Chapter 12

Identical Particles

12.9 Problems

12.9.1 Two Bosons in a Well

Two identical spin-zero bosons are placed in a 1−dimensional square potential well with infinitely high walls, i.e., $V = 0$ for $0 < x < L$, otherwise $V = \infty$. The normalized single particle energy eigenstates are

$$u_n(x) = \sqrt{\frac{2}{L}} \sin(n\pi x/L)$$

(a) Find the wavefunctions and energies for the ground state and the first two excited states of the system.

For the single-particle states

$$E_n = n^2 \frac{\pi^2 \hbar^2}{8ma^2} = \varepsilon n^2$$

Because this well is not centered on zero, the single-particle eigenstates are given by(choosing $L = 2a$)

$$u_n(x) = \sqrt{\frac{1}{a}} \sin(n\pi x/2a) = \langle x \mid n \rangle$$

If we write the two-particle states as $|n_1, n_2\rangle$, the ground-state is $|1,1\rangle$ $(E = 2\varepsilon)$. The first excited states are $|2,1\rangle$ $(E = 5\varepsilon)$ and $|1,2\rangle$ $(E = 5\varepsilon)$. The second excited state is $|2,2\rangle$ $(E = 8\varepsilon)$. The overall wavefunction needs to be symmetric for bosons, which $|1,1\rangle$ and $|2,2\rangle$ are already. These therefore pair with a symmetric spin wavefunction, which is always possible, whether or not the bosons have spin zero.

For the first excited state, both symmetric and antisymmetric combinations are possible:

$$\frac{1}{\sqrt{2}} (|2,1\rangle \pm |1,2\rangle)$$

These would need to pair with spin wavefunctions that are symmetric and antisymmetric, respectively. If $S > 0$, then both are possible. If $S = 0$, then only the symmetric space state is possible.

(b) Suppose that the two bosons interact with each other through the perturbing potential

$$H'(x_1, x_2) = -LV_0\delta(x_1 - x_2)$$

Compute the first-order correction to the ground state energy of the system.

The (normalized) ground-state wavefunction is

$$\psi(x_1, x_2) = |1, 1\rangle = \frac{1}{a}\sin(\pi x_1/2a)\sin(\pi x_2/2a)$$

According to first-order perturbation theory, the change in the ground-state energy cause by

$$H'(x_1, x_2) = -2aV_0\delta(x_1 - x_2)$$

is

$$\Delta E = \langle 1, 1| H'(x_1, x_2) |1, 1\rangle = \int\int \psi^*(x_1, x_2)H'(x_1, x_2)\psi(x_1, x_2)dx_1dx_2$$

Thus,

$$\begin{aligned}\Delta E &= -2aV_0 \int\int \psi^*(x_1, x_2)\delta(x_1 - x_2)\psi(x_1, x_2)dx_1dx_2 \\ &= -2aV_0 \int |\psi(x, x)|^2 dx = -\frac{2}{a}V_0 \int_0^{2a} \sin^4\frac{\pi x}{2a}dx = -4V_0 \int_0^1 \sin^4\pi y dy \\ &= -4V_0 \int_0^1 \left(\frac{1 - \cos 2\pi y}{2}\right)^2 dy = -4V_0\frac{3}{8} = -\frac{3}{2}V_0\end{aligned}$$

12.9.2 Two Fermions in a Well

Two identical spin$-1/2$ bosons are placed in a $1-$dimensional square potential well with infinitely high walls, i.e., $V = 0$ for $0 < x < L$, otherwise $V = \infty$. The normalized single particle energy eigenstates are

$$u_n(x) = \sqrt{\frac{2}{L}}\sin(n\pi x/L)$$

(a) What are the allowed values of the total spin angular momentum quantum number, J ? How many possible values are there fore the $z-$component of the total angular momentum?

The allowed values of J range between $s_1 + s_2$ and $|s_1 - s_2|$ in integer steps. Since $s_1 = s_2 = 1/2$, the only allowed values are $J = 1$ and $J = 0$. $J = 1$ allows $m = -1, 0, 1$ and $J = 0$ allows $m = 0$ only. Thus, there are only three allowed values of m.

