\left(-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}\right)^2 + \frac{1}{3!}\left(-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}\right)^3 + \ldots$$

$$= \hat{I}\left(1 - \frac{\left(\frac{\alpha}{2}\right)^2}{2!} + \frac{\left(\frac{\alpha}{2}\right)^4}{4!} - \ldots.\right) - i\vec{\sigma}_{op}\cdot\hat{\alpha}\left(\frac{\left(\frac{\alpha}{2}\right)}{1!} - \frac{\left(\frac{\alpha}{2}\right)^3}{3!} + \ldots.\right)$$

$$= \hat{I}\cos\frac{\alpha}{2} - i(\vec{\sigma}_{op}\cdot\hat{\alpha})\sin\frac{\alpha}{2}$$

Consider an example.

$\vec{\alpha} \rightarrow -90^\circ$ rotation about the *x*-axis or

$$\vec{\alpha} \rightarrow -\frac{\pi}{2}\hat{x}$$

Now we have

$$\hat{\sigma}_z(\hat{\sigma}_x)^n = (-\hat{\sigma}_x)^n\hat{\sigma}_z$$

Using these relations we get

$$e^{-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}}\hat{\sigma}_z e^{\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}} = e^{\frac{i\pi}{4}\hat{\sigma}_x}\hat{\sigma}_z e^{-\frac{i\pi}{4}\hat{\sigma}_x} = e^{\frac{i\pi}{4}\hat{\sigma}_x} e^{\frac{i\pi}{4}\hat{\sigma}_x}\hat{\sigma}_z = e^{\frac{i\pi}{2}\hat{\sigma}_x}\hat{\sigma}_z$$

$$= (\cos\frac{\pi}{2} + i\hat{\sigma}_x \sin\frac{\pi}{2})\hat{\sigma}_z = i\hat{\sigma}_x\hat{\sigma}_z = \hat{\sigma}_y$$

as expected for this particular rotation.

Now the spin degrees of freedom are simply additional degrees of freedom for the system.

The spin degrees of freedom are independent of the spatial degrees of freedom, however.

This means that we can specify them independently or that $\vec{S}_{op}$ commutes with all operators that depend on 3-dimensional space

$$\left[\vec{S}_{op}, \vec{r}_{op}\right] = 0 \quad , \quad \left[\vec{S}_{op}, \vec{p}_{op}\right] = 0 \quad , \quad \left[\vec{S}_{op}, \vec{L}_{op}\right] = 0$$

To specify completely the state of a *spinning* particle or a system with internal degrees of freedom of any kind we must know

1. the amplitudes for finding the particle at points in space
2. the amplitudes for different spin orientations

By convention, we choose $\hat{z}$ as the spin quantization direction for describing state vectors.

The total state vector is then a direct-product state of the form

$$|\psi\rangle = |\text{external}\rangle \otimes |\text{internal}\rangle$$

and the amplitudes are

$\langle \vec{r}, \hat{z}+ \mid \psi \rangle =$ probability amplitude for finding the particle at $\vec{r}$ with spin up in the $\hat{z}$ direction

$\langle \vec{r}, \hat{z}- \mid \psi \rangle =$ probability amplitude for finding the particle at $\vec{r}$ with spin down in the $\hat{z}$ direction

where

$$\langle \vec{r}, \hat{z}+ \mid \psi \rangle = \langle \vec{r} \mid \psi_{external} \rangle \langle \hat{z}+ \mid \psi_{\text{internal}} \rangle$$

and so on.

The total probability density for finding a particle at $\vec{r}$ is then the sum of two terms

$$|\langle \vec{r}, \hat{z}+ \mid \psi \rangle|^2 + |\langle \vec{r}, \hat{z}- \mid \psi \rangle|^2$$

which represents a sum over all the ways of doing it.

The total angular momentum of such a *spinning* particle is the sum of its orbital and spin angular momenta

$$\vec{J}_{op} = \vec{L}_{op} + \vec{S}_{op}$$

$\vec{J}_{op}$ is now the generator of rotations in 3-dimensional space and in spin space or it affects both external and internal degrees of freedom.

If we operate with $e^{-i\vec{\alpha}\cdot\vec{J}_{op}/\hbar}$ on the basis state $|\vec{r}_0, \hat{m}+\rangle$, where the particle is definitely at $\vec{r}_0$ with spin up (+ $\hbar$ /2) in the $\hat{m}$ direction, then we get a new state $|\vec{r}'_0, \hat{n}+\rangle$ where

$$\vec{r}\,'_0 = \vec{r}_0 + \vec{\alpha} \times \vec{r}_0 \text{ and } \hat{n} = \hat{m} + \vec{\alpha} \times \hat{m}$$

Since $[\vec{S}_{op}, \vec{L}_{op}] = 0$ we have

$$e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{J}_{op}} = e^{-\frac{i}{\hbar}(\vec{\alpha}\cdot\vec{L}_{op}+\vec{\alpha}\cdot\vec{S}_{op})}$$

$$= e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}} e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}_{op}} e^{-\frac{i}{\hbar}\vec{\alpha}\cdot[\vec{S}_{op},\vec{L}_{op}]}$$

$$= e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}} e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}_{op}}$$

This implies that

$$e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{J}_{op}} \left|\vec{r}_0, \hat{m}+\right\rangle = e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{L}_{op}} e^{-\frac{i}{\hbar}\vec{\alpha}\cdot\vec{S}_{op}} \left|\vec{r}_0, \hat{m}+\right\rangle = \left|\vec{r}\,'_0, \hat{n}+\right\rangle$$

and that $e^{-i\vec{\alpha}\cdot\vec{L}op/\hbar}$ carries out the rotation of the spatial degrees of freedom, while $e^{-i\vec{\alpha}\cdot\vec{S}op/\hbar}$ carries out the rotation of the spin degrees of freedom.

If

$$|\psi'\rangle = e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{J}_{op}} |\psi\rangle$$

then the wave function of $|\psi'\rangle$ is

$$\langle\vec{r}_0, \hat{m}+ \mid \psi'\rangle = \langle\vec{r}_0, \hat{m}+| e^{\frac{i}{\hbar}\vec{\alpha}\cdot\vec{J}_{op}} |\psi\rangle = \langle\vec{r}\,'_0, \hat{n}+ \mid \psi\rangle$$

This is the wavefunction of $|\psi\rangle$ evaluated at the rotated point with a rotated spin quantization direction.

The *spin representation* of rotations has a feature which is strikingly different from that of rotations in 3-dimensional space.

Consider a rotation by 2π in spin space.

This implies that

$$e^{-i\pi\vec{\sigma}_{op}\cdot\vec{\alpha}} = \cos\pi - i\vec{\sigma}_{op}\cdot\vec{\alpha}\sin\pi = -\hat{I}$$

A 2π rotation in spin space is represented by $-\hat{I}$.

Since the rotations $\vec{\alpha}$ and $\vec{\alpha} + 2\pi\vec{\alpha}$ are physically equivalent, we must say that the spin representation of rotations is *double-valued*, i.e.,

$$e^{-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}} \text{ and } e^{-\frac{i}{2}\vec{\sigma}_{op}\cdot(\vec{\alpha}+2\pi\hat{\alpha})} = -e^{-\frac{i}{2}\vec{\sigma}_{op}\cdot\vec{\alpha}}$$

represent the same rotation.

One must rotate by 4π in spin space to return to original state!

Problems: Chapter 6: 10, 13, 23, 32

10. A matrix element

Show for the one dimensional simple harmonic oscillator

$$\langle 0|\, e^{ik\hat{x}}\, |0\rangle = \exp\left[-k^2 \langle 0|\, \hat{x}^2\, |0\rangle /2\right]$$

where $\hat{x}$ is the position operator.

We want to evaluate

$$\langle 0|\, e^{ik\hat{x}}\, |0\rangle = \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} \langle 0|\, \hat{x}^n\, |0\rangle$$

Now

$$\begin{aligned}
&\langle 0|\, \hat{x}^0\, |0\rangle = \langle 0 \mid 0\rangle = 1 \\
&\langle 0|\, \hat{x}\, |0\rangle = \sqrt{\tfrac{\hbar}{2m\omega}} \langle 0|\, (\hat{a}+\hat{a}^+)\, |0\rangle = 0 \rightarrow \langle 0|\, \hat{x}^n\, |0\rangle = 0 \quad n\ odd \\
&\langle 0|\, \hat{x}^2\, |0\rangle = \tfrac{\hbar}{2m\omega} \langle 0|\, (\hat{a}+\hat{a}^+)^2\, |0\rangle = \tfrac{\hbar}{2m\omega} \langle 0|\, \hat{a}\hat{a}^+\, |0\rangle = \tfrac{\hbar}{2m\omega} \\
&\langle 0|\, \hat{x}^4\, |0\rangle = \tfrac{\hbar}{2m\omega} \langle 0|\, (\hat{a}\hat{a}\hat{a}^+\hat{a}^+ + \hat{a}\hat{a}^+\hat{a}\hat{a}^+)\, |0\rangle = 3\left(\tfrac{\hbar}{2m\omega}\right)^2 \\
&\langle 0|\, \hat{x}^6\, |0\rangle = 15\left(\tfrac{\hbar}{2m\omega}\right)^3 \quad , \quad \langle 0|\, \hat{x}^8\, |0\rangle = 105\left(\tfrac{\hbar}{2m\omega}\right)^4 \\
&\langle 0|\, \hat{x}^{2n}\, |0\rangle = \left(\prod_{\substack{j\le 2n \\ j\ odd}} j\right)\left(\tfrac{\hbar}{2m\omega}\right)^n = \tfrac{(2n)!}{2^n n!}\left(\tfrac{\hbar}{2m\omega}\right)^n
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle 0|\, e^{ik\hat{x}}\, |0\rangle &= \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} \langle 0|\, \hat{x}^n\, |0\rangle = 1 - \frac{k^2}{2!} \langle 0|\, \hat{x}^2\, |0\rangle + \frac{k^4}{4!} \langle 0|\, \hat{x}^4\, |0\rangle - \frac{k^6}{6!} \langle 0|\, \hat{x}^6\, |0\rangle + \ldots \\
&= 1 - \frac{k^2}{2!}\frac{\hbar}{2m\omega} + \frac{k^4}{4!} 3\left(\frac{\hbar}{2m\omega}\right)^2 - \frac{k^6}{6!} 15\left(\frac{\hbar}{2m\omega}\right)^3 + \ldots \\
&= 1 - \frac{1}{1!}\frac{k^2}{2} \langle 0|\, \hat{x}^2\, |0\rangle + \frac{1}{2!}\left(\frac{k^2}{2} \langle 0|\, \hat{x}^2\, |0\rangle\right)^2 - \frac{1}{3!}\left(\frac{k^2}{2} \langle 0|\, \hat{x}^2\, |0\rangle\right)^3 + \ldots. \\
&= e^{-\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle}
\end{aligned}$$

Alternatively, we can use the result

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]}$$

to get

$$\langle 0| e^{ik\hat{x}} |0\rangle = e^{\frac{\hbar k^2}{4m\omega}} \langle 0| e^{ik\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^+\right)} |0\rangle = e^{\frac{\hbar k^2}{4m\omega}} \langle 0| e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}} e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+} |0\rangle$$

Now expanding the exponential operators we have

$$\langle 0| e^{ik\hat{x}} |0\rangle = e^{\frac{\hbar k^2}{4m\omega}} \langle 0| \left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a} + \frac{1}{2}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^2 \hat{a}^2 + ...\right)$$

$$\times \left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}^+ + \frac{1}{2}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^2 \hat{a}^{+\,2} + ...\right)$$

$$= e^{\frac{\hbar k^2}{4m\omega}} \left(1 - \frac{k^2\hbar}{2m\omega} + \frac{k^4\hbar^2}{8m^2\omega^2} - ....\right) = e^{\frac{\hbar k^2}{4m\omega}} e^{-\frac{\hbar k^2}{2m\omega}} = e^{-\frac{\hbar k^2}{4m\omega}}$$

Since

$$\langle 0| \hat{x}^2 |0\rangle = \frac{\hbar}{2m\omega}$$

we have

$$\langle 0| e^{ik\hat{x}} |0\rangle = e^{-\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle}$$

as above.

13. Coherent States

Coherent states are defined to be eigenstates of the annihilation or lowering operator in the harmonic oscillator potential. Each coherent state has a complex label z and is given by $|z\rangle = e^{z\hat{a}^+}|0\rangle$.

We have

$$|z\rangle = e^{z\hat{a}^+}|0\rangle$$

(a) Show that $\hat{a}|z\rangle = z|z\rangle$

$$\hat{a}|z\rangle = \hat{a}e^{z\hat{a}^+}|0\rangle = \sum_{n=0}^{\infty}\frac{z^n}{n!}\hat{a}(\hat{a}^+)^n|0\rangle = \sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\hat{a}\left(\frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle\right)$$

$$= \sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\hat{a}|n\rangle = \sum_{n=1}^{\infty}\frac{z^n}{\sqrt{n!}}\sqrt{n}|n-1\rangle = z\sum_{n=1}^{\infty}\frac{z^{n-1}}{\sqrt{(n-1)!}}|n-1\rangle$$

$$= z\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle = z\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\left(\frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle\right) = ze^{z\hat{a}^+}|0\rangle = z|z\rangle$$

(b) Show that $\langle z_1 \mid z_2\rangle = e^{z_1^* z_2}$

$$\langle z_1 \mid z_2\rangle = \langle 0|e^{z*_1 a^+}e^{z_2\hat{a}^+}|0\rangle = \left(\sum_{m=0}^{\infty}\frac{z*_1^m}{\sqrt{m!}}\langle m|\right)\left(\sum_{n=0}^{\infty}\frac{z_2^n}{\sqrt{n!}}|n\rangle\right)$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{z_2^n}{\sqrt{n!}}\frac{z*_1^m}{\sqrt{m!}}\langle m \mid n\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{z_2^n}{\sqrt{n!}}\frac{z*_1^m}{\sqrt{m!}}\delta_{mn}$$

$$= \sum_{n=0}^{\infty}\frac{z_2^n}{\sqrt{n!}}\frac{z*_1^n}{\sqrt{n!}} = \sum_{n=0}^{\infty}\frac{z_2^n z*_1^n}{n!} = e^{z*_1 z_2}$$

(c) Show that the completeness relation takes the form

$$\int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z} = \int \frac{dxdy}{\pi} e^{z\hat{a}^+} |0\rangle \langle 0| e^{z^* \hat{a}} e^{-z^* z}$$
$$= \sum_{m,n} \int \frac{dxdy}{\pi} \frac{z^m (\hat{a}^+)^m}{m!} |0\rangle \langle 0| \frac{(z*)^n (\hat{a})^n}{n!} e^{-z^* z}$$
$$= \sum_{m,n} \int_0^{2\pi} \frac{d\varphi}{\pi} \int_0^{\infty} r dr \frac{r^m e^{im\varphi} (\hat{a}^+)^m}{m!} |0\rangle \langle 0| \frac{r^n e^{-in\varphi} (\hat{a})^n}{n!} e^{-r^2}$$

where we have used $z = re^{i\varphi}$. Now

$$\int_0^{2\pi} \frac{d\varphi}{\pi} e^{i(m-n)\varphi} = 2\delta_{mn}$$

Therefore, doing the m sum we have

$$\int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z} = \sum_n \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr \left(\frac{(\hat{a}^+)^n}{\sqrt{n!}} |0\rangle \right) \left(\langle 0| \frac{(\hat{a})^n}{\sqrt{n!}} \right)$$
$$= \sum_n \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr \left(|n\rangle \right) \left(\langle n| \right) = \sum_n |n\rangle \langle n| \frac{1}{n!} \int_0^{\infty} r r^{2n} e^{-r^2} dr$$

Now using $r^2 = x$ we have

$$\int_0^\infty r r^{2n} e^{-r^2} dr = \int_0^\infty x^n e^{-x} dx = n!$$

so that

$$\int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z} = \sum_n |n\rangle \langle n| = \hat{I}$$

This unusual form of the completeness relation reflects the fact that the coherent states form an *overcomplete* set of states.

$$\hat{I} = \sum_n |n\rangle \langle n| = \int \frac{dxdy}{\pi} |z\rangle \langle z| e^{-z^* z}$$

where $|n\rangle$ is a standard harmonic oscillator energy eigenstate, $\hat{I}$ is the identity operator, $z = x + iy$, and the integration is taken over the whole $x - y$ plane(use polar coordinates).

23. Neutrino Oscillations

It is generally recognized that there are at least three different kinds of neutrinos. They can be distinguished by the reactions in which the neutrinos are created or absorbed. Let us call these three types of neutrino ν_e, ν_μ and ν_τ. It has been speculated that each of these neutrinos has a small but finite rest mass, possibly different for each type. Let us suppose, for this exam question, that there is a small perturbing interaction between these neutrino types, in the absence of which all three types of neutrinos have the same nonzero rest mass M_0. The Hamiltonian of the system can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

where

$$\hat{H}_0 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} \rightarrow \text{ no interactions present}$$

and

$$\hat{H}_1 = \begin{pmatrix} 0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & 0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & 0 \end{pmatrix} \rightarrow \text{ effect of interactions}$$

where we have used the basis

$$|\nu_e\rangle = |1\rangle \quad , \quad |\nu_\mu\rangle = |2\rangle \quad , \quad |\nu_\tau\rangle = |3\rangle$$

(a) First assume that $\omega_1 = 0$, i.e., no interactions. What is the time development operator? Discuss what happens if the neutrino initially was in the state

$$|\psi(0)\rangle = |\nu_e\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \text{ or } |\psi(0)\rangle = |\nu_\mu\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ or } |\psi(0)\rangle = |\nu_\tau\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

What is happening physically in this case?

(b) Now assume that $\omega_1 \neq 0$, i.e., interactions are present. Also assume that at $t = 0$ the neutrino is in the state

$$|\psi(0)\rangle = |\nu_e\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

What is the probability as a function of time, that the neutrino will be in each of the other two states?

(c) An experiment to detect the *neutrino oscillations* is being performed. The flight path of the neutrinos is 2000 meters. Their energy is $100\,GeV$. The sensitivity of the experiment is such that the presence of 1% of neutrinos different from those present at the start of the flight can be measured with confidence. Let $M_0 = 20\,eV$. What is the smallest value of $\hbar\omega_1$ that can be detected? How does this depend on M_0? Don't ignore special relativity.

We will do this problem in two equivalent ways, (1) differential equation method and (2) linear algebraic method.

We have

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} + \begin{pmatrix} 0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & 0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & 0 \end{pmatrix} = \begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}$$

differential equation method: The Schrodinger equation is

$$\frac{\hbar}{i}\frac{\partial\psi}{\partial t} + \hat{H}\psi = 0$$

where

$$\psi = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = a_1 |\nu_1\rangle + a_2 |\nu_2\rangle + a_3 |\nu_3\rangle$$

and

$$|\nu_1\rangle = |\nu_e\rangle \quad , \quad |\nu_2\rangle = |\nu_\mu\rangle \quad , \quad |\nu_3\rangle = |\nu_\tau\rangle$$

are basis states and

$$a_i = \text{ probability amplitude to have } |\nu_i\rangle$$

This gives the matrix equation

$$i\hbar \begin{pmatrix} \dot{a}_1 \\ \dot{a}_2 \\ \dot{a}_3 \end{pmatrix} = \begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

(a) Let $\omega_1 = 0$. then we have

$$a_1(t) = e^{-iM_0 t/\hbar} a_1(0)$$
$$a_2(t) = e^{-iM_0 t/\hbar} a_2(0)$$
$$a_3(t) = e^{-iM_0 t/\hbar} a_3(0)$$

or

$$\begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \end{pmatrix} = \hat{U}(t) \begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix} = e^{-iM_0 t/\hbar} \begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix}$$

If the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$, then

$$\begin{pmatrix} a_1(0) \\ a_2(0) \\ a_3(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |\nu_1\rangle \rightarrow \begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \end{pmatrix} = e^{-iM_0 t/\hbar} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |\nu_1\rangle$$

or the neutrino stays in the state $|\nu_1\rangle$ or we do not have any oscillations between basis states. The same is true for the other cases.

(b) Let $\omega_1 \neq 0$. Again we assume the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$. Then we have the equations

$$\begin{aligned} i\hbar\dot{a}_1 &= M_0 a_1 + \hbar\omega_1 a_2 + \hbar\omega_1 a_3 \\ i\hbar\dot{a}_2 &= M_0 a_2 + \hbar\omega_1 a_1 + \hbar\omega_1 a_3 \\ i\hbar\dot{a}_3 &= M_0 a_3 + \hbar\omega_1 a_1 + \hbar\omega_1 a_2 \end{aligned}$$

with boundary conditions

$$a_1(0) = 1 \quad , \quad a_2(0) = 0 \quad , \quad a_3(0) = 0$$

Let

$$\begin{aligned} a_1(t) &= e^{-iM_0 t/\hbar} b_1(t) \rightarrow b_1(0) = 1 \\ a_2(t) &= e^{-iM_0 t/\hbar} b_2(t) \rightarrow b_2(0) = 0 \\ a_3(t) &= e^{-iM_0 t/\hbar} b_3(t) \rightarrow b_3(0) = 0 \end{aligned}$$

so that we get the new equations

$$\begin{aligned} \dot{b}_1 &= -i\omega_1(b_2 + b_3) \\ \dot{b}_2 &= -i\omega_1(b_1 + b_3) \\ \dot{b}_3 &= -i\omega_1(b_1 + b_2) \end{aligned}$$

Since there is no way to distinguish $b_2(t)$ and $b_3(t)$ in these equations we must have $b_2(t) = b_3(t)$ in this model., which gives the new equations

$$\begin{aligned} \dot{b}_1 &= -2i\omega_1 b_2 \\ \dot{b}_2 &= -i\omega_1 b_2 - i\omega_1 b_1 \end{aligned}$$

These give

$$\begin{aligned} \ddot{b}_2 &= -i\omega_1 \dot{b}_2 - i\omega_1 \dot{b}_1 = -i\omega_1 \dot{b}_2 - 2\omega_1^2 b_2 \\ \ddot{b}_2 &+ i\omega_1 \dot{b}_2 + 2\omega_1^2 b_2 = 0 \end{aligned}$$

We assume the solution $b_2(t) = e^{i\alpha t}$. Substitution converts the differential equation into an algebraic equation for the allowed values of α.

$$-\alpha^2 + \omega_1\alpha + 2\omega_1^2 = 0 \rightarrow \alpha = -2\omega_1 \ , \ +\omega_1$$

Therefore, the most general solution is

$$b_2(t) = Ae^{i\omega_1 t} + Be^{-2i\omega_1 t}$$

Now,

$$b_2(0) = A + B = 0 \rightarrow B = -A$$

so that

$$b_2(t) = A(e^{i\omega_1 t} - e^{-2i\omega_1 t}) = b_3(t)$$

Returning to the equation for $b_1(t)$, we then have

$$\dot{b}_1 = -2i\omega_1 b_2 = -2i\omega_1 A(e^{i\omega_1 t} - e^{-2i\omega_1 t})$$

so that

$$b_1(t) = -2i\omega_1 A\left(\frac{1}{i\omega_1}e^{i\omega_1 t} + \frac{1}{2i\omega_1}e^{-2i\omega_1 t}\right) = -2A\left(e^{i\omega_1 t} + \frac{1}{2}e^{-2i\omega_1 t}\right)$$

Now

$$b_1(0) = -3A = 1 \rightarrow A = -\frac{1}{3}$$

so that

$$b_1(t) = \tfrac{2}{3}\left(e^{i\omega_1 t} + \tfrac{1}{2}e^{-2i\omega_1 t}\right)$$
$$b_2(t) = -\tfrac{1}{3}(e^{i\omega_1 t} - e^{-2i\omega_1 t}) = b_3(t)$$

Finally,

$$P(\nu_e \to \nu_\mu; t) = |a_2(t)|^2 = |b_2(t)|^2 = \left| -\frac{1}{3}(e^{i\omega_1 t} - e^{-2i\omega_1 t}) \right|^2$$
$$= \frac{1}{9}\left|(e^{i\omega_1 t} - e^{-2i\omega_1 t})\right|^2 = \frac{1}{9}(2 - 2\cos 3\omega_1 t) = \frac{2}{9}(1 - \cos 3\omega_1 t)$$
$$= P(\nu_e \to \nu_\tau; t)$$

(c) The time of flight of the ν_e is $\Delta t = \ell/v$ in laboratory time. Therefore, the proper time is

$$\Delta\tau = \frac{\Delta t}{\gamma} = \Delta t\sqrt{1 - \frac{v^2}{c^2}} \approx \frac{\ell}{c}\frac{M_0}{E}$$

where $E =$ the total energy of the ν_e in the rest frame.

For $P(\nu_e \to \nu_\mu; t) \geq 0.01$ or

$$\frac{2}{9}(1 - \cos 3\omega_1 \Delta\tau) \geq 0.01$$

we require that

$$1 - \cos 3\omega_1 \Delta\tau \geq 0.045$$
$$0.955 \geq \cos 3\omega_1 \Delta\tau \approx 1 - \tfrac{9}{2}(\omega_1 \Delta\tau)^2$$
$$\omega_1 \geq \tfrac{\sqrt{2}}{3}\sqrt{0.045}\,\tfrac{cE}{\ell M_0} \approx 0.1\,\tfrac{cE}{\ell M_0}$$
$$\hbar\omega_1 \geq 0.05\,eV$$

linear algebraic method: Let us find the eigenvalues and eigenvectors of $\hat{H}$.

The characteristic equation for the eigenvalues is

$$\begin{vmatrix} M_0 - E & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 - E & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 - E \end{vmatrix} = 0 = (M_0 - E)^3 - 3\,(M_0 - E)\,(\hbar\omega_1)^2 + 2\,(\hbar\omega_1)^3$$

or letting $\alpha = (M_0 - E)$ and $\beta = \hbar\omega_1$ we have the equation

$$\alpha^3 - 3\beta^2\alpha + 2\beta^3 = 0 \rightarrow \alpha = \beta,\ \beta,\ -2\beta$$

Therefore, the eigenvalues are

$$E_1 = M_0 + \hbar\omega_1\ ,\ E_2 = E_3 = M_0 - \hbar\omega_1\ (2 - \text{folddegeneracy})$$

Now we obtain the eigenvectors. For $E_1 = M_0 + \hbar\omega_1$ we have

$$\hat{H}\,|E_1\rangle = E_1\,|E_1\rangle = (M_0 + \hbar\omega_1)\,|E_1\rangle$$

or

$$\begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = (M_0 + \hbar\omega_1) \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

or

$$\begin{aligned} -2a + \ \ b + \ \ c &= 0 \\ a - 2b + \ \ c &= 0 \\ a + \ \ b - 2c &= 0 \end{aligned}$$

which imply that

$$a = b = c = \frac{1}{\sqrt{3}} (normalized\ to\ 1)$$

or

$$|E_1\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

In a similar manner, for $E_2 = E_3 = M_0 - \hbar\omega_1$ we have

$$|E_2\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \quad , \quad |E_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

Therefore,

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \sum_n |E_n\rangle \langle E_n \mid \psi(0)\rangle = \frac{1}{\sqrt{3}} |E_1\rangle + \frac{1}{\sqrt{6}} |E_2\rangle + \frac{1}{\sqrt{2}} |E_3\rangle$$

Using $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$, we have

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle = \frac{1}{\sqrt{3}} e^{-iE_1 t/\hbar} |E_1\rangle + \frac{1}{\sqrt{6}} e^{-iE_2 t/\hbar} |E_2\rangle + \frac{1}{\sqrt{2}} e^{-iE_3 t/\hbar} |E_3\rangle$$

Then,

$$P(\nu_e \to \nu_\tau; t) = |\langle \nu_\tau \mid \psi(t)\rangle|^2$$

where

$$|\nu_\tau\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

or

$$\begin{aligned} P(\nu_e \to \nu_\tau; t) &= \left| \frac{1}{\sqrt{3}} e^{2i\omega_1 t} \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{6}} e^{-i\omega_1 t} \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} e^{-i\omega_1 t} \frac{1}{\sqrt{2}} \right|^2 \\ &= \frac{1}{9} \left| e^{3i\omega_1 t} - 1 \right|^2 = \frac{2}{9}(1 - \cos 3\omega_1 t) \end{aligned}$$

as above.

32. Deuteron model

Consider the motion of a particle of mass $m = 0.8 \times 10^{-24}\, gm$ in the well shown in the figure below:

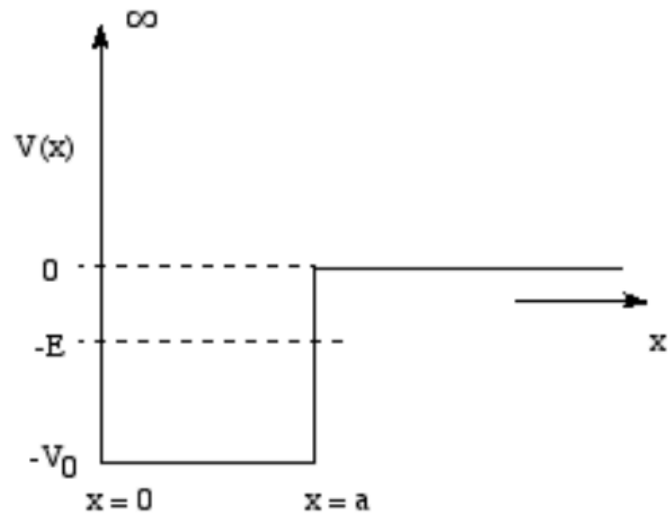


Figure 6.9: Deuteron Model

The size of the well (range of the potential) is $a = 1.4 \times 10^{-13}\, cm$. If the binding energy of the system is $2.2\, MeV$, find the depth of the potential V_0 in MeV. This is a model of the deuteron in one dimension.

We have two regions to consider. We let $E = -|E|$. For $0 \leq x \leq a$

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad , \quad \frac{\hbar^2 k^2}{2m} = V_0 - |E|$$

For $x \geq a$

$$\psi_{II}(x) = Ce^{-\gamma x} \quad , \quad \frac{\hbar^2 \gamma^2}{2m} = |E|$$

We now impose boundary conditions at $x = 0$ and $x = a$:

$$\begin{aligned}
&\psi_I(0) = 0 \rightarrow A = -B \rightarrow \psi_I(x) = A \sin kx \\
&\psi_I(a) = \psi_{II}(a) \rightarrow A \sin ka = Ce^{-\gamma a} \\
&\psi_I'(a) = \psi_{II}'(a) \rightarrow kA \cos ka = -\gamma Ce^{-\gamma a}
\end{aligned}$$

These give

$$\tan ka = -\frac{k}{\gamma} \rightarrow \tan\left(\frac{2m\left|E\right|}{\hbar^2}a^2\right)^{1/2}\left(\frac{V_0}{\left|E\right|}-1\right)^{1/2} = -\left(\frac{V_0}{\left|E\right|}-1\right)^{1/2}$$

Now,

$$\left(\frac{2m\left|E\right|}{\hbar^2}a^2\right)^{1/2} = \left(\frac{2(0.8\times10^{-27})(2.2\times10^{6}\times1.6\times10^{-19})}{(1.05\times10^{-34})^2}(1.4\times10^{-15})^2\right)^{1/2} = 0.32$$

Therefore, we have

$$\tan 0.32\left(\frac{V_0}{\left|E\right|}-1\right)^{1/2} = -\left(\frac{V_0}{\left|E\right|}-1\right)^{1/2}$$

This is solved by

$$\left(\frac{V_0}{\left|E\right|}-1\right)^{1/2} \approx 5.5 \rightarrow V_0 = 31.25\left|E\right| = 66.55\,MeV$$

Superselection Rules

Let us expand on this important point(double-valuedness) discussed last time involving 2π rotations.

The 2π rotation transformation operator is given by

$$\hat{U}_{\hat{n}}(2\pi) = e^{-\frac{2\pi i}{\hbar}\hat{n}\cdot\vec{J}_{op}}$$

When operating on the angular momentum state vectors we have

$$\hat{U}_{\hat{n}}(2\pi)\,|j,m\rangle = e^{-\frac{2\pi i}{\hbar}\hat{n}\cdot\vec{J}_{op}}\,|j,m\rangle = e^{-2\pi ij}\,|j,m\rangle = (-1)^{2j}\,|j,m\rangle$$

This says that it has no effect if j = integer and multiplies by -1 if j = half- integer.

We usually think of a rotation through 2π as a trivial operation that changes nothing in a physical system.

This belief implies that we are assuming all dynamical variables are invariant under 2π rotations or that

$$\hat{U}_{\hat{n}}(2\pi)\hat{A}\hat{U}^{\dagger}_{\hat{n}}(2\pi) = \hat{A}$$

where $\hat{A}$ is any physical observable.

But, as we have seen above, $\hat{U}_{\hat{n}}(2\pi)$ is not equal to a trivial operator (not equal to the identity operator for all physical states and operators).

This says that invariance(or not) under $\hat{U}_{\hat{n}}(2\pi)$ may lead to nontrivial consequences.

I note that the consequences that arise from invariance of an observable are not identical to those that arise from invariance of a state.

Let $\hat{U}$ = a unitary operator that leaves the observable $\hat{F}$ invariant or that we have

$$\left[\hat{U}, \hat{F}\right] = 0$$

Now consider a state that is not invariant under the transformation $\hat{U}$.

If it is a pure state represented by $|\psi\rangle$, then $|\psi'\rangle = \hat{U}\,|\psi\rangle \neq |\psi\rangle$.

The expectation value of $\hat{F}$ in the state $|\psi\rangle$ is

$$\left\langle \hat{F} \right\rangle = \langle \psi' | \hat{F} | \psi' \rangle = \langle \psi | \hat{U}^{+} \hat{F} \hat{U} | \psi \rangle = \langle \psi | \hat{U}^{+} \hat{U} \hat{F} | \psi \rangle = \langle \psi | \hat{F} | \psi \rangle$$

which implies that the observable statistical properties of $\hat{F}$ are the same in the two states $|\psi\rangle$ and $|\psi'\rangle$.

This conclusion certainly holds for $\hat{U}(2\pi)$.

Does anything else hold?

Is there something peculiar to $\hat{U}(2\pi)$?

It turns out that $\hat{U}\,(2\pi)$ divides the vector space into two subspaces:

1. integer angular momentum - has states $|+\rangle$ where

$$\hat{U}(2\pi)\,|+\rangle = |+\rangle$$

2. half-integer angular momentum - has states $|-\rangle$ where

$$\hat{U}(2\pi)\,|-\rangle = -\,|-\rangle$$

Now for any invariant physical observable $\hat{B}$ (where $[\ \hat{U}, \hat{B}\ ] = 0$), we have

$$\langle +|\,\hat{U}(2\pi)\hat{B}\,|-\rangle = \langle +|\,\hat{B}\hat{U}(2\pi)\,|-\rangle$$
$$\langle +|\,\hat{B}\,|-\rangle = -\,\langle +|\,\hat{B}\,|-\rangle$$
$$\rightarrow \langle +|\,\hat{B}\,|-\rangle = 0$$

This says that all physical observables have vanishing matrix elements between states with integer angular momentum and states with half-integer angular momentum (states in the two subspaces).

This is called a **superselection rule**.

A superselection rule says that there is *no observable distinction* among vectors of the form

$$|\psi_\varphi\rangle = |+\rangle + e^{i\varphi}\,|-\rangle$$

for different values of the phase ϕ.

This is so because

$$\langle \psi_\varphi|\,\hat{B}\,|\psi_\varphi\rangle = \langle +|\,\hat{B}\,|+\rangle + \langle -|\,\hat{B}\,|-\rangle$$

and this is independent of ϕ.

What about a more general state represented by the state operator

$$\hat{W} = \sum_{i,j} w_{ij} \left|i\right\rangle \left\langle j\right|$$

If we break up the basis for the space into + and – subspaces, i.e.,

$$\text{basis set} = \{\{+ \text{ states}\}, \{- \text{ states}\}\}$$

then the matrix representation of $\hat{W}$ partitions into four blocks(size determined by how many states)

$$\hat{W} = \begin{pmatrix} \hat{W}_{++} & \hat{W}_{+-} \\ \hat{W}_{-+} & \hat{W}_{--} \end{pmatrix}$$

While, for any physical observable, the same partitioning scheme produces

$$\hat{B} = \begin{pmatrix} \hat{B}_{++} & 0 \\ 0 & \hat{B}_{--} \end{pmatrix}$$

i.e., there is no mixing between the subspaces.

This gives

$$\left\langle \hat{B} \right\rangle = Tr\left(\hat{W}\hat{B}\right) = Tr_{+}\left(\hat{W}_{++}\hat{B}_{++}\right) + Tr_{-}\left(\hat{W}_{--}\hat{B}_{--}\right)$$

where $Tr_{\pm}$ implies a trace only over the particular subspace.

The cross matrix elements $\hat{W}_{+-}$ and $\hat{W}_{-+}$ do not contribute to the expectation value of the observables, or interference between vectors of the $|+\rangle$ and $|-\rangle$ types is not observable.

All equations of motion decouple into two separate equations in each of the two subspaces and no cross-matrix elements of $\hat{W}$ between the two subspaces ever contribute.

If we assume that the cross matrix elements are zero initially, then they will never develop(become nonzero) in time.

What is the difference between a generator $\hat{U}(2\pi)$ of a superselection rule and a symmetry operation that is generated by a universally conserved quantity such as the displacement operator

$$e^{-\frac{i}{\hbar}\vec{a}\cdot\vec{P}_{op}}$$

which is generated by the total momentum $\vec{P}_{op}$?

The Hamiltonian of any closed system is invariant under both transformations.

Both give rise to a quantum number that must be conserved in any transition.

In this example the quantum numbers are

± 1 for $U(2\pi)$ and the total momentum

The difference is that there exist observables that do not commute with $\vec{P}_{op}$ and $\vec{Q}_{op}$, but there are no observables that do not commute with $\hat{U}(2\pi)$.

By measuring the position one can distinguish states that differ only by a displacement, but there is no way to distinguish between states that differ only by a 2π rotation.

The superselection rules from $\hat{U}(2\pi)$, which separates the integer and half-integer angular momentum states, is the only such rule in the quantum mechanics of stable particles (non-relativistic quantum mechanics).

In Quantum Field Theory(relativistic quantum mechanics), where particles can be created and annihilated, the total electric charge operator generates another superselection rule, provided that one assumes all observables are invariant under gauge transformations.

This says that no interference can be observed between states of different total charge because there are no observables that do not commute with the charge operator.

In a theory of stable particles, the charge of each particle and hence the total charge is an invariant.

Thus, the total charge operator is simply a multiple of $\hat{I}$.

Every operator commutes with $\hat{I}$ implying that the charge superselection rule is trivial in non-relativistic quantum mechanics.

stop

Now let us return to the normal world and our earlier discussion.

The techniques that we have developed for the spin = 1/2 system can be applied to any two-state system.

Here is an example of a two-sided box solved using both the Schrodinger and Heisenberg pictures.

A Box with 2 Sides

Let us consider a box containing a particle in a state $|\psi\rangle$.

The box is divided into two halves (**R**ight and **L**eft) by a thin partition.

The only property that we will assign to the particle is whether it is on the **R**ight or **L**eft side of the box.

This means that the system has only two states, namely, $|R\rangle$ and $|L\rangle$ that must have the properties

$$\langle R \mid \psi \rangle = \text{ amplitude to find the particle on right side if in state } |\psi\rangle$$
$$\langle L \mid \psi \rangle = \text{ amplitude to find the particle on leftt side if in state } |\psi\rangle$$

We also suppose that the particle can tunnel through the thin partition and that

$$\frac{d}{dt}\langle R \mid \psi \rangle = \frac{K}{i\hbar}\langle L \mid \psi \rangle \quad , \quad K \text{ real}$$

How does this system develop in time?

We solve this problem in two ways, namely, using the Schrodinger and Heisenberg pictures.

Schrodinger Picture (states depend on time)

We define the general system state vector

$$|\psi\rangle = \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \langle R \mid \psi \rangle \\ \langle L \mid \psi \rangle \end{pmatrix}$$
$$= \psi_R \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_L \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$= \psi_R |R\rangle + \psi_L |L\rangle$$

two state systems can always be written this way

The time-dependent Schrodinger equation (in matrix form) is

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar\begin{pmatrix}\frac{\partial\psi_R}{\partial t}\\ \frac{\partial\psi_L}{\partial t}\end{pmatrix} = \hat{H}\begin{pmatrix}\psi_R\\ \psi_L\end{pmatrix}$$

Now we are given that

$$\frac{d\psi_R}{dt} = \frac{K}{i\hbar}\psi_L \rightarrow \frac{d\psi_R^*}{dt} = -\frac{K}{i\hbar}\psi_L^*$$

The state vector must remain normalized as it develops in time so that

$$\langle\psi \mid \psi\rangle = |\psi_R|^2 + |\psi_L|^2 = 1$$

$$\frac{\partial\langle\psi \mid \psi\rangle}{\partial t} = 0 = \frac{\partial\psi_R^*}{\partial t}\psi_R + \psi_R^*\frac{\partial\psi_R}{\partial t} + \frac{\partial\psi_L^*}{\partial t}\psi_L + \psi_L^*\frac{\partial\psi_L}{\partial t}$$

$$0 = -\frac{K}{i\hbar}\psi_L^*\psi_R + \psi_R^*\frac{K}{i\hbar}\psi_L + \frac{\partial\psi_L^*}{\partial t}\psi_L + \psi_L^*\frac{\partial\psi_L}{\partial t}$$

$$0 = \psi_L\left(\frac{\partial\psi_L^*}{\partial t} + \frac{K}{i\hbar}\psi_R^*\right) + \psi_L^*\left(\frac{\partial\psi_L}{\partial t} - \frac{K}{i\hbar}\psi_R\right)$$

which says that

$$\frac{d\psi_L}{dt} = \frac{K}{i\hbar}\psi_R \rightarrow \frac{d\psi_L^*}{dt} = -\frac{K}{i\hbar}\psi_R^*$$

Therefore we have

$$K\begin{pmatrix}\psi_L\\ \psi_R\end{pmatrix} = \hat{H}\begin{pmatrix}\psi_R\\ \psi_L\end{pmatrix}$$

which says that

$$\hat{H} = K\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

try it to see that it works!

The eigenvalues of $\hat{H}$ are $\pm K$ and its eigenvectors are

$$|\pm K\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

Note that for $\hat{\wp}$ = parity operator (switches right and left) we have

$$\hat{\wp}\,|\pm K\rangle = \pm\,|\pm K\rangle$$

so these are also states of definite parity.

If the initial state of the system is $|\psi(0)\rangle = \begin{pmatrix} \psi_R(0) \\ \psi_L(0) \end{pmatrix}$

then we can write this state in terms of energy eigenstates as

$$|\psi(0)\rangle = \begin{pmatrix} \psi_R(0) \\ \psi_L(0) \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \left(\psi_R(0) + \psi_L(0)\right) |+K\rangle + \frac{1}{\sqrt{2}} \left(\psi_R(0) - \psi_L(0)\right) |-K\rangle$$

Since we know the time dependence of energy eigenstates

$$|\pm K\rangle_t = e^{\mp \frac{i}{\hbar} Kt}\,|\pm K\rangle$$

the time dependence of $|\psi(t)\rangle$ is given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(\psi_R(0) + \psi_L(0)\right) e^{-\frac{i}{\hbar} Kt}\,|+K\rangle + \frac{1}{\sqrt{2}} \left(\psi_R(0) - \psi_L(0)\right) e^{+\frac{i}{\hbar} Kt}\,|-K\rangle$$

or

$$|\psi(t)\rangle = \frac{1}{2}\begin{pmatrix} (\psi_R(0)+\psi_L(0))\,e^{-\frac{i}{\hbar}Kt} + (\psi_R(0)-\psi_L(0))\,e^{+\frac{i}{\hbar}Kt} \\ (\psi_R(0)+\psi_L(0))\,e^{-\frac{i}{\hbar}Kt} - (\psi_R(0)-\psi_L(0))\,e^{+\frac{i}{\hbar}Kt} \end{pmatrix}$$

$$= \left(\psi_R(0)\cos\frac{Kt}{\hbar} - i\psi_L(0)\sin\frac{Kt}{\hbar}\right)|R\rangle$$

$$+ \left(-i\psi_R(0)\sin\frac{Kt}{\hbar} + \psi_L(0)\cos\frac{Kt}{\hbar}\right)|L\rangle$$

switching to energy basis is so powerful!

Therefore, the probability that the particle is on the **R**ight side at time *t* is

$$P_R = |\langle R \mid \psi(t)\rangle|^2 = \left|\psi_R(0)\cos\frac{Kt}{\hbar} - i\psi_L(0)\sin\frac{Kt}{\hbar}\right|^2$$

Now suppose that

$$\psi_R(0) = \frac{1}{\sqrt{2}} \text{ and } \psi_L(0) = e^{i\delta}\psi_R(0)$$

This says that the particle was equally probable to be on either side at $t = 0$, but that the probability amplitudes differed by a phase factor.

In this case, we get

$$P_R = \frac{1}{2}\left(1 + \sin\delta\sin\frac{2Kt}{\hbar}\right)$$

That is how the Schrodinger picture works!

Heisenberg Picture (operators depend on time)

Let us define an operator $\hat{Q}$ such that for a state vector

$$|\psi\rangle = \psi_R|R\rangle + \psi_L|L\rangle$$

we have

$$\langle\psi|\hat{Q}|\psi\rangle = |\psi_R|^2 = \text{ probability that particle is on right side}$$

This says that

$$\langle\psi|\,\hat{Q}\,|\psi\rangle = |\psi_R|^2 = \langle\psi\mid R\rangle\langle R\mid\psi\rangle$$

or

$$\hat{Q} = |R\rangle\langle R| = \text{ pure state projection operator } = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \hat{I} + \hat{\sigma}_z$$

and that the expectation value of the pure state projection operator is equal to the probability of being in that state.

This agrees with our earlier rules/discussions.

Now we have

$$\hat{H} = K\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = K\hat{\sigma}_x$$

Therefore

$$\hat{Q}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{Q}e^{-\frac{i}{\hbar}\hat{H}t}$$

Now as we saw earlier

$$e^{\frac{i}{\hbar}\hat{H}t} = e^{\frac{i}{\hbar}K\hat{\sigma}_x t} = \cos\frac{Kt}{\hbar}\hat{I} + i\sin\frac{Kt}{\hbar}\hat{\sigma}_x$$

Thus,

$$\begin{aligned}
\hat{Q}(t) &= \left(\cos\frac{Kt}{\hbar}\hat{I} + i\sin\frac{Kt}{\hbar}\hat{\sigma}_x\right)\left(\hat{I} + \hat{\sigma}_z\right)\left(\cos\frac{Kt}{\hbar}\hat{I} - i\sin\frac{Kt}{\hbar}\hat{\sigma}_x\right) \\
&= \cos^2\frac{Kt}{\hbar} + \sin^2\frac{Kt}{\hbar} + \cos^2\frac{Kt}{\hbar}\hat{\sigma}_z - i\sin\frac{Kt}{\hbar}\cos\frac{Kt}{\hbar}\left[\hat{\sigma}_z, \hat{\sigma}_x\right] + \sin^2\frac{Kt}{\hbar}\hat{\sigma}_x\hat{\sigma}_z\hat{\sigma}_x \\
&= 1 + \cos^2\frac{Kt}{\hbar}\hat{\sigma}_z + 2\sin\frac{Kt}{\hbar}\cos\frac{Kt}{\hbar}\hat{\sigma}_y - \sin^2\frac{Kt}{\hbar}\hat{\sigma}_z \\
&= 1 + \cos\frac{2Kt}{\hbar}\hat{\sigma}_z + \sin\frac{2Kt}{\hbar}\hat{\sigma}_y
\end{aligned}$$

Then

$$P_R(t) = \langle\psi(0)|\,\hat{Q}(t)\,|\psi(0)\rangle$$

where

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|R\rangle + \frac{e^{i\delta}}{\sqrt{2}}|L\rangle$$

Now

$$\hat{\sigma}_z|R\rangle = |R\rangle \quad , \quad \hat{\sigma}_z|L\rangle = -|L\rangle$$
$$\hat{\sigma}_y|R\rangle = -i|L\rangle \quad , \quad \hat{\sigma}_y|L\rangle = i|R\rangle$$

and we get

$$P_R = \frac{1}{2}(1 + \sin\delta \sin\frac{2Kt}{\hbar})$$ as before.

That is how the Heisenberg picture works!

Magnetic Resonance

How does an experimentalist observe the spin of a particle?

Classically, a spinning charge distribution will have an associated magnetic moment.

In non-relativistic quantum mechanics particles with internal spin degrees of freedom also have magnetic moments which are connected to their angular momentum.

We write for the magnetic moment operator (in terms of the angular momentum operators)

$$\vec{M}_{op} = \vec{M}_{op}^{orbital} + \vec{M}_{op}^{spin}$$
$$= g_\ell \frac{q}{2mc}\vec{L}_{op} + g_s \frac{q}{2mc}\vec{S}_{op} = \frac{q}{2mc}\left(g_\ell \vec{L}_{op} + g_s \vec{S}_{op}\right)$$

where, as we shall derive later,

$$g_{j\ell s} = 1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}$$

$$g_\ell = g_{jj0} = 1 \text{ and } g_s = g_{j0j} = 2$$

Therefore we have

$$\vec{M}_{op} = \frac{q}{2mc}\left(\vec{L}_{op} + 2\vec{S}_{op}\right) = \frac{q}{2mc}\left(\vec{J}_{op} + \vec{S}_{op}\right)$$

which says that $\vec{M}_{op}$ is not (in general) parallel to $\vec{J}_{op}$.

The energy operator or contribution to the Hamiltonian operator from the magnetic moment in a magnetic field $\vec{B}(\vec{r},t)$ is

$$\hat{H}_M = -\vec{M}_{op} \cdot \vec{B}(\vec{r},t)$$

Spin measurement experiments are designed to detect the effects of this extra contribution to the system energy and thus detect the effects of spin angular momentum.

We will return to a full discussion of the effect of $\hat{H}_M$ on the energy levels of atoms, etc later.

For now we will restrict our attention to spin space and investigate the effect of the spin contribution to $\hat{H}_M$ on the states of a particle.

We will use

$$\hat{H}_{spin} = -\frac{g}{2}\frac{q}{mc}\vec{B} \cdot \bar{S}_{op}$$

where we have replaced g_s by g.

We have not set $g = 2$ since it turns out that it is not exactly that value(due to relativistic effects).

In the Schrodinger picture we have

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}_{spin} |\psi(t)\rangle$$

If we ignore spatial dependences (worry only about spin effects), we have

$$|\psi(t)\rangle = \begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix}$$

$$i\hbar \frac{d}{dt} \begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix} = -\frac{g}{2}\frac{q}{mc} \vec{B} \cdot \bar{S}_{op} \begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix}$$

$$= -\frac{g}{4}\frac{q\hbar}{mc} \vec{B} \cdot \vec{\sigma}_{op} \begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix}$$

$$= -\frac{g}{4}\frac{q\hbar}{mc} \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix} \begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix}$$

This represents two coupled differential equations for the time dependence of the amplitudes $\langle + | \psi \rangle$ and $\langle - | \psi \rangle$. When solved, the solution tells us the time dependence of the measurable probabilities.

We can see the physics of the motion best in the Heisenberg picture, where the operators, instead of the states, move in time.

In this case, we have

$$i\hbar \frac{d\hat{S}_i(t)}{dt} = \left[\hat{S}_i(t), \hat{H}_{spin}(t)\right]$$

$$= -\frac{gq}{2mc} \left[\hat{S}_i(t), \hat{S}_j(t)\right] B_j(t) = -i\frac{gq\hbar}{2mc} \varepsilon_{ijk} \hat{S}_k(t) B_j(t)$$

for each component.

The operators are all time-dependent Heisenberg picture operators.

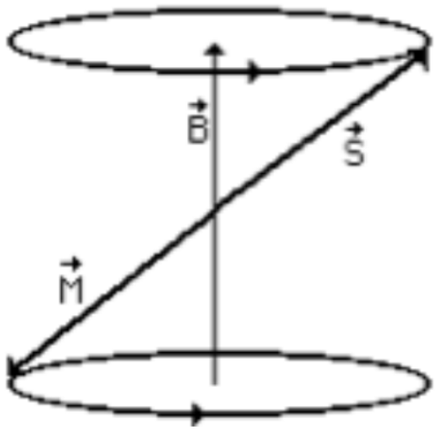
This gives

$$\frac{d\vec{S}_{op}(t)}{dt} = \frac{gq}{2mc}\vec{S}_{op}(t) \times \vec{B}(t) = \vec{M}_{spin}(t) \times \vec{B}(t)$$

The right-hand-side is the *torque* exerted by the magnetic field on the magnetic moment.

In operator language, this equation implies that the rate of change of the spin angular momentum vector equals the applied torque.

This implies that the spin vector with $q < 0$ precesses in a positive sense about the magnetic field direction as shown in the Figure below.



Motion of Spin

Suppose that $\vec{B}(t) = B_0\ \hat{z}$ (independent of t). We then have

$$\frac{d\hat{S}_z(t)}{dt} = 0$$

$$\frac{d\hat{S}_x(t)}{dt} = \frac{gqB_0}{2mc}\hat{S}_y(t)$$

$$\frac{d\hat{S}_y(t)}{dt} = -\frac{gqB_0}{2mc}\hat{S}_x(t)$$

These coupled differential equations have the solutions

$$\hat{S}_x(t) = \hat{S}_x(0)\cos\omega_0 t + \hat{S}_y(0)\sin\omega_0 t$$
$$\hat{S}_y(t) = -\hat{S}_x(0)\sin\omega_0 t + \hat{S}_y(0)\cos\omega_0 t$$
$$\hat{S}_z(t) = \hat{S}_z(0)$$

where

$$\omega_0 = \frac{gqB_0}{2mc}$$

Now suppose that at $t = 0$, the spin is in the $+x$-direction, which says that

$$\left\langle \hat{S}_x(0) \right\rangle = \langle \hat{x}+ | \, \hat{S}_x(0) \, | \hat{x}+ \rangle = \frac{\hbar}{2}$$
$$\left\langle \hat{S}_y(0) \right\rangle = \left\langle \hat{S}_z(0) \right\rangle = 0$$

Therefore, the expectation values of the solutions become

$$\left\langle \hat{S}_x(t) \right\rangle = \frac{\hbar}{2}\cos\omega_0 t$$
$$\left\langle \hat{S}_y(t) \right\rangle = -\frac{\hbar}{2}\sin\omega_0 t$$
$$\left\langle \hat{S}_z(0) \right\rangle = 0$$

which says that the expectation value of the spin vector rotates in a negative sense in the x–y plane (precession about the z-axis).

Now let us return to the Schrodinger picture to see what precession looks like there.

We will do the calculation a couple of different ways - best way to learn.

First we use the time-development operator. For $\vec{B} = B\,\hat{n}$ we have

$$\hat{H} = -\frac{gq\hbar B}{4mc}\vec{\sigma}_{op}\cdot\hat{n}$$

If we define

$$\omega_L = \frac{qB}{mc} = \text{ Larmor frequency}$$

and let $g = 2$ we have

$$\hat{H} = -\frac{1}{2}\hbar\omega_L\vec{\sigma}_{op}\cdot\hat{n}$$

In the Schrodinger picture

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}_{spin}(t)\,|\psi(t)\rangle$$

When $\hat{H}_{\text{spin}}(t)$ is time-independent, we have the solution

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle$$

where

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$$

or

$$|\psi(t)\rangle = e^{i\frac{\omega_L t}{2}\vec{\sigma}_{op}\cdot\hat{n}}\,|\psi(0)\rangle$$

Since $\hat{n}$ = a unit vector, we have $(\vec{\sigma}_{\text{op}}\cdot\hat{n}) = \hat{I}$, which gives, as before,

$$|\psi(t)\rangle = \left(\cos\frac{\omega_L t}{2} + i(\vec{\sigma}_{op}\cdot\hat{n})\sin\frac{\omega_L t}{2}\right)|\psi(0)\rangle$$

This is the solution to the Schrodinger equation in this case.

Now let

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\hat{z}\uparrow\rangle = |\hat{z}+\rangle = |+\rangle$$

From earlier we have

$$\vec{\sigma}_{op}\cdot\hat{n} = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}$$

We then have

$$\begin{aligned} |\psi(t)\rangle &= \cos\frac{\omega_L t}{2}|+\rangle + i\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}|+\rangle \sin\frac{\omega_L t}{2} \\ &= \cos\frac{\omega_L t}{2}|+\rangle + i\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\sin\frac{\omega_L t}{2} \\ &= \cos\frac{\omega_L t}{2}|+\rangle + i\sin\frac{\omega_L t}{2}\begin{pmatrix} n_z \\ n_x + in_y \end{pmatrix} \\ &= \cos\frac{\omega_L t}{2}|+\rangle + i\sin\frac{\omega_L t}{2}\left(n_z|+\rangle + (n_x + in_y)|-\rangle\right) \\ &= \left(\cos\frac{\omega_L t}{2} + in_z\sin\frac{\omega_L t}{2}\right)|+\rangle + i(n_x + in_y)\sin\frac{\omega_L t}{2}|-\rangle \end{aligned}$$

This says that as the initial state $|+\rangle$ develops in time it picks up some amplitude to be in the $|-\rangle$ state.

Special Case

Let

$$\hat{n} = \hat{y} \rightarrow \vec{B} \text{ is in the } y\text{- direction}$$

$$n_y = 1\ ,\ n_x = n_z = 0$$

This gives

$$|\psi(t)\rangle = \cos\frac{\omega_L t}{2}|+\rangle - \sin\frac{\omega_L t}{2}|-\rangle$$

which implies that $\langle \hat{s}_z \rangle$ flips with frequency $\nu = \omega_L/4\pi$ or that the spin vector is precessing around the direction of the magnetic field.

Finally, let us just solve the Schrodinger equation directly so you can see the procedure.