(b) If single-particle spin eigenstates are denoted by $|\uparrow\rangle = u$ and $|\downarrow\rangle = d$, construct the two-particle spin states that are either symmetric or antisymmetric. How many states of each type are there?

Symmetric ("triplet") states are

$$u(1)u(2), d(1)d(2) \quad and \quad \frac{u(1)d(2) + u(2)d(1)}{\sqrt{2}}$$

The antisymmetric ("singlet") state is

$$\frac{u(1)d(2) - u(2)d(1)}{\sqrt{2}}$$

(c) Show that the $j = 1$, $m = 1$ state must be symmetric. What is the symmetry of the $J = 0$ state?

The $m = 1$ state requires both particles to be spin up. Thus, it must be $J = 1$. We thus need the symmetric state $u(1)u(2)$. The $J = 0$ is antisymmetric.

(d) What is the ground-state energy of the two-particle system, and how does it depend on the overall spin state?

The overall wavefunction of the 2-particle system must be antisymmetric under exchange of spin and space labels (these are fermions). If the wavefunction factorizes into $\psi = u(space) \times v(spin)$, then the symmetries of u and v must be opposite. Therefore, if $J = 0$ (v is antisymmetric), u must be symmetric, and vice-versa.

A symmetric ground-state is possible:

$$u(1, 2) = u_1(1)u_1(2)$$

but, an antisymmetric space state only allows one particle in the lowest single-particle state allows only one particle in the lowest single-particle state:

$$\frac{u(1)d(2) - u(2)d(1)}{\sqrt{2}}$$

The single-particle energies are

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

where $k = \pi/L$ for the u_1 state and $k = 2\pi/l$ for the u_2 state. The symmetric ground-state energy is thus

$$E_{symm} = 2\frac{\hbar^2\left(\frac{\pi}{L}\right)^2}{2m} = \frac{\hbar^2\pi^2}{mL^2}$$

whereas the antisymmetric ground state energy is 5/2 larger, i.e.,

$$E_{anti} = \frac{\hbar^2\left(\frac{\pi}{L}\right)^2}{2m} + \frac{\hbar^2\left(\frac{2\pi}{L}\right)^2}{2m} = \left(\frac{1}{2}+2\right)\frac{\hbar^2\pi^2}{mL^2} = \frac{5}{2}E_{symm}$$

12.9.3 Two spin$-1/2$ particles

The Hamiltonian for two spin$-1/2$ particles, one with mass m_1 and the other with m_2, is given by

$$\hat{H} = \frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(r) + \left(\frac{1}{4} - \frac{\vec{S}_1\cdot\vec{S}_2}{\hbar^2}\right)V_b(r)$$

where $|\vec{r}| = \vec{r}_1 - \vec{r}_2$, $|\vec{r}| = r$ and

$$V_a(r) = \begin{cases} 0 & \text{for } r < a \\ V_0 & \text{for } r > a \end{cases} \quad , \quad V_b(r) = \begin{cases} 0 & \text{for } r < b \\ V_0 & \text{for } r > b \end{cases}$$

with $b < a$ and V_0 very large (assume V_0 is infinite where appropriate) and positive.

(a) Determine the normalized position-space energy eigenfunction for the ground state. What is the spin state of the ground state? What is the degeneracy?

For a system of 2 spin $= 1/2$ particles, the eigenstates of $\vec{S}_1\cdot\vec{S}_2$ are the total spin states $|S, S_z\rangle$ since

$$\vec{S}_1\cdot\vec{S}_2\,|S,S_z\rangle = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right)|S,S_z\rangle = \frac{\hbar^2}{2}\left(S(S+1) - \frac{3}{2}\right)|S,S_z\rangle$$

We have allowed total spin values $S = 0, 1$ so that

$$\vec{S}_1\cdot\vec{S}_2\,|1,M\rangle = \frac{\hbar^2}{4}\,|1,M\rangle \quad , \quad \vec{S}_1\cdot\vec{S}_2\,|0,0\rangle = -\frac{3\hbar^2}{4}\,|0,0\rangle$$