We have

$$i\hbar\frac{d}{dt}\begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix} = -\frac{1}{2}\frac{q\hbar}{mc}\begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}\begin{pmatrix} \langle \hat{n}+ \mid \psi(t)\rangle \\ \langle \hat{n}- \mid \psi(t)\rangle \end{pmatrix}$$

If we choose $\hat{n} = \hat{x}$, then we have

$$i\hbar\frac{d}{dt}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = -\frac{1}{2}\hbar\omega_L\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$$

where $a(t) = \langle \hat{n}+ \mid \psi(t)\rangle$ and $b(t) = \langle \hat{n}- \mid \psi(t)\rangle$

and $|a|^2 + |b|^2 = 1$

This gives two coupled differential equations

$$\dot{a} = i\frac{\omega_L}{2}b \text{ and } \dot{b} = i\frac{\omega_L}{2}a$$

which are solved as follows:

$$(\dot{a} + \dot{b}) = i\frac{\omega_L}{2}(\dot{a} + \dot{b}) \rightarrow a + b = (a(0) + b(0))e^{i\frac{\omega_L}{2}t}$$

$$(\dot{a} - \dot{b}) = -i\frac{\omega_L}{2}(\dot{a} - \dot{b}) \rightarrow a - b = (a(0) - b(0))e^{-i\frac{\omega_L}{2}t}$$

or

$$a(t) = a(0)\cos\frac{\omega_L}{2}t + ib(0)\sin\frac{\omega_L}{2}t$$

$$b(t) = ia(0)\sin\frac{\omega_L}{2}t + b(0)\cos\frac{\omega_L}{2}t$$

For the initial state

$$|\psi(0)\rangle = \begin{pmatrix} a(0) \\ b(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

we get

$$a(t) = \cos\frac{\omega_L}{2}t \quad , \quad b(t) = i\sin\frac{\omega_L}{2}t$$

and

$$a(t) = \cos\frac{\omega_L}{2}t \quad , \quad b(t) = i\sin\frac{\omega_L}{2}t$$

as before.

Spin Resonance

Let us now consider the addition of an **oscillating** magnetic field **perpendicular** to the applied field $\vec{B} = B_0\,\hat{z}$.

In particular, we add the field

$$\vec{B}_1 = B_1\cos\omega t\hat{x}$$

In the Schrodinger picture, we then have the equation of motion

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = -\frac{e\hbar}{2mc}\frac{g}{2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t\hat{\sigma}_x\right)|\psi(t)\rangle$$

new term

Now we first make the transformation (shift to rotating coordinate system since we know that if the extra field were not present the spin would just be precessing about the direction of the applied field)

$$|\psi(t)\rangle = e^{i\frac{\omega t}{2}\hat{\sigma}_z}|\psi'(t)\rangle$$ —> precession now built in!!

which gives

$$i\hbar\frac{d}{dt}\left(e^{i\frac{\omega t}{2}\hat{\sigma}_z}|\psi'(t)\rangle\right) = -\frac{e\hbar}{2mc}\frac{g}{2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t\hat{\sigma}_x\right)e^{i\frac{\omega t}{2}\hat{\sigma}_z}|\psi'(t)\rangle$$

$$i\hbar e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\frac{d}{dt}\left(e^{i\frac{\omega t}{2}\hat{\sigma}_z}|\psi'(t)\rangle\right)$$

$$= -\frac{e\hbar}{2mc}\frac{g}{2}\left(B_0 e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\hat{\sigma}_z e^{i\frac{\omega t}{2}\hat{\sigma}_z} + B_1\cos\omega t e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\hat{\sigma}_x e^{i\frac{\omega t}{2}\hat{\sigma}_z}\right)|\psi'(t)\rangle$$

or

$$i\hbar e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\left(e^{i\frac{\omega t}{2}\hat{\sigma}_z}\frac{d}{dt}|\psi'(t)\rangle + i\frac{\omega}{2}\hat{\sigma}_z e^{i\frac{\omega t}{2}\hat{\sigma}_z}|\psi'(t)\rangle\right)$$

$$= -\frac{e\hbar}{2mc}\frac{g}{2}\left(B_0\hat{\sigma}_z + B_1\cos\omega t e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\hat{\sigma}_x e^{i\frac{\omega t}{2}\hat{\sigma}_z}\right)|\psi'(t)\rangle$$

Now

$$\cos\omega t e^{-i\frac{\omega t}{2}\hat{\sigma}_z}\hat{\sigma}_x e^{i\frac{\omega t}{2}t\hat{\sigma}_z} = \cos\omega t\hat{\sigma}_x e^{i\omega t\hat{\sigma}_z}$$

$$= \hat{\sigma}_x(\cos^2\omega t + i\hat{\sigma}_z\cos\omega t\sin\omega t)$$

$$= \hat{\sigma}_x(\frac{1}{2} + \frac{1}{2}\cos 2\omega t + i\hat{\sigma}_z\frac{1}{2}\sin 2\omega t)$$

$$= \frac{\hat{\sigma}_x}{2} + \frac{1}{2}(\hat{\sigma}_x\cos 2\omega t + i\hat{\sigma}_x\hat{\sigma}_z\sin 2\omega t)$$

$$= \frac{\hat{\sigma}_x}{2} + \frac{1}{2}(\hat{\sigma}_x\cos 2\omega t + \hat{\sigma}_y\sin 2\omega t)$$

Defining

$$\omega_0 = \frac{geB_0}{4mc} \text{ and } \omega_1 = \frac{geB_1}{4mc}$$

we get

$$i\hbar \frac{d}{dt} |\psi'(t)\rangle$$

$$= \left(\left(\frac{\omega - \omega_0}{2} \right) \hat{\sigma}_z - \frac{\omega_1}{2} \hat{\sigma}_x \right) |\psi'(t)\rangle$$

$$+ \frac{\omega_1}{2} \left(\hat{\sigma}_x \cos 2\omega t + \hat{\sigma}_y \sin 2\omega t \right) |\psi'(t)\rangle$$

The two higher frequency terms produce high frequency wiggles in $|\psi'(t)\rangle$.

Since we will be looking at the average motion of the spin vector (expectation values changing in time), these terms will average to zero and we can neglect them in this discussion.

We thus have

$$i\hbar \frac{d}{dt} |\psi'(t)\rangle = \left(\left(\frac{\omega - \omega_0}{2} \right) \hat{\sigma}_z - \frac{\omega_1}{2} \hat{\sigma}_x \right) |\psi'(t)\rangle$$

which has a solution

$$|\psi'(t)\rangle = e^{-i\frac{\Omega t}{2}\hat{\sigma}} |\psi'(0)\rangle$$

$$\Omega = \left[(\omega - \omega_0)^2 + \omega_1^2 \right]^{1/2} \text{ and } \hat{\sigma} = \frac{\omega - \omega_0}{\Omega} \hat{\sigma}_z - \frac{\omega_1}{\Omega} \hat{\sigma}_x$$

We note that

$$\hat{\sigma}^2 = \frac{(\omega - \omega_0)^2 + \omega_1^2}{\Omega^2} \hat{I} = \hat{I}$$

The final solution to the original problem (again neglecting the higher frequency terms) is then (after leaving the rotating system)

$$|\psi(t)\rangle = e^{-i\frac{\omega t}{2}\hat{\sigma}_z} e^{-i\frac{\Omega t}{2}\hat{\sigma}} |\psi(0)\rangle$$

Example

Let us choose

$$|\psi(0)\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We get

$$|\psi(t)\rangle = e^{-i\frac{\omega t}{2}\hat{\sigma}_z} e^{-i\frac{\Omega t}{2}\hat{\sigma}} |+\rangle = e^{-i\frac{\omega t}{2}\hat{\sigma}_z} \left(\cos\frac{\Omega t}{2} - i\hat{\sigma}\sin\frac{\Omega t}{2}\right)|+\rangle$$

$$= e^{-i\frac{\omega t}{2}\hat{\sigma}_z} \left(\cos\frac{\Omega t}{2}|+\rangle - i\frac{\omega-\omega_0}{\Omega}\sin\frac{\Omega t}{2}\hat{\sigma}_z|+\rangle + i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}\hat{\sigma}_x|+\rangle\right)$$

Now using

$$\hat{\sigma}_z|+\rangle = |+\rangle \text{ and } \hat{\sigma}_x|+\rangle = |-\rangle$$

$$e^{-i\frac{\omega t}{2}\hat{\sigma}_z} = \cos\frac{\omega t}{2} - i\sin\frac{\omega t}{2}\hat{\sigma}_z$$

we have

$$|\psi(t)\rangle = A^{(+)}|+\rangle + A^{(-)}|-\rangle$$

$$A^{(+)} = \cos\frac{\omega t}{2}\cos\frac{\Omega t}{2} - i\sin\frac{\omega t}{2}\cos\frac{\Omega t}{2}$$

$$- i\frac{\omega-\omega_0}{\Omega}\cos\frac{\omega t}{2}\sin\frac{\Omega t}{2} - \frac{\omega-\omega_0}{\Omega}\sin\frac{\omega t}{2}\sin\frac{\Omega t}{2}$$

$$A^{(-)} = -i\frac{\omega_1}{\Omega}\cos\frac{\omega t}{2}\sin\frac{\Omega t}{2} + \frac{\omega_1}{\Omega}\sin\frac{\omega t}{2}\sin\frac{\Omega t}{2}$$

Therefore, the amplitude for spin flip to the state $|\hat{z}\downarrow\rangle = |-\rangle$ at time t is

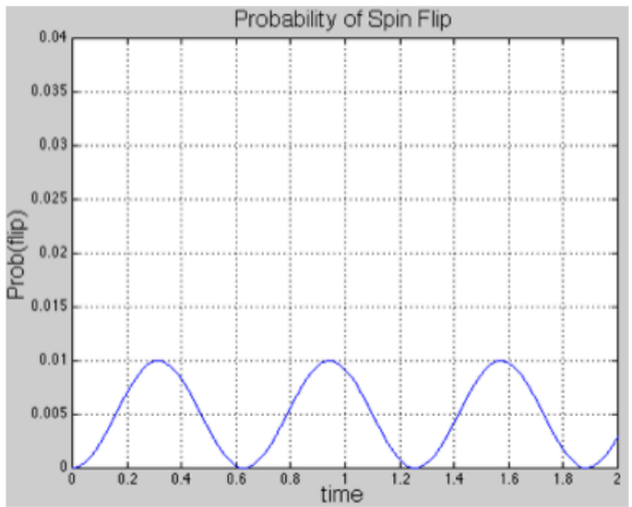
$$\langle - \,|\, \psi(t)\rangle = A^{(-)} = -i\frac{\omega_1}{\Omega}\cos\frac{\omega t}{2}\sin\frac{\Omega t}{2} + \frac{\omega_1}{\Omega}\sin\frac{\omega t}{2}\sin\frac{\Omega t}{2}$$

$$= -i\frac{\omega_1}{\Omega}\sin\frac{\Omega t}{2}e^{i\frac{\omega t}{2}}$$

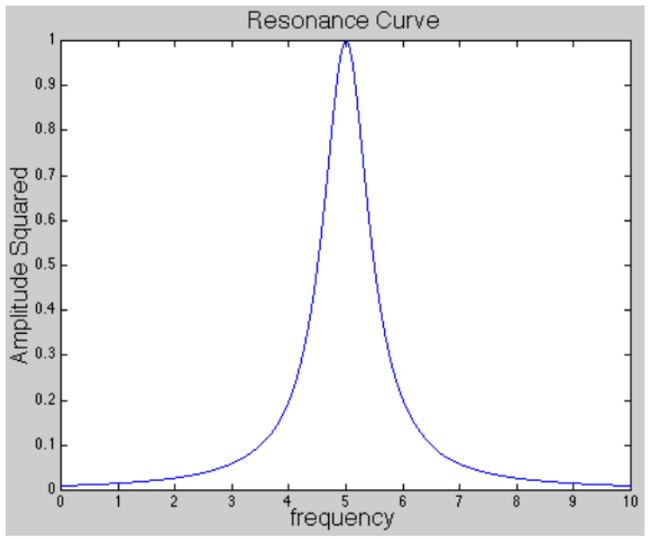
and the probability of spin flip is $$P_{flip}(t) = |\langle - \,|\, \psi(t)\rangle|^2 = \frac{\omega_1^2}{\Omega^2}\sin^2\frac{\Omega t}{2} = \frac{\omega_1^2}{2\Omega^2}(1-\cos\Omega t)$$

What is happening to the spin vector?

If we plot $P_{\text{flip}}(t)$ versus t as in the Figure below left we get



Spin=Flip Probability versus Time



Resonance Curve

where the peak values are given by ω_1^2/Ω^2.

What is the value of ω_1^2/Ω^2 and can it be large? This spin resonance process is used to determine a wide variety of spin properties of systems.

If we plot ω_1^2/Ω^2 versus ω (the frequency of the added field) we get as in Figure above right the result The peak occurs at $\omega - \omega_0 \approx 0$ (called a ***resonance***).

Therefore, if $\omega - \omega_0 \gg \omega_1$ (called **off-resonance**), the maximum probability for spin flip is small(that corresponds to the Figure left).

However, if $\omega - \omega_0 \approx 0$, which corresponds to resonance, the maximum probability ≈ 1 and the spin has flipped with certainty.

The spin system preferentially absorbs energy (flipping spin) near resonance.

Addition of Angular Momentum (the fundamental rule)

A derivation of the addition process for arbitrary angular momentum values is very complex.

We can, however, learn and understand all of the required steps within the context of a special case, namely, combining two spin = 1/2 systems into a new system.

We will present the general derivation after the special case.

Addition of Two Spin = 1/2 Angular Momenta

We define

$$\vec{S}_{1,op} = \text{ spin operator for system 1}$$
$$\vec{S}_{2,op} = \text{ spin operator for system 2}$$

The operators for system 1 are assumed to be independent of the operators for system 2, which implies that

$$\left[\hat{S}_{1i}, \hat{S}_{2j}\right] = 0 \text{ for all } i \text{ and } j$$

We characterize each system by eigenvalue/eigenvector equations

$$\vec{S}^2_{1,op}\left|s_1, m_1\right\rangle = \hbar^2 s_1(s_1+1)\left|s_1, m_1\right\rangle$$
$$\hat{S}_{1,z}\left|s_1, m_1\right\rangle = \hbar m_1 \left|s_1, m_1\right\rangle$$
$$\vec{S}^2_{2,op}\left|s_2, m_2\right\rangle = \hbar^2 s_2(s_2+1)\left|s_2, m_2\right\rangle$$
$$\hat{S}_{2,z}\left|s_2, m_2\right\rangle = \hbar m_2 \left|s_2, m_2\right\rangle$$

where

$$s_1 = s_2 = \frac{1}{2} \text{ and } m_1 = \pm\frac{1}{2}\,,\; m_2 = \pm\frac{1}{2}$$

Since both s_1 and s_2 are fixed and unchanging during this addition process we will drop them from the arguments and subscripts to lessen the complexity of the equations.

Each space (1 and 2) is 2-dimensional and thus each has two ($2s + 1 = 2$) basis states corresponding to the number of m-values in each case

$$\left|s_1 = \frac{1}{2}, m_1 = \frac{1}{2}\right\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle_1 = |\uparrow\rangle_1 = |+\rangle_1$$
$$\left|s_1 = \frac{1}{2}, m_1 = -\frac{1}{2}\right\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_1 = |\downarrow\rangle_1 = |-\rangle_1$$
$$\left|s_2 = \frac{1}{2}, m_2 = \frac{1}{2}\right\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle_2 = |\uparrow\rangle_2 = |+\rangle_2$$
$$\left|s_2 = \frac{1}{2}, m_2 = -\frac{1}{2}\right\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle_2 = |\downarrow\rangle_2 = |-\rangle_2$$

This means that there are 4 possible basis states for the combined system that we can construct using the direct product procedure.

We label them as

$$|\uparrow\uparrow\rangle = |++\rangle = |+\rangle_1 \otimes |+\rangle_2 \quad , \quad |\uparrow\downarrow\rangle = |+-\rangle = |+\rangle_1 \otimes |-\rangle_2$$
$$|\downarrow\uparrow\rangle = |-+\rangle = |-\rangle_1 \otimes |+\rangle_2 \quad , \quad |\downarrow\downarrow\rangle = |--\rangle = |-\rangle_1 \otimes |-\rangle_2$$

so that the first symbol in the combined states corresponds to system 1 and the second symbol to system 2.

These are not the only possible basis states as we shall see (they are the simplest to find).

The "1" operators operate only on the "1" part of the direct product, for example,

$$\vec{S}_{1,op}^2 |+-\rangle = \hbar^2 s_1(s_1+1) |+-\rangle = \frac{3}{4}\hbar^2 |+-\rangle$$

$$\hat{S}_{1,z} |+-\rangle = \hbar m_1 |+-\rangle = \frac{\hbar}{2} |+-\rangle$$

$$\vec{S}_{2,op}^2 |+-\rangle = \hbar^2 s_2(s_2+1) |+-\rangle = \frac{3}{4}\hbar^2 |+-\rangle$$

$$\hat{S}_{2,z} |+-\rangle = \hbar m_2 |+-\rangle = -\frac{\hbar}{2} |+-\rangle$$

The total spin angular momentum operator for the combined system is

$$\vec{S}_{op} = \vec{S}_{1,op} + \vec{S}_{2,op}$$

It obeys the same commutation rules as the individual system operators, i.e.,

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\varepsilon_{ijk}\hat{S}_k$$

This tells us to look for the same kind of angular momentum eigenstates and eigenvalues

$$\vec{S}_{op}^2 |s,m\rangle = \hbar^2 s(s+1) |s,m\rangle$$

$$\hat{S}_z |s,m\rangle = \hbar m |s,m\rangle$$

To proceed, we need to derive some relations.

Squaring the total spin operator we have

$$\vec{S}_{op}^2 = \left(\vec{S}_{1,op} + \vec{S}_{2,op}\right)^2 = \vec{S}_{1,op}^2 + \vec{S}_{2,op}^2 + 2\vec{S}_{1,op} \cdot \vec{S}_{2,op}$$

$$= \frac{3}{4}\hbar^2 \hat{I} + \frac{3}{4}\hbar^2 \hat{I} + 2\hat{S}_{1z}\hat{S}_{2z} + 2\hat{S}_{1x}\hat{S}_{2x} + 2\hat{S}_{1y}\hat{S}_{2y}$$

Now using

$$\hat{S}_{1\pm} = \hat{S}_{1x} \pm i\hat{S}_{1y} \text{ and } \hat{S}_{2\pm} = \hat{S}_{2x} \pm i\hat{S}_{2y}$$

we have

$$2\hat{S}_{1x}\hat{S}_{2x} + 2\hat{S}_{1y}\hat{S}_{2y} = \hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+}$$

and therefore

$$\vec{S}_{op}^{2} = \frac{3}{2}\hbar^2\hat{I} + 2\hat{S}_{1z}\hat{S}_{2z} + \hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+}$$

Now suppose we choose the four states $|{+}{+}\rangle$, $|{+}{-}\rangle$, $|{-}{+}\rangle$, $|{-}{-}\rangle$ as the orthonormal basis for the 4-dimensional vector space of the combined system.

We then ask the following question.

Are these basis states also eigenstates of the spin operators for the combined system?

We have

$$\begin{aligned}\hat{S}_z|{+}{+}\rangle &= (\hat{S}_{1z} + \hat{S}_{2z})|{+}\rangle_1 \otimes |{+}\rangle_2 = (\hat{S}_{1z}|{+}\rangle_1) \otimes |{+}\rangle_2 + |{+}\rangle_1 \otimes (\hat{S}_{2z}|{+}\rangle_2) \\ &= (\frac{\hbar}{2}|{+}\rangle_1) \otimes |{+}\rangle_2 + |{+}\rangle_1 \otimes (\frac{\hbar}{2}|{+}\rangle_2) = (\frac{\hbar}{2} + \frac{\hbar}{2})|{+}\rangle_1 \otimes |{+}\rangle_2 \\ &= \hbar|{+}{+}\rangle\end{aligned}$$

and similarly

$$\hat{S}_z|{+}{-}\rangle = 0$$

$$\hat{S}_z|{-}{+}\rangle = 0$$

$$\hat{S}_z|{-}{-}\rangle = -\hbar|{-}{-}\rangle$$

This says that the direct-product basis states are eigenvectors of (total) $\hat{S}_z$ and that the eigenvalues are $m = 1, 0, -1$ and 0 (a second time).

Since each value s of the total angular momentum of the combined system must have $2s + 1$ associated m-values, these results tell us that the combined system will have

$$s = 1 \rightarrow m = 1, 0, -1 \text{ and } s = 0 \rightarrow m = 0$$

which accounts for all of the four states.

What about the $\vec{S}^2_{op}$ operator?

We have

$$\vec{S}^2_{op} |{+}{+}\rangle = \left(\frac{3}{2}\hbar^2 \hat{I} + 2\hat{S}_{1z}\hat{S}_{2z} + \hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+} \right) |{+}{+}\rangle$$

$$= \left(\frac{3}{2}\hbar^2 + 2\frac{\hbar}{2}\frac{\hbar}{2} + \hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+} \right) |{+}{+}\rangle$$

Now using

$$\hat{S}_{1+} |{+}{+}\rangle = 0 = \hat{S}_{+} |{+}{+}\rangle$$

we get

$$\vec{S}^2_{op} |{+}{+}\rangle = 2\hbar^2 |{+}{+}\rangle = \hbar^2 1(1+1) |{+}{+}\rangle$$

or the state $|{+}{+}\rangle$ is also an eigenstate of $\vec{S}^2_{op}$ with $s = 1$

$$|{+}{+}\rangle = |s = 1, m = 1\rangle = |1, 1\rangle$$

Similarly, we have

$$|{-}{-}\rangle = |s = 1, m = -1\rangle = |1, -1\rangle$$

or the state $|{-}{-}\rangle$ is also an eigenstate of $\vec{S}^2_{op}$ with $s = 1$

In the same manner we can show that $|{+}{-}\rangle$ and $|{-}{+}\rangle$ are not eigenstates of $\vec{S}^2_{op}$.

So the simple direct-product states are *not* appropriate to describe the combined system if we want to characterize it using

$$\vec{S}_{op}^2 \text{ and } \hat{S}_z$$

However, since the direct-product states are a complete basis set, we should be able to construct the remaining two eigenstates of $\vec{S}_{op}^2$ and $\hat{S}_z$ as linear combinations of the direct-product states

$$|s,m\rangle = \sum_{m_1,m_2} a_{smm_1m_2} |m_1,m_2\rangle$$

where we have left out the s_1 and s_2 dependence in the states and coefficients.

In a formal manner, we can identify the so-called ***Clebsch-Gordon coefficients*** $a_{smm_1m_2}$ by using the orthonormality of the direct-product basis states.

We have

$$\langle m_1', m_2' \mid s,m\rangle = \sum_{m_1,m_2} a_{smm_1m_2} \langle m_1', m_2' \mid m_1,m_2\rangle$$

$$= \sum_{m_1,m_2} a_{smm_1m_2} \delta_{m_1'm_1} \delta_{m_2'm_2} = a_{smm_1'm_2'}$$

where we have used

$$\langle m_1', m_2' \mid m_1,m_2\rangle = \delta_{m_1'm_1} \delta_{m_2'm_2}$$

This does not help us actually compute the coefficients because we do not know the states $|s,m\rangle$.

A procedure that works in this case and that can be generalized, is the following.

We already found that $|{+}{+}\rangle = |1,1\rangle$ and $|{-}{-}\rangle = |1,-1\rangle$.

Now we define the operators

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y = (\hat{S}_{1x} + \hat{S}_{2x}) \pm i(\hat{S}_{1y} + \hat{S}_{2y}) = \hat{S}_{1\pm} + \hat{S}_{2\pm}$$

These are the raising and lowering operators for the combined system and thus they satisfy the relations

$$\hat{S}_{\pm}|s,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}\,|s,m\pm 1\rangle$$

This gives

$$\hat{S}_{+}|1,1\rangle = 0 = \hat{S}_{-}|1,-1\rangle$$

as we expect.

If, however, we apply $\hat{S}_{-}$ to the topmost state (maximum s and m values) we get

$$\begin{aligned}\hat{S}_{-}|1,1\rangle &= \hbar\sqrt{1(1+1)-1(1-1)}\,|1,0\rangle = \hbar\sqrt{2}\,|1,0\rangle \\ &= (\hat{S}_{1-}+\hat{S}_{2-})|+\rangle_1\otimes|+\rangle_2 = (\hat{S}_{1-}|+\rangle_1)\otimes|+\rangle_2 + |+\rangle_1\otimes(\hat{S}_{2-}|+\rangle_2) \\ &= \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(\frac{1}{2}-1)}\,|-\rangle_1\otimes|+\rangle_2 \\ &\quad + \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)-\frac{1}{2}(\frac{1}{2}-1)}\,|+\rangle_1\otimes|-\rangle_2 \\ &= \hbar\,|-+\rangle + \hbar\,|+-\rangle\end{aligned}$$

or

$$|1,0\rangle = |s=1,m=0\rangle = \frac{1}{\sqrt{2}}|-+\rangle + \frac{1}{\sqrt{2}}|+-\rangle$$

Note that the only terms that appear on the right hand side are those that have $m = m_1 + m_2$.

We can easily see that this is a general property since

$$\begin{aligned}\hat{S}_z|s,m\rangle = m\hbar\,|s,m\rangle &= \sum_{m_1,m_2} a_{smm_1m_2}(\hat{S}_{1z}+\hat{S}_{2z})|m_1,m_2\rangle \\ &= \hbar\sum_{m_1,m_2} a_{smm_1m_2}(m_1+m_2)|m_1,m_2\rangle\end{aligned}$$

The only way to satisfy this equation is for $m = m_1 + m_2$ in every term in the sum.

Thus, our linear combination should really be written as a single sum of the form

$$|s,m\rangle = \sum_{\substack{m_1,m_2 \\ m_1+m_2=m}} a_{smm_1m_2} |m_1,m_2\rangle = \sum_{m_1} a_{smm_1,m-m_1} |m_1,m-m_1\rangle$$

These three states

$$|1,1\rangle = |{+}{+}\rangle \rightarrow a_{1,1,\frac{1}{2},\frac{1}{2}} = 1$$

$$|1,0\rangle = \frac{1}{\sqrt{2}}(|{-}{+}\rangle + |{+}{-}\rangle) \rightarrow a_{1,1,-\frac{1}{2},\frac{1}{2}} = a_{1,1,\frac{1}{2},-\frac{1}{2}} = \frac{1}{\sqrt{2}}$$

$$|1,-1\rangle = |{-}{-}\rangle \rightarrow a_{1,1,-\frac{1}{2},-\frac{1}{2}} = 1$$

are called a *triplet*.

The state $|s=0,m=0\rangle = |0,0\rangle$ can then be found as follows: the state has $m=0$, $\hat{S}_z |0,0\rangle = 0$ and thus each state(term) in the linear combination must have $m = m_1 + m_2 = 0$, which means we must be able to write

$$|0,0\rangle = a|{+}{-}\rangle + b|{-}{+}\rangle$$

where

$$|a|^2 + |b|^2 = 1 \text{ (state is normalized to 1)}$$

Now we must also have

$$\langle 1,0 \mid 0,0\rangle = 0 \text{ (since the } |s,m\rangle \text{ states are orthogonal)}$$

which implies that

$$\frac{1}{\sqrt{2}}a + \frac{1}{\sqrt{2}}b = 0 \rightarrow b = -a$$

We then have

$$2|a|^2 = 1 \rightarrow a = \frac{1}{\sqrt{2}} = -b$$

and

$$|0,0\rangle = |s=0, m=0\rangle = \frac{1}{\sqrt{2}}|+-\rangle - \frac{1}{\sqrt{2}}|-+\rangle$$

This is called a *singlet state*.

That completes the construction of the angular momentum states for the combined system of two spin-1/2 systems.

We now *generalize* this procedure for the addition of any two angular momenta.

General Addition of Two Angular Momenta

Given two angular momenta $\vec{J}_{1,op}$ and $\vec{J}_{2,op}$, we have the operators and states for each separate system

$$\vec{J}_{1,op} \rightarrow \vec{J}^2_{1,op}, \hat{J}_{1z}, \hat{J}_{1\pm} \rightarrow |j_1, m_1\rangle$$
$$\vec{J}_{2,op} \rightarrow \vec{J}^2_{2,op}, \hat{J}_{2z}, \hat{J}_{2\pm} \rightarrow |j_2, m_2\rangle$$

with

$$\vec{J}^2_{1,op}|j_1,m_1\rangle = \hbar^2 j_1(j_1+1)|j_1,m_1\rangle, \hat{J}_{1z}|j_1,m_1\rangle = \hbar m_1|j_1,m_1\rangle$$
$$\hat{J}_{1\pm}|j_1,m_1\rangle = \hbar\sqrt{j_1(j_1+1) - m_1(m_1\pm 1)}\,|j_1 \pm 1, m_1\rangle$$
$$\vec{J}^2_{2,op}|j_2,m_2\rangle = \hbar^2 j_2(j_2+1)|j_2,m_2\rangle, \hat{J}_{2z}|j_2,m_2\rangle = \hbar m_2|j_2,m_2\rangle$$
$$\hat{J}_{2\pm}|j_2,m_2\rangle = \hbar\sqrt{j_2(j_2+1) - m_2(m_2\pm 1)}\,|j_2 \pm 1, m_2\rangle$$

Remember that there are $2j_1 + 1$ possible m_1 values and $2j_2 + 1$ possible m_2 values.