Since $\left[\hat{H}, \vec{S}_1\cdot\vec{S}_2\right] = 0$ we can find simultaneous eigenstates of energy and total spin. This means that for

$$\hat{H} = \frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(r) + \left(\frac{1}{4} - \frac{\vec{S}_1\cdot\vec{S}_2}{\hbar^2}\right)V_b(r)$$

with

$$V_a(r) = \begin{cases} 0 & r < a \\ V_0 & r > a \end{cases} \quad , \quad V_b(r) = \begin{cases} 0 & r < b \\ V_0 & r > b \end{cases}$$

we have

$$\begin{aligned} \hat{H}|1,M\rangle &= \left(\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(|r|) + \left(\frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b(r) \right) |1,M\rangle \\ &= \left(\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(|r|) \right) |1,M\rangle \end{aligned}$$

$$\begin{aligned} \hat{H}|0,0\rangle &= \left(\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(|r|) + \left(\frac{1}{4} - \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} \right) V_b(r) \right) |0,0\rangle \\ &= \left(\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V_a(|r|) + V_b(r) \right) |0,0\rangle \end{aligned}$$

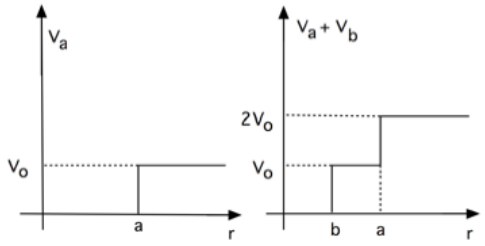
Now we can write

$$\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} = \frac{\hat{\vec{p}}^{\,2}}{2\mu} + \frac{\hat{\vec{\mathcal{P}}}^{2}}{2M} \quad , \quad \vec{p} = \vec{p}_1 - \vec{p}_2 \quad , \quad \vec{P} = \frac{\vec{p}_1 + \vec{p}_2}{M}$$
$$M = m_1 + m_2 \quad , \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

If we choose the CM system, then $\vec{P} = 0$ and we have

$$\begin{aligned} \hat{H}|1,M\rangle &= \left(\frac{\vec{p}^{\,2}}{2\mu} + V_a(|r|) \right) |1,M\rangle \\ \hat{H}|0,0\rangle &= \left(\frac{\vec{p}^{\,2}}{2\mu} + V_a(|r|) + V_b(r) \right) |0,0\rangle \end{aligned}$$

The potentials look like



As $V_0 \to \infty$, the particles in the spin = 1 states are confined in an infinite potential well of radius a, while the particles in the spin = 0 state are confined in a well of radius b.

Since $b < a$, the spin = 1 states will have a lower energy ($1/a^2 < 1/b^2$) than the spin = 0 state.

To determine the energies, we specify a complete set of 2-particle states in the form $|E, L, M, S, M_s\rangle$. Then we have

$$\langle \vec{r}; S=1, M_s | \hat{H} | E, L, M, S, M_s \rangle = \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} \right) + \frac{L(L+1)}{2\mu r^2} R + V_a R \right] Y_{LM} = ERY_{LM}$$

The ground state has $L = 0$. Now writing $u = rR$ we have

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + V_a(r)u = Eu \rightarrow \frac{d^2u}{dr^2} = -\frac{2\mu E}{\hbar^2}u = -k^2 u \quad for \quad r < a$$

and $u = 0$ for $r > a$, where the potential barrier is infinite.

Therefore, the ground state wave function for the spin = 1 states is

$$\langle \vec{r} \mid E, L=0, M=0, S=1, M_s \rangle = \begin{cases} \frac{1}{r}\sqrt{\frac{2}{a}} \sin\frac{n\pi r}{a} Y_{00} | S=1, M_s \rangle & r < a \\ 0 & r > a \end{cases}$$

The ground state is 3-fold degenerate.

(b) What can you say about the energy and spin state of the first excited state? Does your result depend on how much larger a is than b? Explain.

The lowest energy spin = 0 state has energy (for $V_0 \rightarrow \infty$)

$$E_{n=1} = \frac{\hbar^2\pi^2}{2\mu b^2}$$

Since $b < a$, this is higher than the energy of the spin = 1 states.

The 1^{st} excited states for the spin = 1 states have $L = 1$ and therefore

$$\psi = Aj_1(kr)Y_{1M}$$

for the spatial wave function.