Since all of the "1" operators commute with all of the "2" operators, we can find a common eigenbasis for the four operators $\vec{J}_{1,op}^2, \hat{J}_{1z}, \vec{J}_{2,op}^2, \hat{J}_{2z}$ in terms of the direct-product states

$$|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

For the combined system we define total operators as before

$$\vec{J}_{op} = \vec{J}_{1,op} + \vec{J}_{2,op} = \text{ total angular momentum}$$
$$\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}, \left[\vec{J}_{op}^2, \hat{J}_z\right] = 0$$
$$\left[\vec{J}_{op}^2, \hat{J}_{1,op}^2\right] = 0 \quad , \quad \left[\vec{J}_{op}^2, \hat{J}_{2,op}^2\right] = 0$$
$$\left[\hat{J}_{1,op}^2, \hat{J}_z\right] = 0 \quad , \quad \left[\hat{J}_{2,op}^2, \hat{J}_z\right] = 0$$

These commutators imply that we can construct a common eigenbasis of $\vec{J}_{1,op}^2, \hat{J}_{1z}, \vec{J}_{2,op}^2, \hat{J}_{2z}$ using the states $|j_1, j_2, m_1, m_2\rangle$ where

$$\vec{J}_{op}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle \text{ and } \hat{J}_z |j, m\rangle = \hbar m |j, m\rangle$$

There are $2j + 1$ possible m values for each allowed j value.

We cannot use the operators $\hat{J}_{1z}, \hat{J}_{2z}$ to construct the eigenbasis for the combined system because they do not commute with $\vec{J}_{op}^2$.

Remember that in order for a label to appear in a ket vector it must be one of the eigenvalues of a set of commuting observables since only such a set shares a common eigenbasis.

We now determine how to write the $|j_1, j_2, m_1, m_2\rangle$ in terms of the $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ basis.

We have

$$|j_1, j_2, j, m\rangle$$
$$= \sum_{j_1'} \sum_{j_2'} \sum_{m_1} \sum_{m_2} |j_1', j_2', m_1, m_2\rangle \langle j_1', j_2', m_1, m_2 \mid j_1, j_2, j, m\rangle$$

where

$$\langle j_1', j_2', m_1, m_2 \mid j_1, j_2, j, m\rangle = \text{ Clebsch - Gordon coefficients}$$

This corresponds to inserting an identity operator of the form

$$\hat{I} = \sum_{j_1'} \sum_{j_2'} \sum_{m_1} \sum_{m_2} |j_1', j_2', m_1, m_2\rangle \langle j_1', j_2', m_1, m_2|$$

Since

$$\langle j_1', j_2', m_1, m_2| \vec{J}_{1,op}^{\,2} |j_1, j_2, j, m\rangle$$
$$= \hbar^2 j_1'(j_1' + 1) \langle j_1', j_2', m_1, m_2 \mid j_1, j_2, j, m\rangle$$
$$= \hbar^2 j_1(j_1 + 1) \langle j_1', j_2', m_1, m_2 \mid j_1, j_2, j, m\rangle$$

the Clebsch-Gordon(CG) coefficients must vanish unless $j'_1 = j_1$ and similarly unless $j'_2 = j_2$.

Thus we have

$$|j_1, j_2, j, m\rangle = \sum_{m_1} \sum_{m_2} |j_1, j_2, m_1, m_2\rangle \langle j_1, j_2, m_1, m_2 \mid j_1, j_2, j, m\rangle$$

Also, as we saw earlier, since $\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$ we must have

$$\langle j_1, j_2, m_1, m_2| \hat{J}_z |j_1, j_2, j, m\rangle = \hbar(m_1 + m_2) \langle j_1, j_2, m_1, m_2 \mid j_1, j_2, j, m\rangle$$
$$= \hbar m \langle j_1, j_2, m_1, m_2 \mid j_1, j_2, j, m\rangle$$

which implies that the CG coefficients must vanish unless $m_1 + m_2 = m$.

Thus the only non-vanishing coefficients are

$$\langle j_1, j_2, m_1, m_2 \mid j_1, j_2, j, m = m_1 + m_2 \rangle$$

and we can write

$$|j_1, j_2, j, m\rangle = \sum_{m_1} \sum_{m_2 = m - m_1} |j_1, j_2, m_1, m_2\rangle \langle j_1, j_2, m_1, m_2 \mid j_1, j_2, j, m\rangle$$

$$= \sum_{m_1} |j_1, j_2, m_1, m_2 = m - m_1\rangle \langle j_1, j_2, m_1, m_2 = m - m_1 \mid j_1, j_2, j, m\rangle$$

For fixed j_1 and j_2 there are $2j_1 + 1$ possible m_1 values and $2j_2 + 1$ possible m_2 values.

Thus, there are $(2j_1 + 1)(2j_2 + 1)$ linearly independent states of the form

$$|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

and hence the vector space describing the combined system is $(2j_1 + 1)(2j_2 + 1)$ - dimensional.

This says that there must be $(2j_1 + 1)(2j_2 + 1)$ states of the form $|j_1, j_2, j, m\rangle$ also.

We notice that there is only one state with $m = m_1 + m_2 = j_1 + j_2$, namely,

$$m_1 = j_1 \text{ and } m_2 = j_2$$

This state has the *maximum possible m value*.

There are two states with $m = m_1 + m_2 = j_1 + j_2 - 1$, namely,

$$m_1 = j_1 - 1, m_2 = j_2 \text{ and } m_1 = j_1, m_2 = j_2 - 1$$

and so on.

For **example**

$$j_1 = 2\ ,\ j_2 = 1 \rightarrow (2(2)+1))(2(1)+1)) = 15 \text{ states}$$

If we label these states by the m-values only (since j_1 and j_2 do not change) or $|m_1,m_2\rangle$, then we have (in this example)

$$m = 3 \rightarrow 1 \text{ state} \rightarrow |2,1\rangle$$
$$m = 2 \rightarrow 2 \text{ states} \rightarrow |2,0\rangle\ ,\ |1,1\rangle$$
$$m = 1 \rightarrow 3 \text{ states} \rightarrow |1,0\rangle\ ,\ |0,1\rangle\ ,\ |2,-1\rangle$$
$$m = 0 \rightarrow 3 \text{ states} \rightarrow |0,0\rangle\ ,\ |1,-1\rangle\ ,\ |-1,1\rangle$$
$$m = -1 \rightarrow 3 \text{ states} \rightarrow |-1,0\rangle\ ,\ |0,-1\rangle\ ,\ |-2,1\rangle$$
$$m = -2 \rightarrow 2 \text{ states} \rightarrow |-2,0\rangle\ ,\ |-1,-1\rangle$$
$$m = -3 \rightarrow 1 \text{ state} \rightarrow |-2,-1\rangle$$

for a total of 15 states.

The combined system, as we shall see by construction, has these states

$$j = 3 \rightarrow m = 3,2,1,0,-1,-2,-3 \rightarrow 7 \text{ states}$$
$$j = 2 \rightarrow m = 2,1,0,-1,-2 \rightarrow 5 \text{ states}$$
$$j = 1 \rightarrow m = 1,0,-1 \rightarrow 3 \text{ states}$$

for a total of 15 states.

The general rules, which follows from group theory, are

1. The combined system has allowed j values given by

$$j_1 + j_2 \geq j \geq |j_1 - j_2| \text{ in integer steps}$$

2. The total number of states is given by the total number of m-values for all the allowed j-values or

$$\sum_{j=|j_1-j_2|}^{j_1+j_2}(2j+1) = (2j_1+1)(2j_2+1)$$

We write the addition of two angular momenta symbolically as

$$j_1 \otimes j_2 = |j_1 - j_2| \oplus |j_1 - j_2| + 1 \oplus |j_1 - j_2| + 2 \oplus \ldots\ldots \oplus j_1 + j_2 - 1 \oplus j_1 + j_2$$

Examples are required because it is so complicated!!!!

Our original special case of adding two spin = 1/2 systems gives

$$j_1 = j_2 = \frac{1}{2} \rightarrow j = 0, 1 \rightarrow \frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1 \rightarrow 4 \text{ states}$$

which is the result we found earlier.

Other cases are:

$$j_1 = j_2 = 1 \rightarrow j = 0, 1, 2 \rightarrow 1 \otimes 1 = 0 \oplus 1 \oplus 2 \rightarrow 9 \text{ states}$$

$$j_1 = 2, j_2 = 1 \rightarrow j = 1, 2, 3 \rightarrow 2 \otimes 1 = 1 \oplus 2 \oplus 3 \rightarrow 15 \text{ states}$$

$$j_1 = 2, j_2 = 3 \rightarrow j = 1, 2, 3, 4, 5 \rightarrow 2 \otimes 3 = 1 \oplus 2 \oplus 3 \oplus 4 \oplus 5 \rightarrow 35 \text{ states}$$

Actual Construction of States

Notation

1. states labeled $|7, 6\rangle$ are $|j, m\rangle$ states
2. states labeled $|3, 2\rangle_{\otimes}$ are $|m_1, m_2\rangle$ states
3. we suppress the j_1, j_2 labels everywhere

Procedure

1. choose j_1 and j_2
2. write down the direct-product $|m_1, m_2\rangle$ basis
3. determine the allowed j values
4. write down the maximum m state ($m = j_1 + j_2$); it is unique
5. the maximum m-value corresponds to the maximum j-value
6. use the lowering operator to generate all other m-states for this J-value; there are $2j + 1$, i.e.,

$$\hat{J}_- |j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\,|j, m-1\rangle$$

7. find the maximum m-state for the next lowest j-value; it is constructed from the same basis states as in the corresponding m-states for higher j-values; use orthonormality properties to figure out coefficients
8. repeat (6) and (7) until all j-values have been dealt with

Now for More Detailed Examples (we must learn this process by actually doing it)

#1 - Individual system values

$$j_1 = j_2 = \frac{1}{2} \rightarrow m_1, m_2 = \frac{1}{2}, -\frac{1}{2} \text{ (we already did this example)}$$

The basis states are (we use the notation $|+-\rangle$ here instead of $|1/2,-1/2\rangle_{\otimes}$)

$$\begin{array}{lcccccccc} & |++\rangle & , & |+-\rangle & , & |-+\rangle & , & |--\rangle \\ m = m_1 + m_2 = & 1 & & 0 & & -1 & & 0 \end{array}$$

Construction Algebra

Allowed j-values are $j = 1, 0$

$j = 1$ has $2j + 1 = 3$ m-values $= 1, 0, -1$

$j = 0$ has $2j + 1 = 1$ m value $= 0$

$|1,1\rangle = |{+}{+}\rangle$ maximum or topmost (j, m) state is always unique

$$\hat{J}_- |1,1\rangle = \sqrt{2}\hbar\,|1,0\rangle = (\hat{J}_{1-} + \hat{J}_{2-})\,|{+}{+}\rangle = \hbar\,|{+}{-}\rangle + \hbar\,|{-}{+}\rangle$$

$$|1,0\rangle = \tfrac{1}{\sqrt{2}}\,|{+}{-}\rangle + \tfrac{1}{\sqrt{2}}\,|{-}{+}\rangle$$

$$\hat{J}_- |1,0\rangle = \sqrt{2}\hbar\,|1,-1\rangle = (\hat{J}_{1-} + \hat{J}_{2-})\left(\tfrac{1}{\sqrt{2}}\,|{+}{-}\rangle + \tfrac{1}{\sqrt{2}}\,|{-}{+}\rangle\right) = \sqrt{2}\hbar\,|{-}{-}\rangle$$

$|1,-1\rangle = |{-}{-}\rangle$

We must now have $|0,0\rangle = a\,|{+}{-}\rangle + b\,|{-}{+}\rangle$ (Rule 7) with

$$|a|^2 + |b|^2 = 1 \text{ and } \langle 1,0\,|\,,0,0\rangle = \tfrac{1}{\sqrt{2}}a + \tfrac{1}{\sqrt{2}}b = 0$$

which gives

$$a = -b = \tfrac{1}{\sqrt{2}}$$

or

$$|0,0\rangle = \tfrac{1}{\sqrt{2}}\,|{+}{-}\rangle - \tfrac{1}{\sqrt{2}}\,|{-}{+}\rangle$$

All the $j-$values are now done.

We end up with the Clebsch-Gordon coefficients.

#2 - Individual system values

$$j_1 = j_2 = 1 \rightarrow m_1, m_2 = 1, 0, -1$$

The basis states are

$$\begin{array}{lccccc} & |1,1\rangle_\otimes & |1,0\rangle_\otimes & |1,-1\rangle_\otimes & |0,1\rangle_\otimes & |0,0\rangle_\otimes \\ m = m_1 + m_2 = & 2 & 1 & 0 & 1 & 0 \end{array}$$

$$\begin{array}{lcccc} & |0,-1\rangle_\otimes & |-1,1\rangle_\otimes & |-1,0\rangle_\otimes & |-1,-1\rangle_\otimes \\ m = m_1 + m_2 = & -1 & 0 & -1 & -2 \end{array}$$

Construction Algebra

Allowed j-values are $j = 2, 1, 0$

$j = 2$ has $2j + 1 = 3$ m-values $= 2, 1, 0, -1, -2$

$j = 1$ has $2j + 1 = 3$ m-values $= 1, 0, -1$

$j = 0$ has $2j + 1 = 1$ m value $= 0$

$|2,2\rangle = |1,1\rangle_\otimes$ maximum or topmost (j, m) state is always unique

$$\hat{J}_- |2,2\rangle = 2\hbar |2,1\rangle = (\hat{J}_{1-} + \hat{J}_{2-}) |1,1\rangle_\otimes = \sqrt{2}\hbar |1,0\rangle_\otimes + \sqrt{2}\hbar |0,1\rangle_\otimes$$

$$|2,1\rangle = \tfrac{1}{\sqrt{2}} |1,0\rangle_\otimes + \tfrac{1}{\sqrt{2}} |0,1\rangle_\otimes$$

$$\begin{aligned} \hat{J}_- |2,1\rangle = \sqrt{6}\hbar |2,0\rangle &= (\hat{J}_{1-} + \hat{J}_{2-}) \left(\tfrac{1}{\sqrt{2}} |1,0\rangle_\otimes + \tfrac{1}{\sqrt{2}} |0,1\rangle_\otimes \right) \\ &= \hbar |1,-1\rangle_\otimes + 2\hbar |0,0\rangle_\otimes + \hbar |-1,1\rangle_\otimes \end{aligned}$$

$$|2,0\rangle = \tfrac{1}{\sqrt{6}} |1,-1\rangle_\otimes + \tfrac{2}{\sqrt{6}} |0,0\rangle_\otimes + \tfrac{1}{\sqrt{6}} |-1,1\rangle_\otimes$$

Continuing we have

$$|2,-1\rangle = \frac{1}{\sqrt{2}}|-1,0\rangle_{\otimes} + \frac{1}{\sqrt{2}}|0,-1\rangle_{\otimes}$$
$$|2,-2\rangle = |-1,-1\rangle_{\otimes}$$

which completes the five $j = 2$ states.

We must now have $|1,1\rangle = a|1,0\rangle_{\otimes} + b|0,1\rangle_{\otimes}$ with

$$|a|^2 + |b|^2 = 1 \text{ and } \langle 2,1|,1,1\rangle = \tfrac{1}{\sqrt{2}}a + \tfrac{1}{\sqrt{2}}b = 0$$

which gives

$$a = -b = \tfrac{1}{\sqrt{2}}$$

or

$$|1,1\rangle = \tfrac{1}{\sqrt{2}}|1,0\rangle_{\otimes} - \tfrac{1}{\sqrt{2}}|0,1\rangle_{\otimes}$$

We now find all of the $j = 1$ states

$$\hat{J}_-|1,1\rangle = \sqrt{2}\hbar|1,0\rangle = (\hat{J}_{1-} + \hat{J}_{2-})(\frac{1}{\sqrt{2}}|1,0\rangle_{\otimes} - \frac{1}{\sqrt{2}}|0,1\rangle_{\otimes})$$
$$= \hbar|1,-1\rangle_{\otimes} - \hbar|-1,1\rangle_{\otimes}$$
$$|1,0\rangle = \frac{1}{\sqrt{2}}|1,-1\rangle_{\otimes} - \frac{1}{\sqrt{2}}|-1,1\rangle_{\otimes}$$

and continuing

$$|1,-1\rangle = \frac{1}{\sqrt{2}}|0,-1\rangle_{\otimes} - \frac{1}{\sqrt{2}}|-1,0\rangle_{\otimes}$$

which completes the three $j = 1$ states.

31. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for $-8/15$ read $-\sqrt{8/15}$.

Notation:

J	J	...
M	M	...

m_1	m_2	
m_1	m_2	Coefficients
.	.	
.	.	
.	.	

1/2×1/2

	$+1$	
$+1/2\ +1/2$	1	0
	0	0

$+1/2\ -1/2$	$1/2$	$1/2$	1
$-1/2\ +1/2$	$1/2$	$-1/2$	-1
	$-1/2\ -1/2$		1

1×1/2

	$3/2$	
$+1\ +1/2$	1	$+1/2\ +1/2$

$+1\ -1/2$	$1/3$	$2/3$
$0\ +1/2$	$2/3$	$-1/3$

$0\ -1/2$	$2/3$	$1/3$
$-1\ +1/2$	$1/3$	$-2/3$
	$-1\ -1/2$	

2×1

	3	
$+2\ +1$	1	$+2\ \ +2$

$+2\ \ 0$	$1/3$	$2/3$
$+1\ +1$	$2/3$	$-1/3$

$+2\ -1$	$1/15$	$1/3$
$+1\ \ 0$	$8/15$	$1/6$
$0\ +1$	$6/15$	$-1/2$

$+2\ -1$	$1/15$	$1/3$
$+1\ \ 0$	$8/15$	$1/6$
$0\ +1$	$6/15$	$-1/2$

$+1\ -1$	$1/5$	$1/2$
$0\ \ 0$	$3/5$	0
$-1\ +1$	$1/5$	$-1/2$

$0\ -1$	$6/15$	$1/2$
$-1\ \ 0$	$8/15$	$-1/6$
$-2\ +1$	$1/15$	$-1/3$

$-1\ -1$	$2/3$	$1/3$
$-2\ \ 0$	$1/3$	$-2/3$
	$-2\ -1$	

1×1

	2	
$+1\ +1$	1	$+1\ \ +1$

$+1\ \ 0$	$1/2$	$1/2$
$0\ +1$	$1/2$	$-1/2$

$+1\ -1$	$1/6$	$1/2$
$0\ \ 0$	$2/3$	0
$-1\ +1$	$1/6$	$-1/2$

$+1\ -1$	$1/6$	$1/2$
$0\ \ 0$	$2/3$	0
$-1\ +1$	$1/6$	$-1/2$

$0\ -1$	$1/2$	$1/2$
$-1\ \ 0$	$1/2$	$-1/2$
	$-1\ -1$	

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

2×1/2

	5/2	
$+2\ \ 1/2$	1	$+5/2\ \ 3/2$

$+2\ -1/2$	$2/5$	$4/5$
$+1\ +1/2$	$4/5$	$-1/5$

$+1\ -1/2$	$2/5$	$3/5$
$0\ +1/2$	$3/5$	$-2/5$

$0\ -1/2$	$3/5$	$2/5$
$-1\ +1/2$	$2/5$	$-3/5$

$-1\ -1/2$	$4/5$	$1/5$
$-2\ +1/2$	$1/5$	$-4/5$
	$-2\ -1/2$	

3/2×1/2

	2	
$+3/2\ +1/2$	1	$+2\ \ +1$

$+3/2\ -1/2$	$1/4$	$3/4$
$+1/2\ +1/2$	$3/4$	$-1/4$

$+1/2\ -1/2$	$1/2$	$1/2$
$-1/2\ +1/2$	$1/2$	$-1/2$

$-1/2\ -1/2$	$3/4$	$1/4$
$-3/2\ +1/2$	$1/4$	$-3/4$
	$-3/2\ -1/2$	

3/2×1

	5/2	
$+3/2\ +1$	1	$+3/2\ +3/2$

$+3/2\ \ 0$	$2/5$	$3/5$
$+1/2\ +1$	$3/5$	$-2/5$

$+3/2\ -1$	$1/10$	$2/5$
$+1/2\ \ 0$	$3/5$	$1/15$
$-1/2\ +1$	$3/10$	$-8/15$

$+1/2\ -1$	$3/10$	$8/15$
$-1/2\ \ 0$	$3/5$	$-1/15$
$-3/2\ +1$	$1/10$	$-2/5$

$-1/2\ -1$	$3/10$	$2/5$
$-3/2\ \ 0$	$2/5$	$-3/5$
	$-3/2\ -1$	

$$d^j_{m',m} = (-1)^{m-m'} d^j_{m,m'} = d^j_{-m,-m'}$$

$$d^\ell_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

3/2×3/2

	3	
$+3/2\ +3/2$	1	$+2\ \ +2$

$+3/2\ +1/2$	$1/2$	$1/2$
$+1/2\ +3/2$	$1/2$	$-1/2$

$+3/2\ -1/2$	$1/5$	$1/2$
$+1/2\ +1/2$	$3/5$	0
$-1/2\ +3/2$	$1/5$	$-1/2$

$+3/2\ -3/2$	$1/20$	$1/4$
$+1/2\ -1/2$	$9/20$	$1/4$
$-1/2\ +1/2$	$9/20$	$-1/4$
$-3/2\ +3/2$	$1/20$	$-1/4$

$+1/2\ -3/2$	$1/5$	$1/2$
$-1/2\ -1/2$	$3/5$	0
$-3/2\ +1/2$	$1/5$	$-1/2$

$-1/2\ -3/2$	$1/2$	$1/2$
$-3/2\ -1/2$	$1/2$	$-1/2$
	$-3/2\ -3/2$	

2×3/2

	7/2	
$+2\ +3/2$	1	$+5/2\ +5/2$

$+2\ +1/2$	$3/7$	$4/7$
$+1\ +3/2$	$4/7$	$-3/7$

$+2\ -1/2$	$1/7$	$16/35$
$+1\ \ 1/2$	$4/7$	$1/35$
$0\ \ 3/2$	$2/7$	$-18/35$

$+2\ -1/2$	$1/7$	$16/35$
$+1\ \ 1/2$	$4/7$	$1/35$
$0\ \ 3/2$	$2/7$	$-18/35$

$-2\ -3/2$	$1/35$	$6/35$
$-1\ -1/2$	$12/35$	$5/14$
$0\ \ 1/2$	$18/35$	$-3/35$
$-1\ \ 3/2$	$4/35$	$-27/70$

$+2\ -3/2$	$4/35$	$27/70$
$0\ -1/2$	$18/35$	$3/35$
$-2\ \ 1/2$	$12/35$	$-5/14$
$-2\ \ 3/2$	$1/35$	$-6/35$

$0\ -3/2$	$2/7$	$18/35$
$-1\ -1/2$	$4/7$	$-1/35$
$-2\ \ 1/2$	$1/7$	$-16/35$

$-1\ -3/2$	$4/7$	$3/7$
$-2\ -1/2$	$3/7$	$-4/7$
	$-2\ -3/2$	

2×2

	4	
$+2\ +2$	1	$+3\ \ +3$

$+2\ +1$	$1/2$	$1/2$
$+1\ +2$	$1/2$	$-1/2$

$+2\ \ 0$	$3/14$	$1/2$
$+1\ \ 1$	$4/7$	0
$0\ \ 2$	$3/14$	$-1/2$

$+2\ -1$	$1/14$	$3/10$
$+1\ \ 0$	$3/7$	$1/5$
$0\ \ 1$	$3/7$	$-1/5$
$-1\ \ 2$	$1/14$	$-3/10$

$+2\ -2$	$1/70$	$1/10$
$+1\ -1$	$8/35$	$2/5$
$0\ \ 0$	$18/35$	0
$-1\ \ 1$	$8/35$	$-2/5$
$-2\ \ 2$	$1/70$	$-1/10$

$+1\ -2$	$1/14$	$3/10$
$0\ -1$	$3/7$	$1/5$
$-1\ \ 0$	$3/7$	$-1/5$
$-2\ \ 1$	$1/14$	$-3/10$

$0\ -2$	$3/14$	$1/2$
$-1\ -1$	$4/7$	0
$-2\ \ 0$	$3/14$	$-1/2$

$-1\ -2$	$1/2$	$1/2$
$-2\ -1$	$1/2$	$-1/2$
	$-2\ -2$	

$$d^{3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,1/2} = -\sqrt{3}\frac{1+\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-1/2} = \sqrt{3}\frac{1-\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2}$$

$$d^{3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2}$$

$$d^{3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2}$$

$$d^2_{2,2} = \left(\frac{1+\cos\theta}{2}\right)^2$$

$$d^2_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

$$d^2_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta$$

$$d^2_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta$$

$$d^2_{2,-2} = \left(\frac{1-\cos\theta}{2}\right)^2$$

$$d^2_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^2_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^2_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1)$$

$$d^2_{0,0} = \left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

$$d^0_{0,0} = \cos\theta \qquad d^{1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^1_{1,1} = \frac{1+\cos\theta}{2}$$

$$d^{1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2} \qquad d^1_{1,0} = -\frac{\sin\theta}{\sqrt{2}}$$

$$d^1_{1,-1} = \frac{1-\cos\theta}{2}$$

$$(j_1 j_2 m_1 m_2 | j_1 j_2 J M) = (-1)^{j-j_1-j_2}(j_2 j_1 m_2 m_1 | j_2 j_1 J M)$$

Figure 31.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

We must now have $|0,0\rangle = a\,|1,-1\rangle_\otimes + b\,|0,0\rangle_\otimes + c\,|-1,1\rangle_\otimes$ with

$$|a|^2 + |b|^2 = 1 \text{ and } \langle 2,0\,|\,,0,0\rangle = \tfrac{1}{\sqrt{6}}a + \tfrac{2}{\sqrt{6}}b + \tfrac{1}{\sqrt{6}}c = 0$$

$$\text{and } \langle 1,0\,|\,,0,0\rangle = \tfrac{1}{\sqrt{6}}a - \tfrac{1}{\sqrt{6}}c = 0$$

which gives

$$a = -b = c = \tfrac{1}{\sqrt{3}}$$

or

$$|0,0\rangle = \tfrac{1}{\sqrt{3}}\,|1,-1\rangle_\otimes - \tfrac{1}{\sqrt{3}}\,|0,0\rangle_\otimes + \tfrac{1}{\sqrt{3}}\,|-1,1\rangle_\otimes$$

All the *j*-values are now done.

Two- and Three-Dimensional Systems

We now turn our attention to 2– and 3–dimensional systems that can be solved analytically.

In the position representation, the wave function

$$\psi(\vec{r}) = \langle \vec{r} \mid \psi \rangle$$

contains all the information that is knowable about the state of a physical system.

The equation that determines the wave function is the Schrodinger equation, which we derived from the energy eigenvalue equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

The general form of the Schrodinger equation in three dimensions is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

We will use a succession of concrete examples to elucidate the solution techniques and the physical principles that are involved.

2- and 3-Dimensional Infinite Wells

2-Dimensional Infinite Square Well - Cartesian Coordinates

The potential energy function is

$$V(x,y) = \begin{cases} 0 & |x| < \frac{a}{2} \text{ and } |y| < \frac{a}{2} \rightarrow \text{ region I} \\ \infty & \text{otherwise} \rightarrow \text{ region II} \end{cases}$$

This is a simple extension of the 1–dimensional infinite well problem, but it is useful because it illustrates all the ideas we will need for more complicated problems.

In region I
$$\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2} = -\frac{2mE}{\hbar^2}\psi(x,y)$$

In region II
$$\psi(x,y) = 0$$

since the potential is infinite over an extended region.

We solve this equation by the separation of variables (SOV) technique.

We assume
$$\psi(x,y) = X(x)Y(y)$$

Upon substitution we get

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2}$$

Each term on the left-hand side of the equation is a function only of a single variable and hence the only way to satisfy the equation for all x and y is to set each function of a single variable equal to a constant.

We have

$$\frac{1}{X}\frac{d^2X}{dx^2} = -\frac{2mE_x}{\hbar^2} = \text{constant}$$

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -\frac{2mE_y}{\hbar^2} = \text{constant}$$

$$E = E_x + E_y$$

If we choose

$$\frac{2mE_x}{\hbar^2} = k_x^2 \quad , \quad \frac{2mE_y}{\hbar^2} = k_y^2 \quad , \quad \frac{2mE}{\hbar^2} = k^2$$

we get the solutions

$$X(x) = A\sin k_x x + B\cos k_x x$$

$$Y(y) = C\sin k_y y + D\cos k_y y$$

with the boundary conditions

$$X\left(\pm\frac{a}{2}\right) = 0 = Y\left(\pm\frac{a}{2}\right)$$

For the function $X(x)$ each boundary condition implies two solution types

$$A = 0 \text{ or } \sin\frac{k_x a}{2} = 0 \text{ and } B = 0 \text{ or } \cos\frac{k_x a}{2} = 0$$

These are both summarized in the solution

$$X(x) = \begin{cases} \sin \frac{n_x \pi x}{a} & n_x = \text{even} \\ \\ \cos \frac{n_x \pi x}{a} & n_x = \text{odd} \end{cases} \qquad k_x = \frac{n_x \pi}{a} \qquad n_x = \text{integer}$$

and similarly for $Y(y)$

$$Y(y) = \begin{cases} \sin \frac{n_y \pi y}{a} & n_y = \text{even} \\ \\ \cos \frac{n_y \pi y}{a} & n_y = \text{odd} \end{cases} \qquad k_y = \frac{n_y \pi}{a} \qquad n_y = \text{integer}$$

The corresponding energy eigenvalues are

$$E = (n_x^2 + n_y^2)\frac{\pi^2 \hbar^2}{2ma^2} \quad , \quad n_x, n_y = 1, 2, 3, 4 \ldots$$

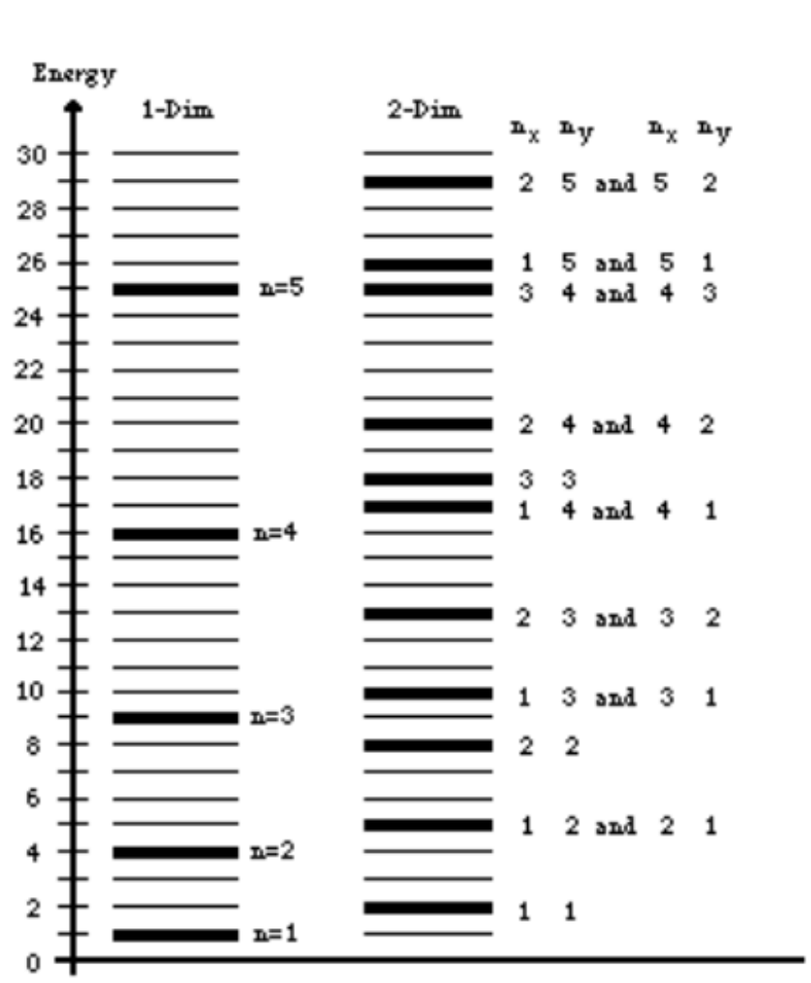
The 1–dimensional result we found earlier was

$$E_{1\,\mathrm{dim}} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad , n = 1, 2, 3, 4 \ldots$$

A plot of these levels for comparison is shown in the Figure;

we choose $\frac{\pi^2 \hbar^2}{2ma^2} = 1$

Comparison of 1D and 2D Infinite Wells



The major change is not only that the level structure gets more complex, but also that a major new feature appears, namely, *degeneracy*.

Several of the 2–dimensional well levels are degenerate, which means that *different sets* of quantum numbers give the *same energy eigenvalue*.

In the energy level diagram above the $E = 5,10,13,17,20,25,26$ and 29 levels are all two-fold degenerate.

This degeneracy arises from the fact that $V(x, y) = V(-x, -y)$ and hence parity is conserved.

This means that the correct physical eigenstates should be simultaneous eigenstates of both the parity and the energy.

The first three wave functions are

$$\psi_{11}(x,y) = \cos\frac{\pi x}{a}\cos\frac{\pi y}{a} \quad , \quad E = E_{11}$$

$$\psi_{12}(x,y) = \cos\frac{\pi x}{a}\sin\frac{2\pi y}{a} \quad , \quad E = E_{12}$$

$$\psi_{21}(x,y) = \sin\frac{2\pi x}{a}\cos\frac{\pi y}{a} \quad , \quad E = E_{21} = E_{12}$$

A simple calculation shows that we have

$$\langle 11 \mid 12\rangle = \langle 11 \mid 21\rangle = 0 \rightarrow \text{ orthogonal and } \langle 21 \mid 12\rangle \neq 0 \rightarrow \text{ not orthogonal}$$

We can construct two new eigenfunctions from the degenerate pair that are orthogonal using the Gram-Schmidt process.

We get

$$\psi_{12}^{+} = \psi_{12} + \psi_{21} \text{ and } \psi_{12}^{-} = \psi_{12} - \psi_{21}$$

We then have

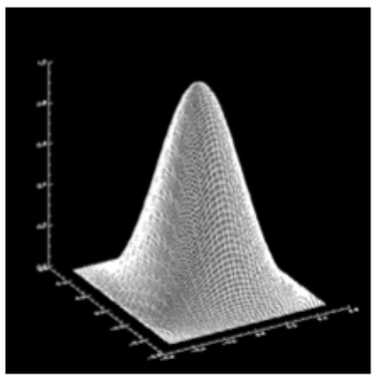
$$\langle 12+ \mid 12- \rangle = 0 \rightarrow \text{ orthogonal}$$

We also note that for the parity operator $\wp$ we have

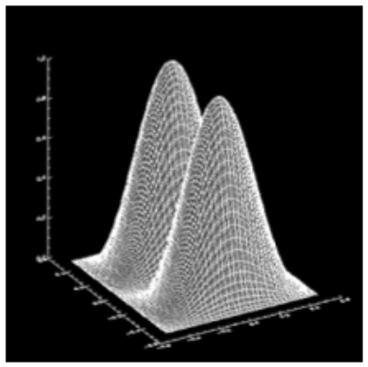
$$\hat{\wp}\,|11\rangle = |11\rangle \quad , \quad \hat{\wp}\,|12+\rangle = |12+\rangle \quad , \quad \hat{\wp}\,|12-\rangle = -|12-\rangle$$

so that the new eigenfunctions are simultaneous eigenstates of parity and energy.

Two of the wave functions are plotted below in the Figures as $|\psi|^2$.



$|\psi_{11}|^2$



$|\psi_{12}^{+}|^2$

Now let us turn to the infinite circular well in two dimensions.

Two-Dimensional Infinite Circular Well

We consider the potential in two dimensions

$$V(r) = \begin{cases} 0 & r < a \\ \infty & r > a \end{cases}$$

The Schrodinger equation in plane-polar coordinates is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right]\psi(r,\varphi)=E\psi(r,\varphi)\qquad r<a$$

$$\psi(r,\varphi)=0\qquad r<a$$

We assume(SOV)

$$\psi(r,\varphi)=R(r)\Phi(\varphi)$$

which gives

$$-\frac{\hbar^2}{2m}\left[\frac{1}{rR}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right)+\frac{1}{r^2}\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}\right]=E\qquad r<a$$

We choose a separation constant

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=-\alpha^2\rightarrow\Phi(\varphi)=B\sin(\alpha\varphi+\delta)$$

The requirement of single-valuedness under a ϕ-rotation of 2π says that

$$\sin(\alpha\varphi+\delta)=\sin(\alpha\varphi+\delta+\alpha\pi)$$

$$\rightarrow\alpha=\text{ integer }=0,1,2,3\ldots$$

Alternatively, we could write

$$\Phi(\varphi)=Be^{i\alpha\varphi}$$

$$\alpha=\text{ integer }=\ldots-3,-2,-1,0,1,2,3,\ldots$$

Substitution of this solution leaves the radial differential equation

$$r^2\frac{d^2R}{dr^2}+r\frac{dR}{dr}+\left[\lambda^2r^2-\alpha^2\right]R=0\text{ where }\lambda^2=\frac{2mE}{\hbar^2}$$

This is Bessel's equation.

The general solution is

$$R(r) = NJ_\alpha(\lambda r) + MY_\alpha(\lambda r)$$

Now $Y_\alpha(\lambda r) \to \infty$ as $r \to 0$.

Therefore, in order to have a normalizable solution in the region $r < a$ (which includes $r = 0$), we must choose $M = 0$ and thus we have

$$R(r) = NJ_\alpha(\lambda r)$$

and the complete solution is then

$$\psi_{k\alpha}(r, \varphi) = R(r)\Phi(\varphi) = NJ_\alpha(\lambda r)e^{i\alpha\varphi}$$

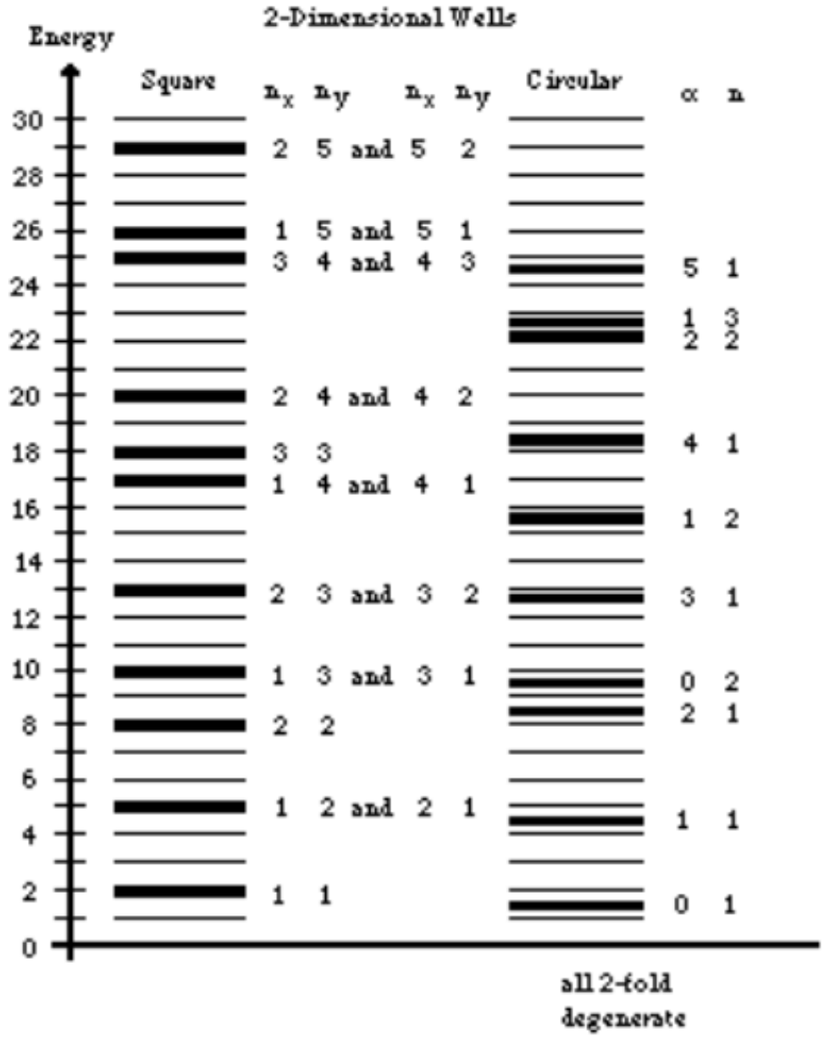
The continuity (or boundary) condition at $r = a$ is

$$\psi_{k\alpha}(a, \varphi) = 0 \to R(a) = 0 \to J_\alpha(\lambda a) = 0$$

Thus, the allowed values of λ and hence the allowed values of E are given by

$$\lambda_{n\alpha}a = z_{n\alpha} = \text{ the } n^{th} \text{ zero of } J_\alpha \to E_{n\alpha} = \frac{\hbar^2}{2ma^2}z_{n\alpha}^2$$

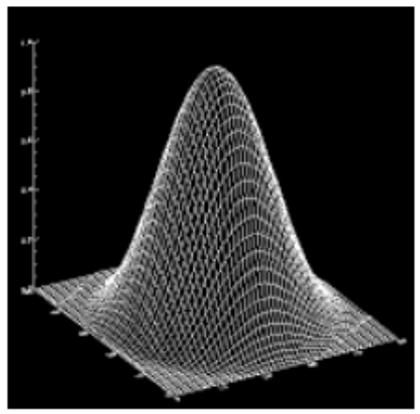
We compare the infinite square and circular wells in 2–dimensions using the energy level diagram in the Figure.



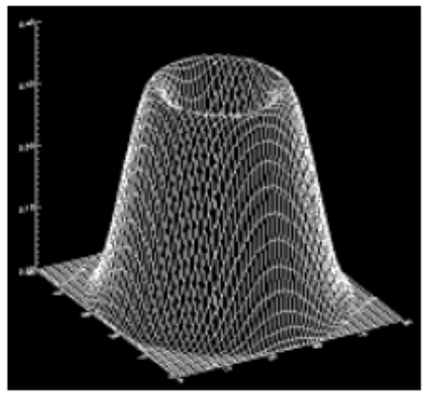
Two Dimensional Wells

Note the rather dramatic differences in both the location and degeneracies for the two sets of energy levels.

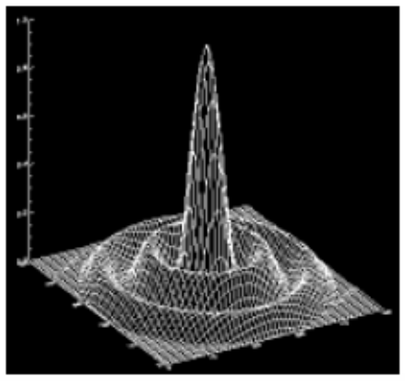
Some of the wave functions for the 2–dimensional circular well are shown in the Figures below.



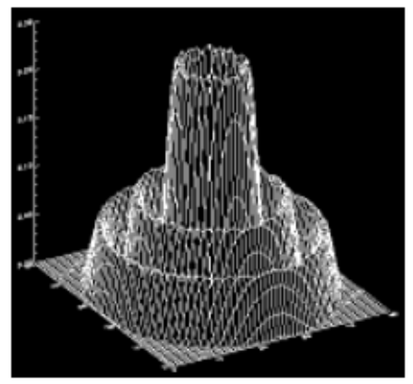
$|\psi_{01}|^2$



$|\psi_{11}|^2$



$|\psi_{03}|^2$



$|\psi_{23}|^2$

The 3–*dimensional infinite square well* is a simple extension of the 2–dimensional infinite square well.

The result for the energies is

$$E = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2ma^2} \quad , \quad n_x, n_y, n_z = 1, 2, 3, 4\ldots$$

The 3–*dimensional infinite spherical well* involves the potential

$$V(r,\theta,\varphi) = \begin{cases} 0 & r < a \quad \text{region I} \\ \infty & r > a \quad \text{region II} \end{cases}$$

The Schrodinger equation is:

Region I

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} = -\frac{2m}{\hbar^2}E$$

Region II

$$\psi(r,\theta,\varphi) = 0$$

The equation in region I can be rewritten in terms of the $\vec{L}^2_{op}$ operator as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) - \frac{\vec{L}^2_{op}\psi}{\hbar^2 r^2} = -\frac{2m}{\hbar^2}E\psi$$

Since the potential energy is spherically symmetric, we have

$$\left[\vec{L}^2_{op}, \hat{H}\right] = 0$$

and thus the operators $\vec{L}^2_{op}$ and $\hat{H}$ have a common eigenbasis.

Earlier, we found the eigenfunctions of $\vec{L}^2_{op}$ to be the spherical harmonics $Y_{\ell m}(\theta,\phi)$, where

$$\vec{L}^2_{op}Y_{\ell m}(\theta,\varphi) = \hbar^2\ell(\ell+1)Y_{\ell m}(\theta,\varphi)$$

Therefore, we can write(SOV)

$$\psi(r,\theta,\varphi) = R_\ell(r)Y_{\ell m}(\theta,\varphi)$$

Substitution of this form of the solution gives the radial equation in region I

$$\frac{d^2R_\ell}{dr^2} + \frac{2}{r}\frac{dR_\ell}{dr} - \frac{\ell(\ell+1)}{r^2}R_\ell + k^2R_\ell = 0$$

where

$$E = \frac{h^2k^2}{2m}$$

In region II we have $R_\ell(r) = 0$.

The most general solution of the radial equation(which is a different form of Bessel's equation) is

$$R_\ell(r) = Aj_\ell(kr) + B\eta_\ell(kr)$$

where

$$j_\ell(kr) = \left(\frac{\pi}{2kr}\right)^{1/2} J_{\ell+1/2}(kr)$$

$$\eta_\ell(kr) = (-1)^{\ell+1}\left(\frac{\pi}{2kr}\right)^{1/2} J_{-\ell-1/2}(kr)$$

are the spherical Bessel functions.

Now $\eta_\ell(kr) \to \infty$ as $r \to 0$.

Therefore, the normalizable solution in region I (which contains $r = 0$) is

$$R_\ell(r) = Aj_\ell(kr)$$

The first few of these functions

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x$$

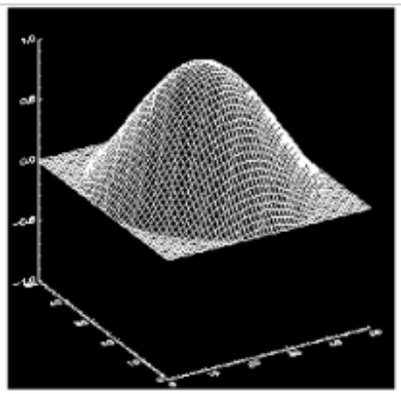
The boundary conditions give

$$j_\ell(k_{n\ell}a) = 0 \text{ where } k_{n\ell} = \text{ the } n^{th} \text{ zero of } j_\ell$$

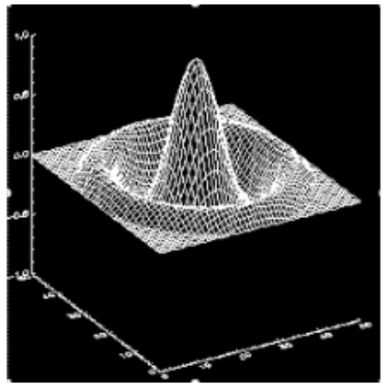
The full solution is

$$\psi_{n\ell m}(\theta,\varphi) = R_{n\ell}(r)Y_{\ell m}(\theta,\varphi) = j_\ell(k_n r)P_\ell^m(\cos\theta)e^{im\varphi}$$

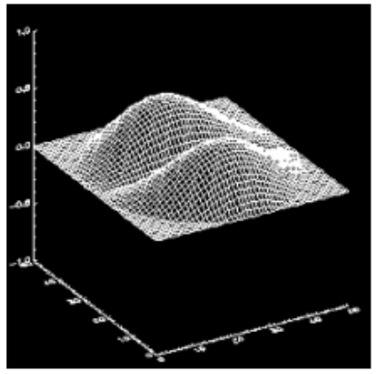
Some of the wavefunctions (absolute squares) are shown in the Figures below.



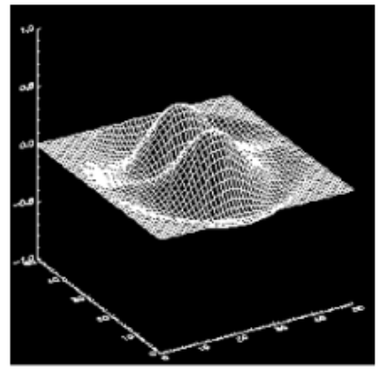
$n\ell m = 100$



$n\ell m = 200$



$n\ell m = 111$



$n\ell m = 211$

3-Dimensional Finite Well

We now consider the potential function in three dimensions

$$V(r) = \begin{cases} -V_0 & r \le a \quad \text{region I} \\ 0 & r > a \quad \text{region II} \end{cases}$$

The Schrodinger equation is

Region I (same as infinite well)

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{2m}{\hbar^2}V_0\psi = -\frac{2m}{\hbar^2}E\psi$$

Region II

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}=-\frac{2m}{\hbar^2}E\psi$$

If we choose $E=-|E|<0$ for bound states, we have

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)-\frac{\vec{L}_{op}^2\psi}{\hbar^2r^2}+\frac{2m}{\hbar^2}V_0\psi=\frac{2m}{\hbar^2}|E|\psi \text{ in region I}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)-\frac{\vec{L}_{op}^2\psi}{\hbar^2r^2}=\frac{2m}{\hbar^2}|E|\psi \text{ in region II}$$

We then write, as before,

$$\psi(\theta,\varphi)=R_\ell(r)Y_{\ell m}(\theta,\varphi)$$

and get

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{\ell(\ell+1)R}{r^2}+\frac{2m}{\hbar^2}V_0R=\frac{2m}{\hbar^2}|E|R \quad \text{in region I}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-\frac{\ell(\ell+1)R}{r^2}=\frac{2m}{\hbar^2}|E|R \quad \text{in region II}$$

which finally becomes

$$\frac{d^2R}{d\rho^2}+\frac{2}{\rho}\frac{dR}{d\rho}+\left[1-\frac{\ell(\ell+1)}{\rho^2}\right]R=0$$

$$\rho=\alpha r \quad , \quad \alpha^2=\frac{2m}{\hbar^2}(V_0-|E|) \quad \text{in region I}$$

and

$$\frac{d^2R}{d\gamma^2} + \frac{2}{\gamma}\frac{dR}{d\gamma} + \left[1 - \frac{\ell(\ell+1)}{\gamma^2}\right]R = 0$$

$$\gamma = i\beta r \quad , \quad \beta^2 = \frac{2m}{\hbar^2}|E| \qquad \text{in region II}$$

The solutions are

$$R(r) = Aj_\ell(\alpha r) \qquad\qquad r \le a$$

$$R(r) = Bh_\ell^{(1)}(i\beta r) = B\left[j_\ell(i\beta r) + i\eta_\ell(i\beta r)\right] \qquad r > a$$

where

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x$$

$$j_\ell(x) = x^\ell\left(-\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}$$

which are *spherical Bessel functions of the 1st kind*, and

$$\eta_0(x) = -\frac{\cos x}{x}$$

$$\eta_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$\eta_2(x) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x$$

$$\eta_\ell(x) = -x^\ell\left(-\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}$$

which are *spherical Bessel functions of the 2nd kind*, and

$$h_0^{(1)}(ix) = -\frac{1}{x}e^{-x}$$

$$h_1^{(1)}(ix) = i\left(\frac{1}{x} + \frac{1}{x^2}\right)e^{-x}$$

$$h_2^{(1)}(ix) = \left(\frac{1}{x} + \frac{3}{x^2} + \frac{3}{x^3}\right)e^{-x}$$

$$h_\ell^{(1)}(ix) = j_\ell(ix) + i\eta_\ell(ix)$$

which are *spherical Hankel functions of the 1st kind*.

There is another independent solution for r > a, namely,

$$h_\ell^{(2)}(ix) = j_\ell(ix) - i\eta_\ell(ix)$$

which is a *spherical Hankel function of the 2nd kind*, but we must exclude it because it behaves like $e^{\beta r}$ as $r \to \infty$ and, hence, is not normalizable

We have also excluded $\eta_\ell(\alpha r)$ from the solution for $r \le a$ because it diverges at $r = 0$.

We note for future reference that we have the asymptotic behaviors

$$j_\ell(x) \underset{x\to 0}{\to} \frac{x^\ell}{1\cdot 3\cdot 5\cdots(2\ell+1)} \text{ and } \eta_\ell(x) \underset{x\to 0}{\to} \frac{1\cdot 3\cdot 5\cdots(2\ell-1)}{x^\ell}$$

$$j_\ell(x) \underset{x\to\infty}{\to} \frac{1}{x}\cos\left[x - \frac{(\ell+1)\pi}{2}\right] \text{ and } \eta_\ell(x) \underset{x\to\infty}{\to} \frac{1}{x}\sin\left[x - \frac{(\ell+1)\pi}{2}\right]$$

$$h_\ell^{(1)}(x) \underset{x\to\infty}{\to} \frac{1}{x}e^{i\left[x - \frac{1}{2}(\ell+1)\pi\right]} \text{ and } h_\ell^{(2)}(x) \underset{x\to\infty}{\to} \frac{1}{x}e^{-i\left[x - \frac{1}{2}(\ell+1)\pi\right]}$$

Since both R and dR/dr are continuous at $r = a$, we can combine the two continuity equations into one using the continuity of the so-called logarithmic derivative

$$\frac{1}{R}\frac{dR}{dr} \text{ at } r = a$$

For *each* value of ℓ this gives a transcendental equation for the energy E.

Examples

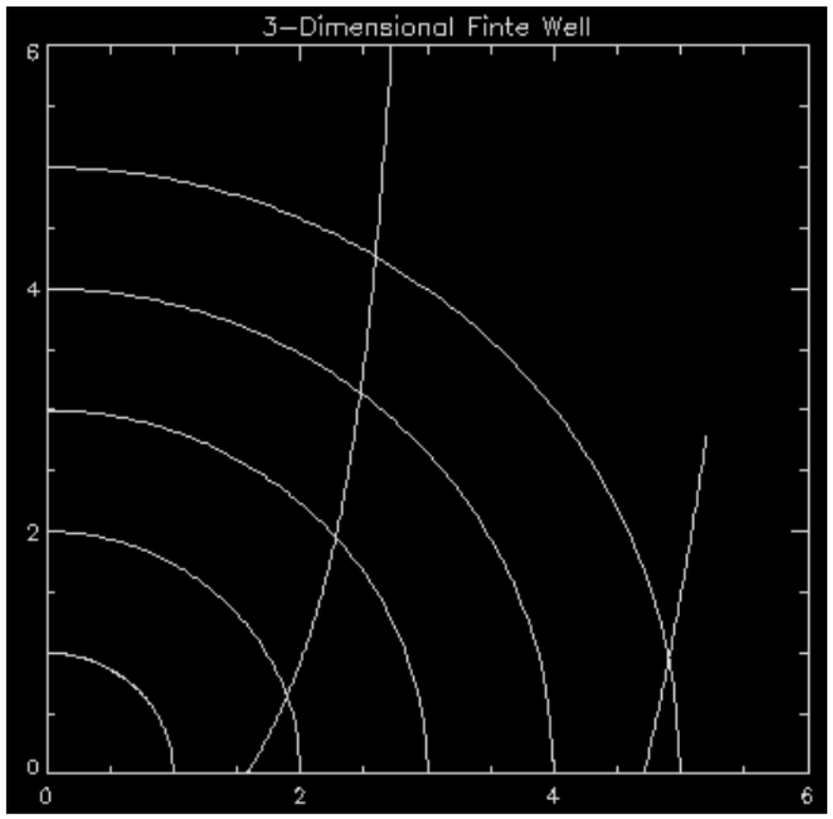
$$\ell = 0 \qquad \xi \cot \xi = -\zeta \quad \text{and} \quad \xi^2 + \zeta^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\xi = \alpha a \quad \text{and} \quad \zeta = \beta a$$

$$\ell = 1 \qquad \frac{\cot \xi}{\xi} - \frac{1}{\xi^2} = \frac{1}{\zeta} + \frac{1}{\zeta^2} v\xi^2 + \zeta^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\xi = \alpha a \quad \text{and} \quad \zeta = \beta a$$

A graphical solution for the $\ell = 0$ case is shown in the Figure.



Graphical Solution

For a given well, only one circle exists on the plot.

The solutions (energy eigenvalues) are given by the intersection of that circle with the cotangent curves.

The big change from the finite well in one dimension is that the quantity

$$\frac{2mV_0a^2}{\hbar^2}$$

must be larger than some minimum value before any bound state exists (this corresponds to the radius of the smallest circle that intersects the cotangent curves).

In particular,

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{\pi}{2}\right)^2 \rightarrow \text{ no solution}$$

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{3\pi}{2}\right)^2 \rightarrow \text{ 1 solution}$$

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{5\pi}{2}\right)^2 \rightarrow \text{ 2 solutions}$$

stop

Two-Dimensional Harmonic Oscillator

The 2-dimensional harmonic oscillator system has the Hamiltonian

$$\begin{aligned}\hat{H} &= \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2\right) + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2) \\ &= \left(\frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right) + \left(\frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2\hat{y}^2\right) \\ &= \hat{H}_x + \hat{H}_y\end{aligned}$$

where we have the commutation relations

$$\left[\hat{H}_x, \hat{H}_y\right] = 0 = \left[\hat{H}, \hat{H}_x\right] = \left[\hat{H}, \hat{H}_y\right]$$

These commutators imply that $\hat{H}$, $\hat{H}_x$ and $\hat{H}_y$ have a common eigenbasis.