Since $j_1(ka) = 0 \rightarrow ka = 4.49$, the lowest energy $L = 1$ states (there are 9 such states with $L = 1$, $M = 0, \pm 1$ and $S = 1$, $M_s = 0, \pm 1$ are the first excited states provided that

$$\frac{\hbar^2(4.49)^2}{2\mu a^2} < \frac{\hbar^2\pi^2}{2\mu b^2}$$

or

$$b < \sqrt{\frac{\pi}{4.49}}a = 0.70a$$

12.9.4 Hydrogen Atom Calculations

We discuss here some useful tricks for evaluating the expectation values of certain operators in the eigenstates of the hydrogen atom.

(a) Suppose we want to determine $\langle 1/r \rangle_{n\ell m}$. We can interpret $\langle \lambda/r \rangle_{n\ell m}$ as the $1^{st}-$order correction due to the perturbation λ/r (same dependence on r as the potential energy). Show that this problem can be solved exactly by just replacing e^2 by $e^2 - \lambda$ everywhere in the original solution. So, the exact energy is

$$E(\lambda) = -\frac{m\left(e^2-\lambda\right)^2}{2n^2\hbar^2}$$

the $1^{st}-$order correction is the term linear in λ, that is,

$$E^{(1)} = \frac{me^2\lambda}{n^2\hbar^2} = \langle \lambda/r \rangle_{n\ell m}$$

Therefore we get

$$\langle 1/r \rangle_{n\ell m} = \frac{me^2}{n^2\hbar^2} = \frac{1}{n^2 a_0}$$

We note (for later use) that

$$E(\lambda) = E^{(0)} + E^{(1)} + ... = E(\lambda = 0) + \lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0} + ...$$

so that one way to extract $E^{(1)}$ from the exact answer is to calculate

$$\lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0}$$

In order to evaluate $\left\langle \frac{1}{r} \right\rangle$ we consider $\frac{\lambda}{r}$ as a perturbation for the hydrogenic atom, where we can think of λ as a *small* constant. The $1^{st}-$order shift in the energy is given by

$$E_n^{(1)} = \left\langle \frac{\lambda}{r} \right\rangle_{n\ell m}$$

which is clearly linear in λ. Since the eigenvalues for the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r}$$

are

$$E_n = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2}$$

the eigenvalues of the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2 - \lambda}{r}$$

are

$$E_n = -\frac{\mu(Ze^2-\lambda)^2}{2\hbar^2 n^2}$$

Now, in perturbation theory E_n is written as a power series in λ so that

$$E_n^{(1)} = \lambda\left(\frac{dE_n}{d\lambda}\right)_{\lambda=0} \rightarrow E_n^{(1)} = \lambda\frac{\mu Ze^2}{\hbar^2 n^2}$$

However, we also have

$$E_n^{(1)} = \left\langle\frac{\lambda}{r}\right\rangle_{n\ell m} = \lambda\frac{\mu Ze^2}{\hbar^2 n^2} \rightarrow \left\langle\frac{1}{r}\right\rangle_{n\ell m} = \frac{\mu Ze^2}{\hbar^2 n^2} = \frac{Z}{a_0 n^2}$$

(b) Evaluate, in a manner similar to part (a), $\left\langle\vec{p}^2/2\mu\right\rangle_{n\ell m}$ by considering the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} + \lambda\frac{\hat{p}^2}{2\mu}$$

Now we assume the full Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r} + \lambda\frac{\hat{p}^2}{2\mu} = (1+\lambda)\frac{\hat{p}^2}{2\mu} - \frac{Ze^2}{r}$$

This is the same as a change in the effective mass of the form

$$\mu \rightarrow \frac{\mu}{1+\lambda}$$

so that the exact energy eigenvalues become

$$E_n = -\frac{\mu c^2 Z^2\alpha^2}{2n^2(1+\lambda)}$$

and therefore

$$E_n^{(1)} = \lambda\left(\frac{dE_n}{d\lambda}\right)_{\lambda=0} \rightarrow E_n^{(1)} = \lambda\frac{\mu c^2 Z^2\alpha^2}{2n^2} = \lambda\left\langle\frac{\vec{p}^2}{2\mu}\right\rangle_{n\ell m}$$

so that

$$\left\langle\frac{\vec{p}^{\,2}}{2\mu}\right\rangle_{n\ell m} = \frac{\mu c^2 Z^2\alpha^2}{2n^2}$$