We label their common state vectors by

$$|E\rangle = |E_x, E_y\rangle = |E_x\rangle\,|E_y\rangle$$

with

$$\hat{H}_x\,|E_x\rangle = E_x\,|E_x\rangle$$

$$\hat{H}_y\,|E_y\rangle = E_y\,|E_y\rangle$$

$$\hat{H}\,|E\rangle = E\,|E\rangle = (\hat{H}_x + \hat{H}_y)\,|E_x\rangle\,|E_y\rangle$$

$$= (E_x + E_y)\,|E\rangle$$

or

$$E = E_x + E_y$$

Now $\hat{H}_x$ (and $\hat{H}_y$) each represent a 1-dimensional oscillator.

This suggests that we define new operators for the x coordinate

$$a_x = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}_x = (a_x^+)^+$$

where

$$[\hat{x}, \hat{p}_x] = i\hbar \rightarrow [\hat{a}_x, a_x^+] = 1$$

and

$$\hat{H}_x = \hbar\omega\left(\hat{a}_x^+\hat{a}_x + \frac{1}{2}\right) = \hbar\omega\left(\hat{N}_x + \frac{1}{2}\right)$$

As we found earlier, $\hat{N}_x$ has an eigenvalue equation

$$\hat{N}_x\,|n_x\rangle = n_x\,|n_x\rangle \quad , \quad n_x = 0, 1, 2, 3, \ldots\ldots$$

We then have

$$\hat{H}_x |n_x\rangle = \hbar\omega \left(\hat{N}_x + \frac{1}{2}\right)|n_x\rangle = \hbar\omega \left(n_x + \frac{1}{2}\right)|n_x\rangle$$

or

$$E_x = \hbar\omega \left(n_x + \frac{1}{2}\right)$$

In a similar manner, we repeat this process for the *y* coordinate

$$a_y = \sqrt{\frac{m\omega}{2\hbar}}\hat{y} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}_y = \left(a_y^+\right)^+$$

$$[\hat{y}, \hat{p}_y] = i\hbar \rightarrow \left[\hat{a}_y, a_y^+\right] = 1$$

$$\hat{H}_y = \hbar\omega \left(\hat{a}_y^+ \hat{a}_y + \frac{1}{2}\right) = \hbar\omega \left(\hat{N}_y + \frac{1}{2}\right)$$

As we found earlier, $\hat{N}_y$ has an eigenvalue equation

$$\hat{N}_y |n_y\rangle = n_y |n_y\rangle \quad , \quad n_y = 0, 1, 2, 3, \ldots\ldots\ldots$$

We then have

$$\hat{H}_y |n_y\rangle = \hbar\omega \left(\hat{N}_y + \frac{1}{2}\right)|n_y\rangle = \hbar\omega \left(n_y + \frac{1}{2}\right)|n_y\rangle$$

or

$$E_y = \hbar\omega \left(n_y + \frac{1}{2}\right)$$

Putting this all together we get

$$E = E_x + E_y = \hbar\omega(n_x + n_y + 1) = \hbar\omega(n + 1)$$

The table below gives the resulting energy level structure.

n_x	n_y	$E/\hbar\omega$	n
0	0	1	0
1	0	2	1
0	1	2	1
0	2	3	2
2	0	3	2
1	1	3	2

Energy Levels - 2D Oscillator

Each energy value, which is characterized by the quantum number n, has a degeneracy equal to $(n + 1)$.

The existence of degeneracy indicates (this is a general rule) that there is another operator that commutes with $\hat{H}$.

Since this is a central force in the x–y plane, it is not difficult to guess that the other operator that commutes with $\hat{H}$ is the angular momentum about the axis perpendicular to the plane (the z–axis), $\hat{L}_z$.

Since all of the x-type operators commute with all of the y-type operators we can write

$$\hat{L}_z = (\vec{r}_{op} \times \vec{p}_{op})_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

Inverting the standard operator definitions we have

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_x + \hat{a}_x^+) \quad , \quad \hat{p}_x = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}_x - \hat{a}_x^+)$$

$$\hat{y} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_y + \hat{a}_y^+) \quad , \quad \hat{p}_y = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}_y - \hat{a}_y^+)$$

which gives

$$\hat{L}_z = \frac{\hbar}{i}(\hat{a}_x^+ \hat{a}_y - \hat{a}_y^+ a_x)$$

Now using

$$\left[\hat{a}_x, \hat{N}_x\right] = \hat{a}_x \quad , \quad \left[\hat{a}_x^+, \hat{N}_x\right] = -\hat{a}_x^+$$
$$\left[\hat{a}_y, \hat{N}_y\right] = \hat{a}_y \quad , \quad \left[\hat{a}_y^+, \hat{N}_y\right] = -\hat{a}_y^+$$

we get

$$\left[\hat{H}_x, \hat{L}_z\right] = \frac{\hbar}{i}(\hat{a}_y \hat{a}_x^+ + \hat{a}_x \hat{a}_y^+) = -\left[\hat{H}_y, \hat{L}_z\right]$$

or

$$\left[\hat{H}, \hat{L}_z\right] = 0$$

Therefore, $\hat{H}$ and $\hat{L}_z$ share a common eigenbasis.

This new eigenbasis will not be an eigenbasis for $\hat{H}_x$ or $\hat{H}_y$ separately since they do not commute with $\hat{L}_z$.

This suggests that we use linear combinations of the degenerate eigenstates to find the eigenstates of $\hat{L}_z$.

This works because linear combinations for fixed n remain eigenstates of $\hat{H}$ (they are no longer eigenstates of $\hat{H}_x$ or $\hat{H}_y$ however).

We define the eigenstates and eigenvalues of $\hat{L}_z$ by the equation

$$\hat{L}_z |m\rangle = m\hbar |m\rangle$$

and the common eigenstates of $\hat{H}$ and $\hat{L}_z$ by $|n,m\rangle$ where

$$\hat{H}\,|n,m\rangle = \hbar\omega(n+1)\,|n,m\rangle$$
$$\hat{L}_z\,|n,m\rangle = m\hbar\,|n,m\rangle$$

For notational clarity we will write the old states as $|n_x\rangle|n_y\rangle$.

For the $n = 0$ states (there is only one) we have

$$\hat{L}_z\,|0,0\rangle = \hat{L}_z\,|0\rangle\,|0\rangle = 0 \rightarrow m = 0\ ,\ n = 0$$

Now we look at the $n = 1$ states.

We let $$|\psi\rangle = a\,|0\rangle\,|1\rangle + b\,|1\rangle\,|0\rangle \ \text{ where } \ |a|^2 + |b|^2 = 1 \ \text{(normalization)}$$

Since the two states that make up the linear combination are both eigenstates of $\hat{H}$ with $n = 1$, the linear combination is an eigenstate of $\hat{H}$ with $n = 1$ for any choice of a and b.

We therefore choose a and b to make this state an eigenstate of $\hat{L}_z$.

We must have

$$\begin{aligned}\hat{L}_z\,|\psi\rangle &= \hat{L}_z\,|1,m\rangle = \hat{L}_z(a\,|0\rangle\,|1\rangle + b\,|1\rangle\,|0\rangle)\\ &= \frac{\hbar}{i}(\hat{a}_x^{+}\hat{a}_y - \hat{a}_y^{+}a_x)(a\,|0\rangle\,|1\rangle + b\,|1\rangle\,|0\rangle)\\ &= m\hbar(a\,|0\rangle\,|1\rangle + b\,|1\rangle\,|0\rangle)\end{aligned}$$

Using

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \quad , \quad \hat{a}^{+}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

we get

$$a\frac{\hbar}{i}\,|1\rangle\,|0\rangle - b\frac{\hbar}{i}\,|0\rangle\,|1\rangle = m\hbar(a\,|0\rangle\,|1\rangle + b\,|1\rangle\,|0\rangle)$$

or

$$ma = ib \quad and \quad mb = -ia$$

Dividing these two equations we get

$$\frac{a}{b} = -\frac{b}{a}$$

which implies that

$$a^2 = -b^2 \rightarrow a = \pm ib$$

and

$$m = -\frac{b}{ia} = \begin{cases} +1 & a = +ib \\ -1 & a = -ib \end{cases}$$

Normalization then says that

$$m = \begin{cases} +1 & a = \frac{1}{\sqrt{2}}, b = -\frac{i}{\sqrt{2}} \\ -1 & a = \frac{1}{\sqrt{2}}, b = +\frac{i}{\sqrt{2}} \end{cases}$$

or

$$|1, \pm 1\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle |1\rangle \mp |1\rangle |0\rangle \right)$$

This gives a new characterization of the first two excited energy levels as shown in the Table.

n	m	$E/\hbar\omega$
0	0	1
1	+1	2
1	-1	2

Energy Levels - (n,m) Characterization

Let us now do the $n = 2$ states.

In the same way we assume

$$|\psi\rangle = a |2\rangle |0\rangle + b |1\rangle |1\rangle + c |0\rangle |2\rangle$$

where normalization gives

$$|a|^2 + |b|^2 + |c|^2 = 1$$

We then have

$$\begin{aligned}
\hat{L}_z |\psi\rangle &= \hat{L}_z |2,m\rangle = m\hbar |\psi\rangle \\
&= m\hbar a |2\rangle |0\rangle + m\hbar b |1\rangle |1\rangle + m\hbar c |0\rangle |2\rangle \\
&= \frac{\hbar}{i}(\hat{a}_x^+ \hat{a}_y - \hat{a}_y^+ \hat{a}_x)(a |2\rangle |0\rangle + b |1\rangle |1\rangle + c |0\rangle |2\rangle) \\
&= \frac{\hbar}{i}\left[\sqrt{2}b |2\rangle |0\rangle + \sqrt{2}(c-a) |1\rangle |1\rangle - \sqrt{2}b |0\rangle |2\rangle\right]
\end{aligned}$$

which gives

$$ma = -i\sqrt{2}b$$

$$mc = +i\sqrt{2}b$$

$$mb = -i\sqrt{2}(c-a)$$

$$\frac{a}{c} = -1 \rightarrow c = -a$$

$$\frac{c}{b} = -\frac{b}{c-a} \rightarrow \frac{a}{b} = -\frac{b}{2a} \rightarrow b^2$$

$$= -2a^2 \rightarrow b = \pm i\sqrt{2a}$$

Putting these pieces all together we have

$$a = \frac{1}{2} = -c \quad , \quad b_\pm = \pm i\frac{\sqrt{2}}{2}$$

This implies the *m*-values

$$m = \begin{cases} \frac{\sqrt{2}b_+}{ia} & +2 \\ \frac{\sqrt{2}b_-}{ia} & -2 \end{cases}$$

or

$$|2,0\rangle = \frac{1}{\sqrt{2}}|2\rangle|0\rangle + \frac{1}{\sqrt{2}}|0\rangle|2\rangle$$

Thus, the final energy levels are as shown in the Table.

n	m	$E/\hbar\omega$
0	0	1
1	+1	2
1	-1	2
2	+2	3
2	0	3
2	-2	3

Energy Levels - (n,m) Characterization

What a strange result?

The allowed *m*-values are separated by $\Delta m = \pm 2$.

Let us look at this system using the Schrodinger equation to help us understand what is happening.

We have (using plane-polar coordinates)

$$-\frac{h^2}{2M}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2}\right)+\frac{1}{2}M\omega^2r^2\psi = E\psi$$

Choosing

$$\psi(r,\varphi) = R(r)\Phi(\varphi)$$

we get

$$-\frac{h^2}{2M}\frac{1}{R}\left(\frac{d^2R}{dr^2}+\frac{1}{r}\frac{dR}{dr}\right)-\frac{h^2}{2Mr^2}\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}+\frac{1}{2}M\omega^2r^2=E$$

Now we must have

$$\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=-m^2=\text{constant}$$

which produces a radial equation of the form

$$-\frac{h^2}{2M}\left(\frac{d^2R}{dr^2}+\frac{1}{r}\frac{dR}{dr}\right)+\left(\frac{h^2m^2}{2Mr^2}+\frac{1}{2}M\omega^2r^2\right)R=ER$$

Now we change the variables using

$$r=\rho y \quad , \quad \rho=\frac{\hbar}{M\omega}$$

and get

$$\frac{d^2R}{dy^2}+\frac{1}{y}\frac{dR}{dy}+\left(\varepsilon-y^2-\frac{m^2}{y^2}\right)R=0$$

where

$$\varepsilon=\frac{E}{\hbar\omega}$$

As with the solution of other differential equations, the procedure to follow is to extract out the asymptotic behavior as $y \to 0, \infty$ and solve the equation for the remaining function by recognizing the well-known equation that results.

As $y \to \infty$ the dominant term will be y^2 and the equation for this behavior is

$$\frac{d^2R}{dy^2}-y^2R=0$$

which has a solution $R \to e^{-y^2/2}$.

As $y \to 0$ the dominant term will be $1/y^2$ and the equation for this behavior is

$$\frac{d^2R}{dy^2} - \frac{m^2}{y^2}R = 0$$

which has a solution $R \to y^{|m|}$, where we have excluded any negative powers since that solution would diverge at $y = 0$.

Therefore we assume $R = y^{|m|}e^{-y^2/2}G(y)$.

Substitution gives the equation for G as

$$\frac{d^2G}{dy^2} + \left(\frac{2|m|+1}{y} - 2y\right)\frac{dG}{dy} + (\varepsilon - 2 - 2|m|)\,G = 0$$

Changing the variable again to $z = y^2$ we have

$$\frac{d^2G}{dz^2} + \left(\frac{|m|+1}{z} - 1\right)\frac{dG}{dz} + \left(\frac{\varepsilon - 2(|m|+1)}{4z}\right)G = 0$$

If we are clever, we recognize this as Laguerre's equation.

If not, we make a series solution substitution

$$G(z) = \sum_{s=0}^{\infty} b_s z^s$$

which gives the recursion relation

$$\frac{b_{s+1}}{b_s} = \frac{s + \frac{|m|+1}{2} - \frac{\varepsilon}{4}}{(s+1)(s+|m|+1)} \to \frac{1}{s} \text{ for large } s$$

This says that unless the series terminates (becomes a polynomial in z) it will behave like $e^z = e^{y^2}$ which implies that the solution for $R(y)$ will diverge for large y and thus, not be normalizable.

If we choose the maximum s-value to be $s_{max} = n_r$, then we can terminate the series by choosing

$$\varepsilon = 2|m| + 2 + 4n_r$$

which then gives us the allowed energy eigenvalues

$$E_{n_r,m} = \hbar\omega(|m| + 2n_r + 1)$$

The polynomial solutions are the generalized Laguerre polynomials $L^{|m|}(z)$.

The first few Laguerre polynomials are

$$L_0^k(z) = 1 \quad , \quad L_1^k(z) = 1 + k - z$$

$$L_2^k(z) = \frac{1}{2}(2 + 3k + k^2 - 2z(k+2) + z^2)$$

The full wave function is

$$\psi_{n_r,m}(r,\varphi) = r^{|m|} e^{-\frac{r^2}{2\rho^2}} L_{n_r}^{|m|}\left(\frac{r^2}{\rho^2}\right) e^{im\varphi}$$

and the energy level structure is shown in the Table.

which is the same structure (with different labels) as in the operator solution.

$E/\hbar\omega$	n_r	m	degeneracy
1	0	0	1
2	0	+1	2
2	0	-1	
3	0	+2	3
3	1	0	
3	0	-2	
4	0	+3	4
4	1	+1	
4	1	-1	
4	0	-3	

Energy Levels - 2D Oscillator

The fact that $\Delta m = 2$ in the 2-dimensional case is one of many peculiarities associated with two dimensions that does not appear three dimensions.

What happens in 3 dimensions?

In Cartesian coordinates we have a simple extension of the 2-dimensional case.

$$E = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right) = \hbar\omega\left(n + \frac{3}{2}\right)$$

The degeneracy is $$\frac{(n+1)(n+2)}{2}$$

The energy level structure is shown in the Table.

$E/\hbar\omega$	n_x	n_y	n_z	n	degeneracy
3/2	0	0	0	0	1
5/2	1	0	0	1	3
5/2	0	1	0	1	
5/2	0	0	1	1	
7/2	2	0	0	2	6
7/2	0	2	0	2	
7/2	0	0	2	2	
7/2	1	1	0	2	
7/2	1	0	1	2	
7/2	0	1	1	2	

Energy Levels - 3D Oscillator

In spherical-polar coordinates, we can follow a procedure similar to the plane- polar 2-dimensional case to get

$$\psi_{n_r,\ell,m}(y,\theta,\varphi) = y^{\ell} e^{-\frac{y^2}{2}} L_{n_r}^{\ell+\frac{1}{2}}(y^2) Y_{\ell m}(\theta,\varphi)$$

where

$$r = \rho y \quad , \quad \rho^2 = \frac{\hbar^2}{M\omega}$$

The corresponding energy values are

$$E_{n_r,\ell} = \hbar\omega(2n_r + \ell + \frac{3}{2})$$

which gives the Table.

$E/\hbar\omega$	n_r	ℓ	$n = 2n_r + \ell$	degeneracy
3/2	0	0	0	1
5/2	0	1	1	3 → m=± 1,0
7/2	1 or 0	0 or 2	2	6 → m=± 2, ± 1

Energy Levels - 3D Oscillator

The 3-Dimensional Delta Function

We now consider a particle is moving in 3-dimensions under the action of the attractive delta function potential given by

$$V(r) = -\frac{\hbar^2}{2M\alpha}\delta(r-a)$$

Since this is a central force we know that we can write the solutions in the form

$$\psi(r,\theta,\varphi) = R(r)Y_{\ell m}(\theta,\varphi)$$

The Schrodinger equation is

$$-\frac{\hbar^2}{2M}\left(\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{\ell(\ell+1)}{r^2}R\right)-\frac{\hbar^2}{2M\alpha}\delta(r-a)R-\frac{\hbar^2k^2}{2M}R=0$$

where, since we are looking for bound states, we have set

$$E = -\frac{\hbar^2k^2}{2M} < 0$$

Now the function $R(r)$ must be continuous everywhere.

But as we saw earlier in the 1-dimensional case, the derivative of R is not continuous for delta functions.

The discontinuity at $r = a$ is found by integrating the radial equation around the point $r = a$.

$$-\frac{\hbar^2}{2M}\int_{a^-}^{a^+} r^2dr\left(\frac{d^2R(r)}{dr^2}+\frac{2}{r}\frac{dR(r)}{dr}-\frac{\ell(\ell+1)}{r^2}R(r)\right)$$

$$-\frac{\hbar^2}{2M\alpha}\int_{a^-}^{a^+} r^2dr\delta(r-a)R(r)-\frac{\hbar^2k^2}{2M}\int_{a^-}^{a^+} r^2drR(r)=0$$

which gives the second boundary (continuity) condition

$$\alpha\left[\frac{dR(a^+)}{dr}-\frac{dR(a^-)}{dr}\right]=-R(a)$$

For $r>a$ and $r<a$ we then have the equation

$$-\frac{\hbar^2}{2M}\left(\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{\ell(\ell+1)}{r^2}R\right)-\frac{\hbar^2k^2}{2M}R=0$$

which has as a solution for the case $\ell=0$

$$R(r)=\frac{1}{r}(Ae^{-kr}+Be^{kr})$$

For $R(r)$ to be well behaved at $r=0$ we must choose $B=-A$.

Therefore, the solution for $r<a$ is

$$R(r)=\frac{c}{r}\sinh kr$$

For $R(r)$ to be well behaved as $r\to\infty$ we must choose $B=0$.

Therefore the solution for $r>a$ is

$$R(r)=\frac{b}{r}e^{-kr}$$

The boundary conditions at $r=a$ then give the equations

$$\frac{c}{a}\sinh ka=\frac{b}{a}e^{-ka}\rightarrow c\sinh ka=be^{-ka}$$

and

$$0=-k\alpha(be^{-ka}+c\cosh ka)+c\sinh ka$$

Eliminating b and c we get a transcendental equation for k (or E)

$$\frac{\alpha}{a} = \frac{1 - e^{-2ka}}{2ka}$$

The right-hand side of this equation has a range

$$0 < \frac{1 - e^{-2ka}}{2ka} < 1$$

Therefore, the allowed range of the parameter α, in order that an $\ell = 0$ bound state exist, is $0 < \alpha < a$.

The Hydrogen Atom

Schrodinger Equation Solution

The potential energy function $V(r) = -\frac{Ze^2}{r}$

represents the attractive Coulomb interaction between an atomic nucleus of charge $+Ze$ and an electron of charge $-e$.

The Schrodinger equation we have been using describes the motion of a single particle in an external field.

In the hydrogen atom, however, we are interested in the motion of two particles (nucleus and electron) that are attracted to each other via the potential above (where r is the separation distance between the two particles).

We start by writing the Schrodinger equation for the two particle system.

It involves six coordinates (three for each particle).

We use Cartesian coordinates to start the discussion.

We have

$$\hat{H} = \frac{\vec{p}_{1,op}^{\,2}}{2m_1} + \frac{\vec{p}_{2,op}^{\,2}}{2m_2} + V(\vec{r}) \quad where \quad \vec{r} = \vec{r}_1 - \vec{r}_2$$

which gives

$$-\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2}\right)\phi(x_1, y_1, z_1, x_2, y_2, z_2)$$
$$-\frac{\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}\right)\phi(x_1, y_1, z_1, x_2, y_2, z_2)$$
$$+ V(x_1 - x_2, y_1 - y_2, z_1 - z_2)\phi(x_1, y_1, z_1, x_2, y_2, z_2)$$
$$= E\phi(x_1, y_1, z_1, x_2, y_2, z_2)$$

We now introduce relative and center-of-mass(CM) coordinates by

$$x = x_1 - x_2 \quad , \quad y = y_1 - y_2 \quad , \quad z = z_1 - z_2$$
$$\vec{r} = (x, y, z)$$
$$MX = m_1 x_1 + m_2 x_2 \quad , \quad M\mathrm{Y} = m_1 y_1 + m_2 y_2 \quad , \quad M\mathrm{Z} = m_1 z_1 + m_2 z_2$$
$$\vec{R} = (X, Y, Z)$$
$$M = m_1 + m_2 = \text{ total mass of the system}$$

Substitution gives

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right)\phi(x, y, z, X, Y, Z)$$
$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\phi(x, y, z, X, Y, Z)$$
$$+ V(x, y, z)\phi(x, y, z, X, Y, Z) = E\phi(x, y, z, X, Y, Z)$$

where

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \text{ the reduced mass}$$

We can now separate the variables by assuming a solution of the form

$$\phi(x, y, z, X, Y, Z) = \psi(x, y, z)\Psi(X, Y, Z)$$

which gives the two equations

$$-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{r}}\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r})$$

$$-\frac{\hbar^2}{2M}\nabla^2_{\vec{R}}\Psi(\vec{R}) = E'\Psi(\vec{R})$$

The second equation says that the CM of the two particles is like a free particle of mass M.

The first equation describes the relative motion of the two particles and is the same as the equation of motion of a particle of mass μ in an external potential energy $V(r)$.

In the hydrogen atom problem we are only interested in the energy levels E associated with the relative motion.

In addition, since the nuclear mass is so much larger than the electron mass, we have

$$\mu \approx m_e = m_{electron}$$

This is a central force so we assume a solution of the form

$$\psi(\vec{r}) = R(r)Y_{\ell m}(\theta, \varphi)$$

and obtain the radial equation

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{Ze^2}{r}R + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}R = ER$$

where $E < 0$ for a bound state.

We follow the same approach as before.

We change the variables so that the equation is in dimensionless form by introducing $\varrho = \alpha r$ where

$$\alpha^2 = \frac{8\mu|E|}{\hbar^2} \quad and \quad \lambda = \frac{2\mu Z e^2}{\alpha\hbar^2} = \frac{Ze^2}{\hbar}\left(\frac{\mu}{2|E|}\right)^{1/2}$$

We get

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{dr}\rho\right) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{\ell(\ell+1)}{\rho^2}\right)R = 0$$

For $\varrho \to \infty$ the equation becomes

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{dr}\rho\right) - \frac{1}{4}R = 0$$

which has the solution

$$R \to \rho^n e^{\pm\frac{1}{2}\rho}$$

where n can have any finite value.

Since we want a normalizable solution, we will look for a solution of the form

$$R \to F(\rho)e^{-\frac{1}{2}\rho}$$

Substitution gives an equation for F

$$\frac{d^2F}{d\rho^2} + \left(\frac{2}{\rho} - 1\right)\frac{dF}{d\rho} + \left[\frac{\lambda - 1}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]F = 0$$

We solve this equation (it is Laguerre's equation) by series substitution.

$$F(\rho) = \rho^s (a_0 + a_1\rho + a_2\rho^2 + \ldots.) = \rho^s L(\rho)$$

where $a_0 \neq 0$ and $s \geq 0$.

We must also have that $F(0)$ is finite.

Substitution gives an equation for L.

$$\rho^2 \frac{d^2L}{d\rho^2} + \rho\left[2(s+1) - \rho\right]\frac{dL}{d\rho} + \left[\rho(\lambda - s - 1) + s(s+1) - \ell(\ell+1)\right]L = 0$$

If we set $\varrho = 0$ in this equation and use the fact that L is a power series we get the condition

$$s(s+1) - \ell(\ell+1) = 0$$

or

$$s = \ell \text{ or } s = -(\ell+1)$$

Since R must be finite at the origin we exclude the second possibility and choose $s = \ell$.

This gives

$$\rho^2 \frac{d^2L}{d\rho^2} + \rho\left[2(\ell+1) - \rho\right]\frac{dL}{d\rho} + \left[\rho(\lambda - \ell - 1)\right]L = 0$$

Substituting the power series gives a recursion relation for the coefficients

$$a_{\nu+1} = \frac{\nu + \ell + 1 - \lambda}{(\nu+1)(\nu+2\ell+2)} a_\nu$$

If the series does not terminate, then this recursion relation behaves like

$$\frac{a_{\nu+1}}{a_\nu} \to \frac{1}{\nu}$$

for large ν.

This corresponds to the series for $\varrho^n e^{\varrho}$.

Since this will give a non-normalizable result, we must terminate the series by choosing

$$\lambda = n = \text{ positive integer } = n' + \ell + 1 = \text{ total quantum number}$$

where n' (= radial quantum number) is the largest power of ϱ in the solution L.

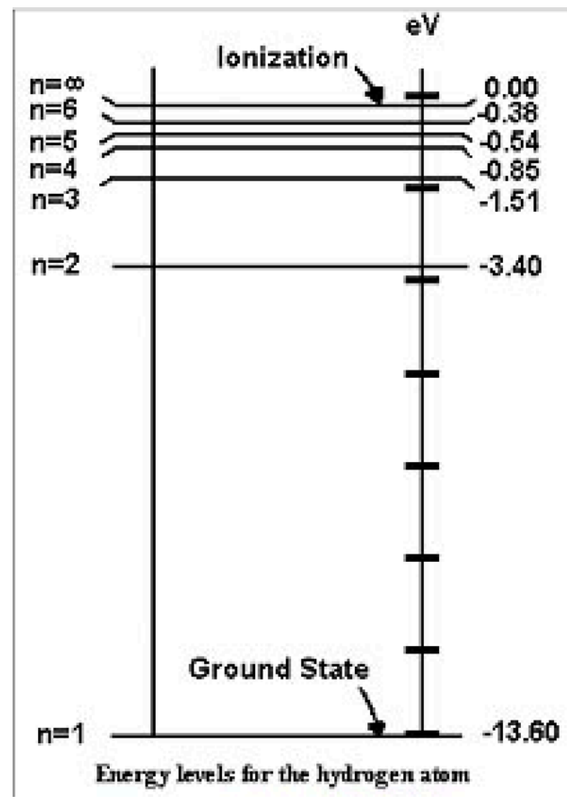
n' and n are non-negative integers, $n = 1,2,3,4,...$

We thus obtain the solution for the energies

$$E_n = -|E_n| = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2} = -\frac{Z^2 e^2}{2a_0 n^2}$$

where

$$a_0 = \text{ Bohr radius } = \frac{\hbar^2}{\mu e^2}$$



Energy levels for the hydrogen atom

Unlike the finite square well, where we had a finite number of bound state levels, in this case, we obtain an infinite set of discrete energies.

This results from the very slow decrease of the Coulomb potential energy with distance.

The Laguerre polynomial solutions are given by the generating function

$$G(\rho, s) = \frac{e^{-\frac{\rho s}{1-s}}}{1-s} = \sum_{q=0}^{\infty} \frac{L_q(\rho)}{q!} s^q \quad , \quad s < 1$$

By differentiating the generating function with respect to ϱ and s we can show that

$$\frac{dL_q}{d\rho} - q\frac{dL_{q-1}}{d\rho} = -qL_{q-1}$$

$$L_{q+1} = (2q + 1 - \rho)L_q - q^2 L_{q-1}$$

The lowest order differential equation involving only L_q that can be constructed from these two equations is

$$\rho\frac{d^2L_q}{d\rho^2}+(1-\rho)\frac{dL_q}{d\rho}+qL_q=0$$

This is not quite our original equation.

However, if we define the associated Laguerre polynomials by

$$L_q^p(\rho)=\frac{d^p}{d\rho^p}L_q(\rho)$$

then differentiating the differential equation p times we get

$$\rho\frac{d^2L_q^p}{d\rho^2}+(p+1-\rho)\frac{dL_q^p}{d\rho}+(q-p)L_q^p=0$$

Setting $\lambda = n$ we then see that the solutions to the Schrodinger equation are

$$L_{n+\ell}^{2\ell+1}(\rho)$$

which are polynomials of order $(n+\ell)-(2\ell+1)=n-\ell-1$ in agreement with the earlier results.

We can differentiate the generating function p times to get

$$G_p(\rho,s)=\frac{(-s)^p e^{-\frac{\rho s}{1-s}}}{(1-s)^{p+1}}=\sum_{q=0}^{\infty}\frac{L_q^p(\rho)}{q!}s^q \quad , \quad s<1$$

Explicitly, we then have

$$L_{n+\ell}^{2\ell+1}(\rho)=\sum_{k=0}^{n-\ell-1}(-1)^{k+1}\frac{[(n+\ell)!]^2\rho^k}{(n-\ell-1-k)!(2\ell+1+k)!k!}$$

The normalized radial wave functions are of the form

$$R_{n\ell}(\rho) = -\left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n\left[(n+\ell)!\right]^3}\right\}^{1/2} e^{-\frac{1}{2}\rho}\rho^{\ell} L_{n+\ell}^{2\ell+1}(\rho)$$

with

$$a_0 = \frac{\hbar^2}{\mu e^2} \text{ and } \rho = \frac{2Z}{na_0} r$$

and

$$\psi_{n\ell m}(r,\theta,\varphi) = R_{n\ell}(r) Y_{\ell m}(\theta,\varphi)$$

The first few radial wave functions are

$$R_{10}(r) = \left(\frac{Z}{a_0}\right)^{3/2} 2e^{-\frac{Zr}{a_0}}$$

$$R_{20}(r) = \left(\frac{Z}{2a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}}$$

$$R_{21}(r) = \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0\sqrt{3}} e^{-\frac{Zr}{2a_0}}$$

What about degeneracy since the energy values do not depend on ℓ and m?

For each value of n, ℓ can vary between 0 and $n-1$, and for each value of these ℓ values m can vary between $-\ell$ and ℓ ($2\ell + 1$ values).

Therefore the total degeneracy of an energy level E_n is given by

$$\sum_{\ell=0}^{n-1} (2\ell+1) = 2\frac{n(n-1)}{2} + n = n^2$$

The degeneracy with respect to *m* is true for any central force (as we have seen in other examples).

The ℓ degeneracy, however, is characteristic of the Coulomb potential alone.

It is called an *accidental degeneracy*.

Some useful expectation values are:

$$\langle r\rangle_{n\ell m} = \frac{a_0}{2Z}\left[3n^2 - \ell(\ell+1)\right] \qquad \left\langle \frac{1}{r}\right\rangle_{n\ell m} = \frac{Z}{a_0 n^2}$$

$$\left\langle \frac{1}{r^2}\right\rangle_{n\ell m} = \frac{Z^2}{a_0^2 n^3(\ell+\frac{1}{2})} \qquad \left\langle \frac{1}{r^3}\right\rangle_{n\ell m} = \frac{Z^3}{a_0^3 n^3 \ell(\ell+\frac{1}{2})(\ell+1)}$$

Algebraic Solution of the Hydrogen Atom

Review of the Classical Kepler Problem

In the classical Kepler problem of an electron of charge -*e* moving in the electric force field of a positive charge *Ze* located at the origin, the angular momentum

$$\vec{L} = \vec{r} \times \vec{p}$$

is constant.

The motion takes place in a plane perpendicular to the constant angular momentum direction.

Newton's second law tells us that the rate of change of the momentum is equal to the force

$$\frac{d\vec{p}}{dt} = -\frac{Ze^2}{r^2}\hat{r} \text{ where } r = |\vec{r}| \text{ and } \hat{r} = \frac{\vec{r}}{r} = \text{ unit vector}$$

The so-called Runge-Lenz vector is defined by

$$\vec{A} = \frac{1}{Ze^2 m}(\vec{L} \times \vec{p}) + \hat{r}$$

If we take its time derivative we find

$$\frac{d\vec{L}}{dt} = 0 \text{ and } \vec{L} = m\vec{r} \times \frac{d\vec{r}}{dt} = mr^2\hat{r} \times \frac{d\hat{r}}{dt} + mr(\hat{r} \times \hat{r})\frac{dr}{dt} = mr^2\hat{r} \times \frac{d\hat{r}}{dt}$$

$$\frac{d\vec{A}}{dt} = \frac{1}{Ze^2m}(\vec{L} \times \frac{d\vec{p}}{dt} + \frac{d\vec{L}}{dt} \times \vec{p}) + \frac{d\hat{r}}{dt} = \frac{1}{Ze^2m}(\vec{L} \times \frac{d\vec{p}}{dt}) + \frac{d\hat{r}}{dt}$$

$$= -\frac{1}{m}(\vec{L} \times \frac{\hat{r}}{r^2}) + \frac{d\hat{r}}{dt} = -(\hat{r} \times \frac{d\hat{r}}{dt}) \times \hat{r} + \frac{d\hat{r}}{dt}$$

$$= -(\frac{d\hat{r}}{dt}(\hat{r} \cdot \hat{r}) - (\hat{r} \cdot \frac{d\hat{r}}{dt})) + \frac{d\hat{r}}{dt} = -\frac{d\hat{r}}{dt} + \frac{d(\hat{r} \cdot \hat{r})}{dt} + \frac{d\hat{r}}{dt} = 0$$

Thus, the vector $\vec{A}$ is a constant of the motion.

It corresponds physically to the length and direction of the fixed semi-major axis of the classical elliptical orbit.

The equation of the elliptical orbit is easily found using the $\vec{A}$ vector.

$$\vec{A} \cdot \vec{r} = ar\cos\theta = \frac{1}{Ze^2m}(\vec{L} \times \vec{p}) \cdot \vec{r} + \hat{r} \cdot \vec{r}$$

$$= -\frac{1}{Ze^2m}\vec{L} \cdot (\vec{r} \times \vec{p}) + r$$

$$ar\cos\theta = -\frac{L^2}{Ze^2m} + r$$

$$\rightarrow \frac{1}{\mathrm{r}} = \frac{Ze^2m}{L^2}(1 - a\cos\theta) \rightarrow \text{ orbit equation (conic sections)}$$

where

$$a = |\vec{A}|$$

= eccentricity and the direction of $\vec{A}$ is from the origin to the aphelion

The Quantum Mechanical Problem

In order to make this useful in quantum mechanics, the classical Runge-Lenz vector must be generalized.

In classical physics

$$\vec{L} \times \vec{p} = -\vec{p} \times \vec{L}$$

In quantum mechanics, this identity is not valid since the components of $\vec{L}_{op}$ do not commute.

The correct quantum mechanical generalization (remember it must be a Hermitian operator if it is a physical observable) of the vector $\vec{A}$ is

$$\vec{A}_{op} = \frac{1}{2Ze^2m}(\vec{L}_{op} \times \vec{p}_{op} - \vec{p}_{op} \times \vec{L}_{op}) + \left(\frac{\vec{r}}{r}\right)_{op}$$

This satisfies $[\hat{H}, \vec{A}_{op}] = 0$, which says $\vec{A}$ is a constant.

It also satisfies $\vec{A}_{op} \cdot \vec{L}_{op} = 0$.

We can derive the following commutators:

$$[\hat{L}_i, \hat{A}_j] = i\hbar\varepsilon_{ijk}\hat{A}_k \quad , \quad [\hat{L}_i, \hat{p}_j] = i\hbar\varepsilon_{ijk}\hat{p}_k \quad , \quad [\hat{L}_i, \hat{r}_j] = i\hbar\varepsilon_{ijk}\hat{r}_k$$

which gives

$$\vec{A}_{op} = \frac{1}{2Ze^2m}(2\vec{L}_{op} \times \vec{p}_{op} + i\hbar\vec{p}_{op}) + \left(\frac{\vec{r}}{r}\right)_{op}$$

We now derive two important properties of $\vec{A}$.

The first property follows from the commutators

$$\left[\left(\vec{L}_{op}\times\vec{p}_{op}\right)_i,\hat{p}_j\right]+\left[\hat{p}_i,\left(\vec{L}_{op}\times\vec{p}_{op}\right)_j\right]=0$$

$$\left[\left(\vec{L}_{op}\times\vec{p}_{op}\right)_i,\left(\vec{L}_{op}\times\vec{p}_{op}\right)_j\right]=-i\hbar\varepsilon_{ijk}\hat{L}_k p^2=-i\hbar\varepsilon_{ijk}p^2\hat{L}_k$$

$$\left[\left(\vec{L}_{op}\times\vec{p}_{op}\right)_i,\frac{\hat{r}_j}{r}\right]+\left[\frac{\hat{r}_i}{r},\left(\vec{L}_{op}\times\vec{p}_{op}\right)_j\right]=2i\hbar\varepsilon_{ijk}\frac{\hat{L}_k}{r}$$

which leads to

$$\left[\hat{A}_i,\hat{A}_j\right]=i\hbar\left(\frac{-2\hat{H}}{Z^2e^4m}\right)\varepsilon_{ijk}\hat{L}_k$$

where

$$\hat{H}=\text{ Hamiltonian }=\frac{\vec{p}_{op}^{\,2}}{2m}-Ze^2\left(\frac{1}{r}\right)_{op}$$

The second property follows from the relations

$$(\vec{L}_{op}\times\vec{p}_{op})\cdot(\vec{L}_{op}\times\vec{p}_{op})=\vec{L}_{op}^2\vec{p}_{op}^2$$

$$\left(\frac{\vec{r}}{r}\right)_{op}\cdot(\vec{L}_{op}\times\vec{p}_{op})+(\vec{L}_{op}\times\vec{p}_{op})\cdot\left(\frac{\vec{r}}{r}\right)_{op}=-\frac{2\vec{L}_{op}^2}{r}+2i\hbar\left(\frac{\vec{r}}{r}\right)_{op}\cdot\vec{p}_{op}$$

$$\vec{p}_{op}\cdot\left(\frac{\vec{r}}{r}\right)_{op}=\left(\frac{\vec{r}}{r}\right)_{op}\cdot\vec{p}_{op}-2i\hbar\left(\frac{1}{r}\right)_{op}$$

$$\vec{p}_{op}\cdot\vec{L}_{op}=\vec{L}_{op}\cdot\vec{p}_{op}=0$$

$$\vec{p}_{op}\cdot(\vec{L}_{op}\times\vec{p}_{op})+(\vec{L}_{op}\times\vec{p}_{op})\cdot\vec{L}_{op}=2i\hbar\vec{p}_{op}^2$$

which lead to

$$\vec{A}_{op}^2=\vec{A}_{op}\cdot\vec{A}_{op}=1+\frac{2\hat{H}}{Z^2e^4m}(\vec{L}_{op}^2+\hbar^2)$$

We now define the two new operators (they are *ladder operators*) by

$$\vec{I}_{op}^{\pm} = \frac{1}{2}\left[\vec{L}_{op} \pm \left(-\frac{2\hat{H}}{Z^2 e^4 m}\right)^{1/2} \vec{A}_{op}\right]$$

Using the relations we have derived for $\left[\hat{A}_i, \hat{A}_j\right]$ and $\left[\hat{L}_i, \hat{A}_j\right]$ we have

$$\left[\vec{I}_{op}^{+}, \vec{I}_{op}^{-}\right] = 0$$

which means they have a common eigenbasis.

We also have

$$\left[\hat{I}_{op,i}^{\pm}, \hat{I}_{op,j}^{\pm}\right] = i\hbar\varepsilon_{ijk}\hat{I}_{op,k}^{\pm}$$

which are the standard angular momentum component commutation relations.

Since they each commute with $\hat{H}$, they also have a common eigenbasis with $\hat{H}$.

Therefore, we can find a set of states such that

$$(\vec{I}_{op}^{\pm})^2 |\psi\rangle = i_{\pm}(i_{\pm}+1)\hbar^2 |\psi\rangle \text{ and } \hat{H}|\psi\rangle = E|\psi\rangle$$

We can show that $(\vec{I}_{op}^{+})^2 = (\vec{I}_{op}^{-})^2$, which implies that $i_+ = i_-$.

We also have(as before)

$$i_+ = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, 3, \ldots$$

Since $\vec{A}_{op} \cdot \vec{L}_{op} = 0$ we get

$$2\left[(\vec{I}_{op}^{+})^2 + (\vec{I}_{op}^{-})^2\right] + \hbar^2 = -\frac{Z^2 e^4 m}{2\hat{H}}$$

$$\left[4i_+(i_+ + 1) + 1\right]\hbar^2 = -\frac{Z^2 e^4 m}{2E}$$

$$E = -\frac{Z^2 e^4 m}{2(2i_+ + 1)^2} = -\frac{Z^2 e^4 m}{2n^2}$$

where we have set $n = 2i_+ + 1 = 1,2,3,4,5,...$, which are the correct energy values for hydrogen.

While the energy depends only on the quantum number i_+ (or n) each state has a degeneracy depending on the number of z-component values for each i_+ value.

This is

$$(2i_+ + 1)(2i_- + 1) = (2i_+ + 1)^2 = n^2$$

which is the correct degeneracy.

The Deuteron

A deuteron is a bound state of a neutron and a proton.

We can consider this system as a single particle with reduced mass

$$\mu = \frac{m_{proton} m_{neutron}}{m_{proton} + m_{neutron}} \approx \frac{m_{proton}}{2} = \frac{m_p}{2}$$

moving in a fixed potential $V(r)$, where r is the proton-neutron separation.

As a first approximation, we assume that the nuclear interaction binding the proton and the neutron into a deuteron is a finite square well in 3–dimensions.

$$V(r) = \begin{cases} -V_0 & r < a \\ 0 & r \geq a \end{cases}$$

The physical properties of the deuteron system are:

1. Almost an $\ell = 0$ state (a small admixture of $\ell = 2$ is present). We will assume $\ell = 0$.

2. Only one bound state exists.

3. The depth and range of the potential is such that the deuteron is weakly bound. The energy level in the potential corresponds to the binding energy of the system, where

$$E = \text{ binding energy } = m_{deuteron}c^2 - (m_{proton} + m_{neutron})c^2 < 0 \quad (7.683)$$

Experimentally, it has been found that $E = -2.228\,MeV$.

4. By weakly bound we mean

$$\frac{|E|}{(m_{proton} + m_{neutron})c^2} << 1 \quad (7.684)$$

In fact, for the deuteron we have

$$\frac{|E|}{(m_{proton} + m_{neutron})c^2} \approx 0.001 \quad (7.685)$$

5. This system is so weakly bound that any small decrease in the radius of the well a or small reduction in the depth of the well V_0 would cause the system to break up (no bound state exists).

We derived the solutions for this potential earlier.

$$R(r) = Aj_0(\alpha r) \qquad r < a$$

$$R(r) = Bh_0^{(1)}(i\beta r) \qquad r \geq a$$

where

$$\alpha^2 = \frac{2m}{\hbar^2}(V_0 - |E|) \text{ and } \beta^2 = \frac{2m}{\hbar^2}|E|$$

The transcendental equation arising from matching boundary conditions at $r = a$ gave us the equations

$$\eta = -\xi \cot \xi \text{ and } \xi^2 + \eta^2 = \frac{2mV_0a^2}{\hbar^2}$$

where

$$\xi = \alpha a \text{ and } \eta = \beta a$$

The graphical solution as shown below in the Figure plots

$$\eta = -\xi \cot \xi \text{ and } \eta^2 = \frac{2mV_0a^2}{\hbar^2} - \xi^2 \text{ versus } \xi$$

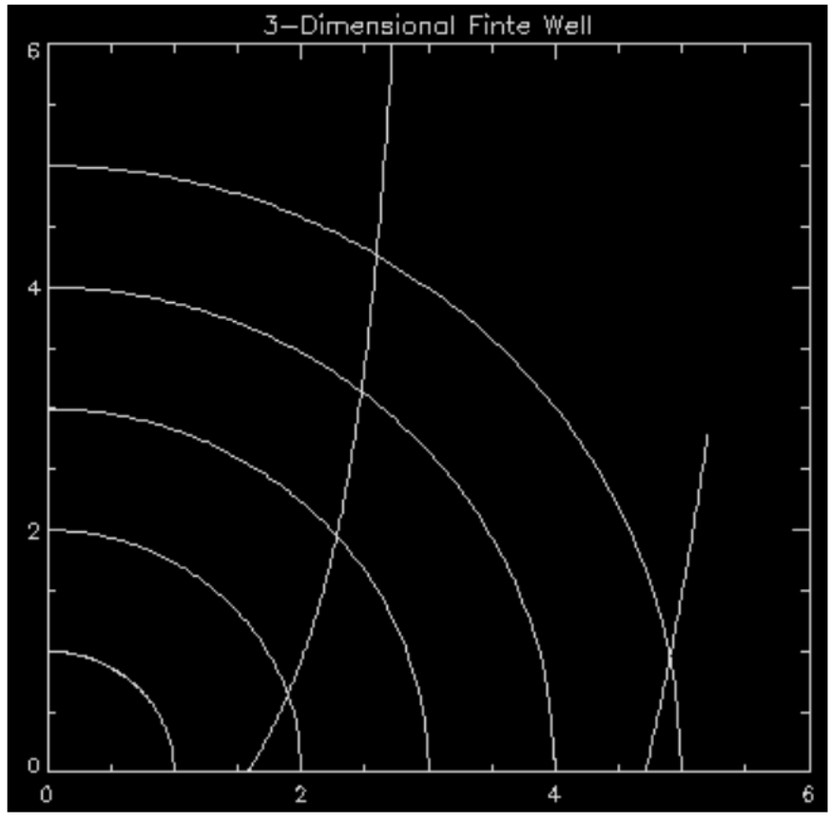
We found a finite number of bound states for given values of the well parameters.

In particular

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{\pi}{2}\right)^2 \rightarrow \text{ no solution}$$

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{3\pi}{2}\right)^2 \rightarrow \text{ 1 solution}$$

$$\frac{2mV_0a^2}{\hbar^2} < \left(\frac{5\pi}{2}\right)^2 \rightarrow \text{ 2 solutions}$$



Deuteron Solution

For the weakly bound deuteron system we expect that

$$\xi = \frac{\pi}{2} + \varepsilon \quad , \quad \varepsilon \ll \frac{\pi}{2}$$

i.e., the radius of the circle is barely large enough to get a single (weakly) bound state.
Substituting into the transcendental equation we get

$$\eta = -\left(\frac{\pi}{2}+\varepsilon\right)\cot\left(\frac{\pi}{2}+\varepsilon\right) = -\left(\frac{\pi}{2}+\varepsilon\right)\frac{\cos\left(\frac{\pi}{2}+\varepsilon\right)}{\sin\left(\frac{\pi}{2}+\varepsilon\right)}$$

$$= -\left(\frac{\pi}{2}+\varepsilon\right)\frac{\cos\left(\frac{\pi}{2}\right)\cos(\varepsilon) - \sin\left(\frac{\pi}{2}\right)\sin(\varepsilon)}{\sin\left(\frac{\pi}{2}\right)\cos(\varepsilon) + \cos\left(\frac{\pi}{2}\right)\sin(\varepsilon)}$$

$$\approx \left(\frac{\pi}{2}+\varepsilon\right)\frac{\sin(\varepsilon)}{\cos(\varepsilon)} \approx \left(\frac{\pi}{2}+\varepsilon\right)\frac{\varepsilon - \frac{\varepsilon^3}{6}}{1-\frac{\varepsilon^2}{2}} \approx \left(\frac{\pi}{2}+\varepsilon\right)\left(\varepsilon - \frac{\varepsilon^3}{6}\right)\left(1+\frac{\varepsilon^2}{2}\right)$$

$$\approx \frac{\pi}{2}\varepsilon + (1+\frac{\pi}{4})\varepsilon^2$$

Now substituting into the circle equation we get

$$\left(\frac{\pi}{2}+\varepsilon\right)^2 + \left(\frac{\pi}{2}\varepsilon + (1+\frac{\pi}{4})\varepsilon^2\right)^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\frac{\pi^2}{4} + \pi\varepsilon + \left(1+\frac{\pi^2}{4}\right)\varepsilon^2 \approx \frac{2mV_0a^2}{\hbar^2}$$

Dropping the small quadratic terms in ε we get

$$\varepsilon \approx \frac{2mV_0a^2}{\pi\hbar^2} - \frac{\pi}{4}$$

Therefore,

$$|E| = \frac{\hbar^2}{2ma^2}\eta^2 \approx \frac{\hbar^2\pi^2}{8ma^2}\left(\frac{2mV_0a^2}{\pi\hbar^2} - \frac{\pi}{4}\right)^2$$

A typical value for the range of the interaction is the order of 2 Fermi or $a \approx 2\times10^{-13}$ cm.

In order to get $|E| \approx 2.3$ MeV, we would need a well depth of $V_0 \approx 42$ M eV which is reasonable (according to experimentalists).

The Deuteron - Another Way

Experiment (scattering) indicates that instead of a square well (very unrealistic) the actual potential is of the form

$$V(r) = -Ae^{-\frac{r}{a}}$$

where

$$A \approx 32MeV \text{ and } a \approx 2.25x10^{-13}cm$$

We can solve for this potential ($\ell = 0$ case) exactly using this clever trick I first learned from Hans Bethe at Cornell University.

The radial equation in this case is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m}{\hbar^2}\left(Ae^{-\frac{r}{a}} - |E|\right)R = 0$$

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2m}{\hbar^2}\left(Ae^{-\frac{r}{a}} - |E|\right)R = 0$$

Now let

$$R(r) = \frac{\chi(r)}{r}$$

which implies that

$$\frac{dR}{dr} = \frac{d\left(\frac{\chi}{r}\right)}{dr} = \frac{1}{r}\frac{d\chi}{dr} - \frac{1}{r^2}\chi$$
$$\frac{d^2R}{dr^2} = -\frac{2}{r^2}\frac{d\chi}{dr} + \frac{1}{r}\frac{d^2\chi}{dr^2} + \frac{2}{r^3}\chi$$

Substitution gives

$$\frac{d^2\chi}{dr^2} + \frac{2m}{\hbar^2}\left(Ae^{-\frac{r}{a}} - |E|\right)\chi = 0$$

We now change the variables using

$$\xi = e^{-\frac{r}{2a}} \rightarrow \frac{d}{dr} = \frac{d\xi}{dr}\frac{d}{d\xi} = -\frac{\xi}{2a}\frac{d}{d\xi}$$
$$\frac{d^2}{dr^2} = \frac{d}{dr}\left(-\frac{\xi}{2a}\frac{d}{d\xi}\right) = \frac{d\xi}{dr}\frac{d}{d\xi}\left(-\frac{\xi}{2a}\frac{d}{d\xi}\right) = \left(\frac{\xi}{2a}\right)^2\frac{d^2}{d\xi^2} + \frac{\xi}{4a^2}\frac{d}{d\xi}$$

We then get the equation

$$\xi^2\frac{d^2\chi}{d\xi^2} + \xi\frac{d\chi}{d\xi} + ((\alpha a)^2\xi^2 - (ka)^2)\chi = 0$$

where

$$(\alpha a)^2 = \frac{2mA}{\hbar^2}a^2 \text{ and } (ka)^2 = \frac{2m|E|}{\hbar^2}a^2$$

Now Bessel's equation has the form

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - \nu^2)y = 0$$

Therefore, we have Bessel's equation with a general solution

$$\chi(r) = CJ_{ka}(\alpha a\xi) + BY_{ka}(\alpha a\xi)$$

$$R(r) = \frac{1}{r}(CJ_{ka}(\alpha a\xi) + BY_{ka}(\alpha a\xi))$$

As $r \to \infty$, $\xi = e^{-r} \to 0$, which implies we must choose **B** = 0 or the solution diverges.

As $r \to 0$, $\xi = e^{-r} \to 1$, which implies we must have

$$J_{ka}(\alpha a) = 0$$

or the solution diverges.

This is then the energy eigenvalue condition.

For the values of *A* and a given earlier we have

$$J_{ka}(6.28) = 0$$

and if we let $|E| = qA$, this becomes

$$J_{1/2}(6.28) = 0$$

Now

$$J_{6.4q}(6.28) = 0$$

Therefore we have

$$6.4q = \frac{1}{2} \to q = \frac{1}{12.8} \to |E| = qA = 2.34\,MeV$$

which is an excellent result for the bound state energy of the deuteron.

Linear Potential

We now consider a *linear* potential energy function given by

$$V(r) = \alpha r - V_0$$

The Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) - \frac{\vec{L}_{op}^2}{\hbar^2 r^2}\psi\right) + (\alpha r - V_0 - E)\psi = 0$$

Since it is a central potential, we can write

$$\psi = R(r)Y_{\ell m}(\theta, \varphi)$$

which implies

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R\right) + (\alpha r - V_0 - E)R = 0$$

If we let

$$\chi(r) = rR(r)$$

we get

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + (\alpha r - V_0 - E + \frac{\hbar^2\ell(\ell+1)}{2mr^2})\chi = 0$$

For $\ell > 0$ there is no closed form solution for this equation and numerical methods must be applied.

For $\ell = 0$, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + (\alpha r - V_0 - E)\chi = 0$$

Now we let

$$\xi = \left(r - \frac{E + V_0}{\alpha}\right)\left(\frac{2m\alpha}{\hbar^2}\right)^{1/3}$$

which implies that

$$\frac{d}{dr} = \frac{d\xi}{dr}\frac{d}{d\xi} = \left(\frac{2m\alpha}{\hbar^2}\right)^{1/3}\frac{d}{d\xi}$$

$$\frac{d^2}{dr^2} = \frac{d}{dr}\left(\frac{d\xi}{dr}\frac{d}{d\xi}\right) = \frac{d\xi}{dr}\frac{d}{d\xi}\left(\left(\frac{2m\alpha}{\hbar^2}\right)^{1/3}\frac{d}{d\xi}\right)$$

$$= \left(\frac{2m\alpha}{\hbar^2}\right)^{2/3}\frac{d^2}{d\xi^2}$$

We then get the equation

$$\frac{d^2\chi}{d\xi^2} - \xi\chi = 0$$

This equation is *not as simple* as it looks.

Let us try a series solution of the form

$$\chi(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$$

Substitution gives the relations

$$a_2 = 0 \text{ and } a_{m+2} = \frac{a_{m-1}}{(m+2)(m+1)}$$

The solution that goes to zero as $\xi \to \pm\infty$ is then of the form

$$\chi(\xi) = c_1 f(\xi) - c_2 g(\xi) = CAi(\xi) = \text{ Airy function}$$

where

$$f(x) = 1 + \frac{1}{3!}x^3 + \frac{1\cdot 4}{6!}x^6 + \frac{1\cdot 4\cdot 7}{9!}x^9 + \ldots$$

$$g(x) = x + \frac{2}{4!}x^4 + \frac{2\cdot 5}{7!}x^7 + \frac{2\cdot 5\cdot 8}{10!}x^{10} + \ldots$$

Now to insure that the wave function is normalizable we must also have

$$\chi(\xi(r=0))=0$$

$$Ai\left(-\frac{E+V_0}{\alpha}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/3}\right)=0$$

This says that

$$-\frac{E_n+V_0}{\alpha}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/3}=z_n=n^{th} \text{ zero of } Ai(\xi)$$

Thus, the allowed energies are given by

$$E_n=-z_n\left(\frac{\hbar^2\alpha^2}{2m}\right)^{1/3}-V_0$$

The first three zeroes are

$$z_1=-2.3381 \quad , \quad z_2=-4.0879 \quad , \quad z_3=-5.5209$$

Programming the numerical method we described in the book for solving the Schrodinger equation allows us to determine *E* values where for simplicity, we have chosen $\hbar = m = \alpha = V_0 = 1$ which gives the $\ell = 0$ energies as

$$E_n=-z_n\left(\frac{1}{2}\right)^{1/3}-1=-0.794z_n-1$$

The general ℓ equation is (in this case)

$$\frac{d^2\chi}{dr^2}-2(r-1-E+\frac{\ell(\ell+1)}{2r^2})\chi=0$$

For $\ell = 0$ we theoretically expect the first three energy values 0.856, 2.246 and 3.384 and the program produces the values 0.855750, 2.24460, 3.38160 which is good agreement.

We now use the linear potential to look at quark-quark bound states at low energies.

Modified Linear Potential and Quark Bound States

Over the past several decades the quark model of elementary particles has had many successes.

Some experimental results are the following:

1. Free (isolated) quarks have never been observed.
2. At small quark separations *color charge* exhibits behavior similar to that of ordinary charge.
3. Quark-Antiquark pairs form bound states.

We can explain some of the features of these experimental results by describing the quark-quark force by an effective potential of the form

$$V(r) = -\frac{A}{r} + Br$$

and using non-relativistic quantum mechanics.

The linear term corresponds to a long-range confining potential that is responsible for the fact that free, isolated quarks have not been observed.

In simple terms, a linear potential of this type means that it costs more and more energy as one of the quarks in a bound system attempts to separate from the other quark.

When this extra energy is twice the rest energy of a quark, a new quark-antiquark pair can be produced.

So instead of the quark getting free, one of the newly created quarks joins with one of the original quarks to recreate the bound pair (so it looks like nothing has happened) and the other new quark binds with the quark attempting to get free into a new meson.

We never see a free quark!

A lot of energy has been expended, but the outcome is the creation of a meson rather than the appearance of free quarks.

The other term, which resembles a Coulomb potential, reflects the fact that at small separations the so-called "color charge" forces behave like ordinary charge forces.

The original observations of quark-quark bound states was in 1974.

The experiments involved bound states of charmed quarks called charmonium (named after the similar bound states of electrons and positrons called positronium).

The observed bound-state energy levels were as shown in the Table:

n	ℓ	$E(GeV)$
1	0	3.097
2	1	3.492
2	0	3.686
3	0	4.105
4	0	4.414

Observed Bound-State Energy Levels

The Schrodinger equation for this potential becomes

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right)-\frac{\vec{L}_{op}^2}{\hbar^2 r^2}\psi\right)+(V(r)-E)\psi=0$$

Since it is a central potential, we can write

$$\psi = R(r)Y_{\ell m}(\theta,\varphi)$$

which implies

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{\ell(\ell+1)}{r^2}R\right)+(V(r)-E)R=0$$

If we let

$$\chi(r)=rR(r)$$

we get

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2}+(V(r)-E+\frac{\hbar^2\ell(\ell+1)}{2mr^2})\chi=0$$

or

$$\frac{d^2\chi}{dr^2}-(aE-\frac{\ell(\ell+1)}{r^2}+\frac{b}{r}-cr)\chi=0$$

We must solve this system numerically.

The same program as earlier works again with a modified potential function.

The results for a set of parameters (a = 0.0385, b = 2.026, c = 34.65) chosen to get the right relationship between the levels are shown in the Table:

n	ℓ	$E(calculated)$	$E(rescaled)$
1	0	656	3.1
2	1	838	3.4
2	0	1160	3.6
3	0	1568	4.1
4	0	1916	4.4

Quark Model-Numerical Results

which is a reasonably good result and indicates that validity of the model.

The rescaled values are adjusted to correspond to the earlier table.

A more exact parameter search produces almost exact agreement.

7-39. Extra(Hidden) Dimensions - and now for something completely different!!

Lorentz Invariance with Extra Dimensions

If string theory is correct, we must entertain the possibility that space-time has more than four dimensions. The number of time dimensions must be kept equal to one - it seems very difficult, if not altogether impossible, to construct a consistent theory with more than one time dimension. The extra dimensions must therefore be spatial.

Can we have Lorentz invariance in worlds with more than three spatial dimensions? The answer is yes. Lorentz invariance is a concept that admits a very natural generalization to space-times with additional dimensions.

We first extend the definition of the invariant interval ds^2 to incorporate the additional space dimensions. In a world of five spatial dimensions, for example, we would write

$$ds^2 = c^2dt^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 - (dx^4)^2 - (dx^5)^2$$

Lorentz transformations are then defined as the linear changes of coordinates that leave ds^2 invariant. This ensures that every inertial observer in the six-dimensional space-time will agree on the value of the speed of light. With more dimensions, come more Lorentz transformations. While in four-dimensional space-time we have boosts in the x^1, x^2 and x^3 directions, in this new world we have boosts along each of the five spatial dimensions. With three spatial coordinates, there are three basic spatial rotations - rotations that mix x^1 and x^2, rotations that mix x^1 and x^3, and finally rotations that mix x^2 and x^3. The equality of the number of boosts and the number of rotations is a special feature of four-dimensional space-time. With five spatial coordinates, we have ten rotations, which is twice the number of boosts.

The higher-dimensional Lorentz invariance includes the lower-dimensional one. If nothing happens along the extra dimensions, then the restrictions of lower-dimensional Lorentz invariance apply. For motion that does not involve the extra dimensions, $dx^4 = dx^5 = 0$, and the expression for ds^2 reduces to that used in four dimensions.

Compact Extra Dimensions

It is possible for additional spatial dimensions to be undetected by low energy experiments if the dimensions are curled up into a compact space of small volume. At this point let us first try to understand what a compact dimension is. We will focus mainly on the case of one dimension. Later we will explain why small compact dimensions are hard to detect.

Consider a one-dimensional world, an infinite line, say, and let x be a coordinate along this line. For each point P along the line, there is a unique real number $x(P)$ called the $x-$coordinate of the point P. A good coordinate on this infinite line satisfies two conditions:

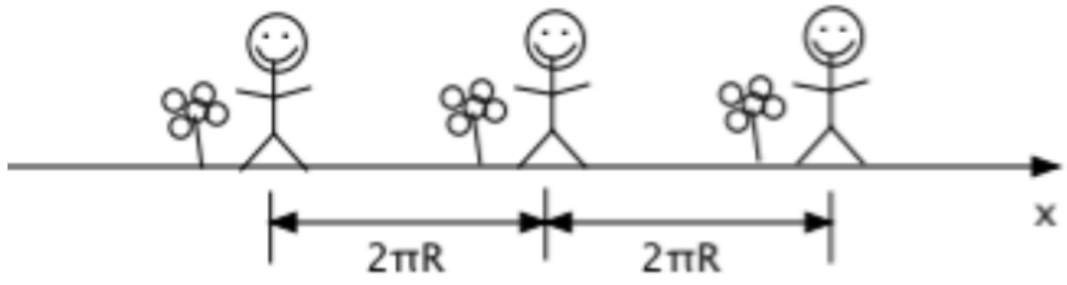
(1) Any two distinct points $P_1 \neq P_2$ have different coordinates $x(P_1) \neq x(P_2)$.

(2) The assignment of coordinates to points are continuous - nearby points have nearly equal coordinates.

If a choice of origin is made for this infinite line, then we can use distance from the origin to define a good coordinate. The coordinate assigned to each point is the distance from that point to the origin, with sign depending upon which side of the origin the point lies.

Imagine you live in a world with one spatial dimension. Suppose you are walking along and notice a strange pattern - the scenery repeats each time you move a distance $2\pi R$ for some value of R. If you meet your friend Phil, you see that there are Phil clones at distances $2\pi R$, $4\pi R$, $6\pi R$, ... down the line as shown in Figure below.

Multiple friends



In fact, there are clones up the line, as well, with the same spacing.

There is no way to distinguish an infinite line with such properties from a circle with circumference $2\pi R$. Indeed, saying that this strange line is a circle *explains* the peculiar property - there really are no Phil clones - you meet the same Phil again and again as you go around the circle!

How do we express this mathematically? We can think of the circle as an open line with an identification, that is, we declare that points with coordinates that differ by $2\pi R$ are the same point. More precisely, two points are declared to be the same point if their coordinates differ by an integer number of $2\pi R$:

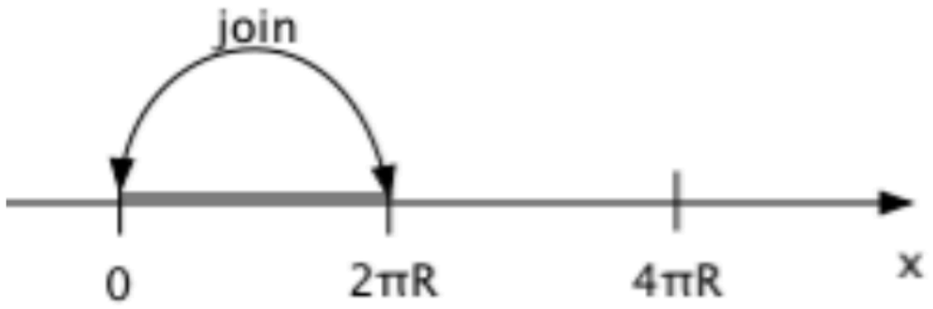
$$P_1 \sim P_2 \leftrightarrow x(P_1) = x(P_2) + 2\pi R n \quad , \quad n \in \mathrm{Z}$$

This is precise, but somewhat cumbersome, notation. With no risk of confusion, we can simply write

$$x \sim x + 2\pi R$$

which should be read as *identify any two points whose coordinates differ by* $2\pi R$. With such an identification, the open line becomes a circle. The identification has turned a non-compact dimension into a compact one. It may seem to you that a line with identifications is only a complicated way to think about a circle. We will see, however, that many physical problems become clearer when we view a compact dimension as an extended one with identifications.

The interval $0 \leq x \leq 2\pi R$ is a *fundamental domain* for the identification as shown in Figure below.



Fundamental domain

A fundamental domain is a subset of the entire space that satisfies two conditions:

(1) no two points . . are identified

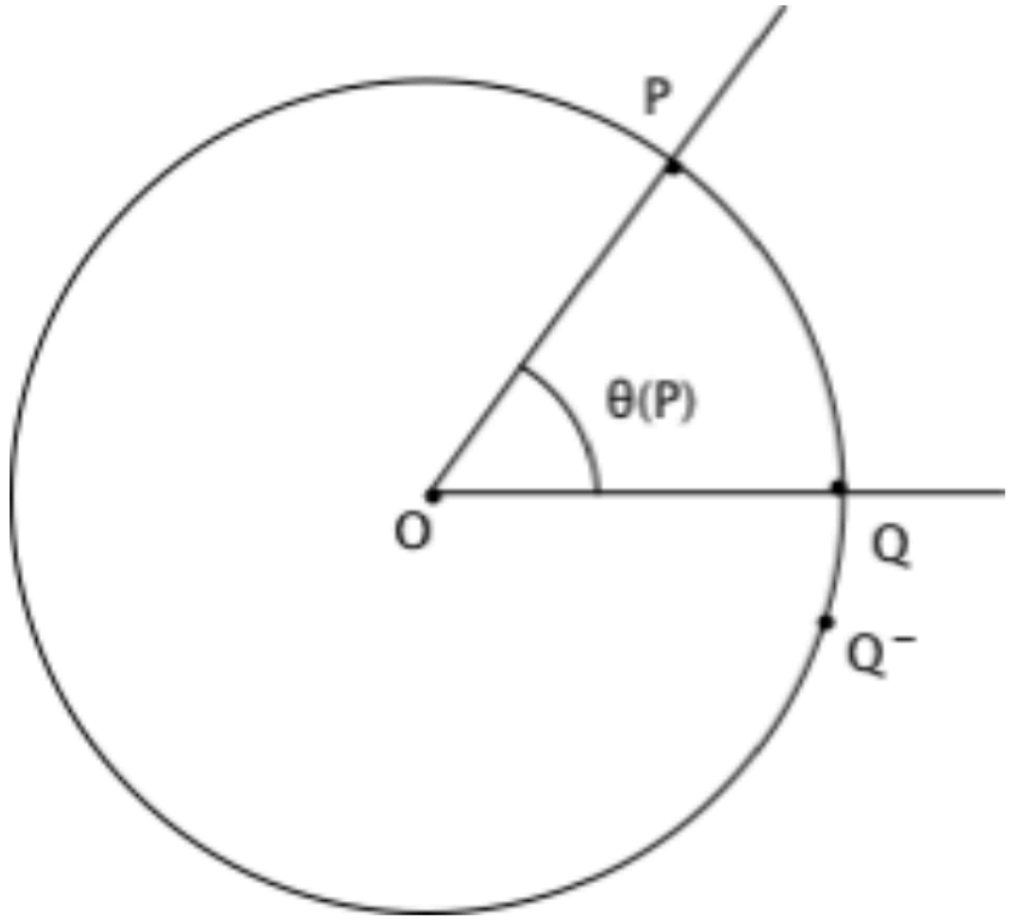
(2) any point in the entire space is related by the identification to some point in the fundamental domain

Whenever possible, as we did here, the fundamental domain is chosen to be a connected region. To build the space implied by the identification, we take the fundamental domain together with its boundary, and implement the identifications on the boundary. In our case, the fundamental domain together with its boundary is the segment $0 \leq x \leq 2\pi R$. In this segment we identify the point $x = 0$ with the point $x = 2\pi R$. The result is the circle.

A circle of radius R can be represented in a two-dimensional plane as the set of points that are a distance R from a point called the center of the circle. Note that the circle obtained above has been constructed directly, without the help of any two-dimensional space. For our circle, there is no point, anywhere, that represents the center of the circle. We can still speak, figuratively, of the radius R of the circle, but in our case, the radius is simply the quantity which multiplied by 2π gives the total length of the circle.

very important ideas!

On the circle, the coordinate x is no longer a good coordinate. The coordinate x is now either multi-valued or discontinuous. This is a problem with any coordinate on a circle. Consider using angles to assign coordinates on the unit circle as shown in Figure below.



Unit circle identification

Fix a reference point Q on the circle, and let O denote the center of the circle. To any point P on the circle we assign as a coordinate the angle $\theta(P) = angle(POQ)$. This angle is naturally multi-valued. The reference point Q, for example, has $\theta(Q) = 0°$ and $\theta(Q) = 360°$. If we force angles to be single-valued by restricting $0° \leq \theta \leq 360°$, for example, then they become discontinuous. Indeed, two nearby points, Q and Q^-, then have very different angles $\theta(Q) = 0°$, while $\theta(Q^-) \sim 360°$. It is easier to work with multi-valued coordinates than it is to work with discontinuous ones.

If we have a world with several open dimensions, then we can apply the identification (´ to one of the dimensions, while doing nothing to the others. The dimension described by x turns into a circle, and the other dimensions remain open. It is possible, of course, to make more than one dimension compact.

stop

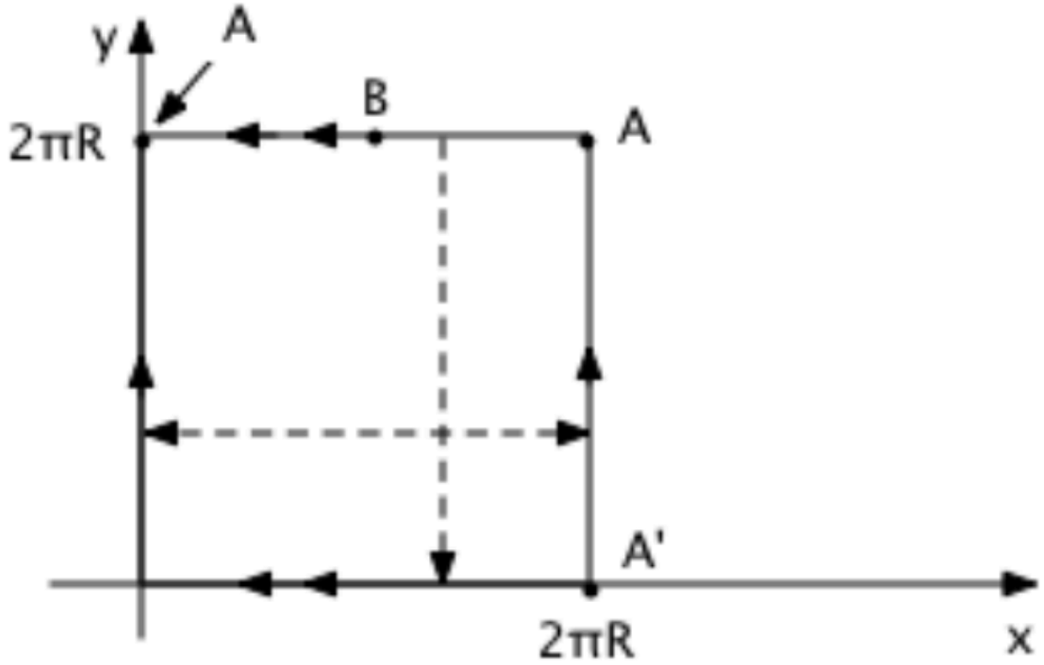
Consider the example, the (x, y) plane, subject to two identifications,

$$x \sim x + 2\pi R \quad , \quad y \sim y + 2\pi R$$

It is perhaps clearer to show both coordinates simultaneously while writing the identifications. In that fashion, the two identifications are written as

$$(x, y) \sim (x + 2\pi R, y) \quad , \quad (x, y) \sim (x, y + 2\pi R)$$

The first identification implies that we can restrict our attention to $0 \leq x \leq 2\pi R$, and the second identification implies that we can restrict our attention to $0 \leq y \leq 2\pi R$. Thus, the fundamental domain can be taken to be the square region $0 \leq x, y < 2\pi R$ as shown in Figure below.



Fundamental domain = square

The identifications are indicated by the dashed lines and arrowheads. To build the space implied by the identifications, we take the fundamental domain together with its boundary, forming the full square $0 \leq x, y < 2\pi R$, and implement the identifications on the boundary. The vertical edges are identified because they correspond to points of the form $(0, y)$ and $(2\pi R, y)$, which are identified by the first equation . This results in the cylinder shown in Figure below.

$(x, y) \sim (x + 2\pi R, y)$

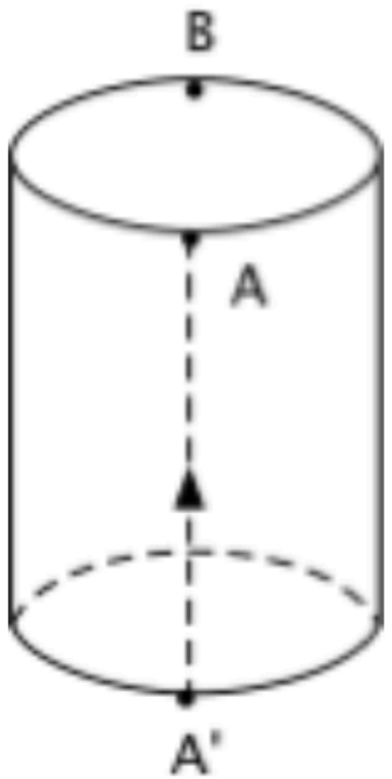


Figure 7.8: Square → cylinder

The horizontal edges are identified because they correspond to points of the form $(x, 0)$ and $(x, 2\pi R)$, which are identified by the second equation . The resulting space is a two-dimensional torus.

$(x, y) \sim (x, y + 2\pi R)$

We can visualize this process in Figure below.



2-dimensional torus

or in words, the torus is visualized by taking the fundamental domain (with its boundary) and gluing the vertical edges as their identification demands. The result is first (vertical) cylinder shown above (the gluing seam is the dashed line). In this cylinder, however, the bottom circle and the top circle must also be glued, since they are nothing other than the horizontal edges of the fundamental domain. To do this with paper, you must flatten the cylinder and then roll it up and glue the circles. The result looks like a flattened doughnut. With a flexible piece of garden hose, you could simply identify the two ends and obtain the familiar picture of a torus.

We have seen how to compactify coordinates using identifications. Some compact spaces are constructed in other ways. In string theory, however, compact spaces that arise from identifications are particularly easy to work with.

Sometimes identifications have fixed points, points that are related to themselves by the identification. For example, consider the real line parameterized by the coordinate x and subject to the identification $x \sim -x$. The point $x = 0$ is the unique fixed point of the identification. A fundamental domain can be chosen to be the half-line $x \geq 0$. Note that the boundary point $x = 0$ must be included in the fundamental domain. The space obtained by the above identification is in fact the fundamental domain $x \geq 0$. This is the simplest example of an *orbifold*, a space obtained by identifications that have fixed points. This orbifold is called an R^1/Z_2 orbifold. Here R^1 stands for the (one-dimensional) real line, and Z_2 describes a basic property of the identification when it is viewed as the transformation $x \to -x$ - if applied twice, it gives back the original coordinate.

Quantum Mechanics and the Square Well

The fundamental relation governing quantum mechanics is

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

In three spatial dimensions the indices i and j run from 1 to 3. The generalization of quantum mechanics to higher dimensions is straightforward. With d spatial dimensions, the indices simply run over the d possible values.

To set the stage for for the analysis of small extra dimensions, let us review the standard quantum mechanics problem involving and infinite potential well.

The time-independent Schrodinger equation(in one-dimension) is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

In the infinite well system we have

$$V(x) = \begin{cases} 0 & \text{if } x \in (0, a) \\ \infty & \text{if } x \notin (0, a) \end{cases}$$

When $x \in (0, a)$, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

The boundary conditions $\psi(0) = \psi(a) = 0$ give the solutions

$$\psi_k(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{k\pi x}{a}\right) \quad , \quad k = 1, 2, ..., \infty$$

The value $k = 0$ is not allowed since it would make the wave-function vanish everywhere. The corresponding energy values are

$$E_k = \frac{\hbar^2}{2m}\left(\frac{k\pi}{a}\right)^2$$

Square Well with Extra Dimensions

We now add an extra dimension to the square well problem. In addition to x, we include a dimension y that is curled up into a small circle of radius R. In other words, we make the identification

$$(x, y) \sim (x, y + 2\pi R)$$

The original dimension x has not been changed(see Figure below). In the figure, on the left we have the original square well potential in one dimension. Here the particle lives on the the line segment shown and on the right, in the (x, y) plane the particle must remain in $0 < x < a$. The direction y is identified as $y \sim y + 2\pi R$.

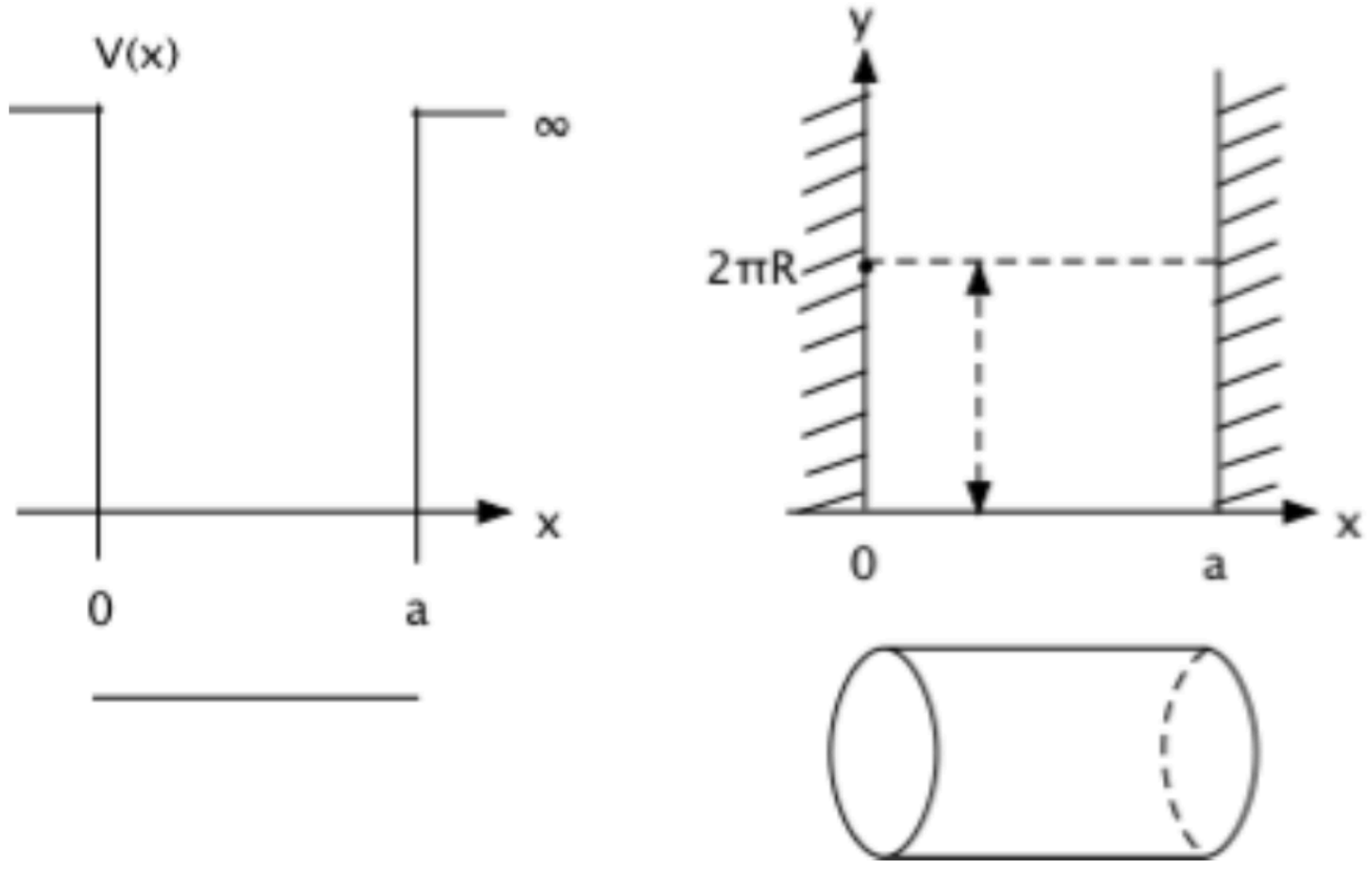


Figure 7.10: Square well with compact hidden dimension

The particle lives on a cylinder, that is, since the y direction has been turned into a circle of circumference $2\pi R$, the space where the particle moves is a cylinder. The cylinder has a length a and a circumference $2\pi R$. The potential energy $V(x, y)$ is given by

$$V(x) = \begin{cases} 0 & \text{if } x \in (0, a) \\ \infty & \text{if } x \notin (0, a) \end{cases}$$

that is, is independent of y.

We want to investigate what happens when R is small and we only do experiments at low energies. Now the only length scale in the one-dimensional infinite well system is the size a of the segment, so small R means $R << a$.

(a) Write down the Schrodinger equation for two Cartesian dimensions.

(b) Use separation of variables to find $x-$dependent and $y-$dependent solutions.

(c) Impose appropriate boundary conditions, namely, and an infinite well in the x dimension and a circle in the y dimension, to determine the allowed values of parameters in the solutions.

(d) Determine the allowed energy eigenvalues and their degeneracy.

(e) Show that the new energy levels contain the old energy levels plus additional levels.

(f) Show that when $R << a$ (a very small (compact) hidden dimension) the first new energy level appears at a very high energy. What are the experimental consequences of this result?

In two dimensions, the Schrodinger equation is given by

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)+V(x,y)\psi(x,y)=E\psi(x,y)$$

Inside the well we have

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)=E\psi(x,y)$$

We use separation of variables to solve this equation. We let

$$\psi(x,y)=\alpha(x)\beta(y)$$

and obtain

$$-\frac{\hbar^2}{2m}\frac{1}{\alpha(x)}\left(\frac{d^2\alpha(x)}{dx^2}\right)-\frac{\hbar^2}{2m}\frac{1}{\beta(y)}\left(\frac{d^2\beta(y)}{dy^2}\right)=E$$

The $x-$dependent and $y-$dependent terms of this equation must separately be constant. We obtain solution of the form

$$\psi_{kl}(x,y)=\alpha_k(x)\beta_l(y)$$

where

$$\alpha_k(x)=c_k\sin\left(\tfrac{k\pi x}{a}\right)$$
$$\beta_l(y)=a_l\sin\left(\frac{ly}{R}\right)+b_l\cos\left(\frac{ly}{R}\right)$$

The physics along the x dimension is unchanged, since the wave-function must still vanish at the ends of the segment. Therefore, the solution $\alpha_k(x)$ takes the same form as earlier and $k = 1, 2, 3, ...$ The boundary condition for $\beta_l(y)$ arises from the identification $y \sim y + 2\pi R$. Since y and $y + 2\pi R$ are coordinates that represent the same point, the wave-function must take the same value at these two arguments:

$$\beta_l(y) = \beta_l(y + 2\pi R)$$

The most general solution contains both sines and cosines in this case. The presence of the cosines allows a non-vanishing *constant* solution for $l = 0$ - we get $\beta_0(y) = b_0$. This solution is key to understanding why a small extra dimension does not change the low energy physics very much.

The energy eigenvalues of the ψ_{kl} are

$$E_{kl} = \frac{\hbar^2}{2m}\left[\left(\frac{k\pi}{a}\right)^2 + \left(\frac{l}{R}\right)^2\right]$$

These energies correspond to doubly degenerate states when $l \neq 0$, because in this case the term

$$\beta_l(y) = a_l \sin\left(\frac{ly}{R}\right) + b_l \cos\left(\frac{ly}{R}\right)$$

contains two linearly independent solutions.

The extra dimension has changed the energy spectrum dramatically. We will see, however, that if $R << a$, then the low-lying part of the spectrum is unchanged. The rest of the spectrum changes, but these changes are not accessible in low energy experiments.

Since $l = 0$ is permitted, the energy levels E_{k0} coincide with the old energy levels E_k ! The new system contains all the energy levels of the old system. However, it also includes additional energy levels. What is the lowest new level? To minimize the energy, each of the terms in the result for E_{kl} must be as low as possible. The minimum occurs when $k = 1$, since $k = 0$ is not allowed, and $l = 1$, since $l = 0$ gives us the old levels. The lowest new energy level is

$$E_{11} = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2 + \left(\frac{1}{R}\right)^2\right]$$

When $R \ll a$, the second term is much larger than the first and thus

$$E_{11} \approx \frac{\hbar^2}{2m}\left(\frac{1}{R}\right)^2$$

This energy is comparable to that of the level k eiegnstate of the original problem where

$$\frac{k\pi}{a} \sim \frac{1}{R} \rightarrow k \sim \frac{1}{\pi}\frac{a}{R}$$

Since R is much smaller than a, k is a very large number. So the first new level appears at an energy far above that of the low-lying original states. We therefore conclude that an extra dimension can remain hidden from experiments at a particular energy level as long as the dimension is small enough. Once the probing energies become sufficiently high, the effect of an extra dimension can be observed.

he quantum mechanics of a string introduces new features not present here. For an extra dimension much smaller than the already small string length ℓ_s, new low-lying states can appear! These correspond to the strings that wrap around the extra dimension. They have no analog in the quantum mechanics of a point particle. In string theory, the conclusion remains true that no new low energy states arise from a small extra dimension, but there is a small qualification - the dimension must not be significantly smaller than ℓ_s.

next