(c) Consider now $\left\langle\lambda/r^2\right\rangle_{n\ell m}$. In this case, an exact solution is possible since the perturbation just modifies the centrifugal term as follows:

$$\frac{\hbar^2\ell(\ell+1)}{2mr^2} + \frac{\lambda}{r^2} = \frac{\hbar^2\ell'(\ell'+1)}{2mr^2}$$

where ℓ' is a function of λ. Now go back to the original hydrogen atom solution and show that the dependence of E on $\ell'(\lambda)$ is

$$E(\ell') = -\frac{mZ^2e^4}{2\hbar^2(k+\ell'+1)^2} = E(\lambda) = E^{(0)} + E^{(1)} + ...$$

Then show that

$$\begin{aligned}\left\langle \lambda/r^2 \right\rangle_{n\ell m} &= E^{(1)}\lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0} = \lambda \left(\frac{dE}{d\ell'}\right)_{\ell'=\ell} \left(\frac{d\ell'}{d\lambda}\right)_{\ell'=\ell} \\ &= \frac{\lambda}{n^3 a_0^2(\ell+1/2)}\end{aligned}$$

or

$$\left\langle 1/r^2 \right\rangle_{n\ell m} = \frac{1}{n^3 a_0^2(\ell+1/2)}$$

A perturbation $\frac{\lambda}{r^2}$ modifies the $\frac{1}{r^2}$ term as follows:

$$\frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + \frac{\lambda}{r^2} = \frac{\hbar^2\ell'(\ell'+1)}{2\mu r^2}$$

so that

$$E(\ell') = -\frac{\mu c^2 Z^2\alpha^2}{2(k+\ell'+1)^2}$$

The old quantum number $n = k + \ell + 1$.

As above we then have

$$\left\langle \frac{\lambda}{r^2} \right\rangle_{n\ell m} = E^{(1)}\lambda \left(\frac{dE}{d\lambda}\right)_{\lambda=0} = \lambda \left(\frac{dE}{d\ell'}\right)_{\ell'=\ell} \left(\frac{d\ell'}{d\lambda}\right)_{\ell'=\ell} = \lambda \frac{\mu c^2 Z^2\alpha^2}{(k+\ell+1)^3} \left(\frac{d\ell'}{d\lambda}\right)_{\ell'=\ell}$$

Now,

$$\begin{aligned}&\tfrac{d}{d\lambda}\left(\tfrac{\hbar^2\ell(\ell+1)}{2\mu r^2} + \tfrac{\lambda}{r^2}\right) = \tfrac{d}{d\lambda}\left(\tfrac{\hbar^2\ell'(\ell'+1)}{2\mu r^2}\right) \\ &\tfrac{1}{r^2} = \tfrac{\hbar^2(2\ell'+1)}{2\mu r^2}\tfrac{d\ell'}{d\lambda} \rightarrow \left(\tfrac{d\ell'}{d\lambda}\right)_{\ell'=\ell} = \tfrac{\mu}{(\ell+1/2)\hbar^2}\end{aligned}$$

Therefore,

$$\left\langle \frac{1}{r^2} \right\rangle_{n\ell m} = \frac{\mu c^2 Z^2\alpha^2}{n^3} \frac{\mu}{(\ell+1/2)\hbar^2} = \frac{Z^2}{n^3 a_0^2(\ell+1/2)}$$

(d) Finally consider $\left\langle \lambda/r^3 \right\rangle_{n\ell m}$. Since there is no such term in the hydrogen Hamiltonian, we resort to different trick. Consider the radial momentum operator

$$p_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

Show that in terms of this operator we may write the radial part of the Hamiltonian

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right)$$

as

$$\frac{p_r^2}{2m}$$

Now show that

$$\langle [H, p_r] \rangle = 0$$

in the energy eigenstates. Using this fact, and by explicitly evaluating the commutator, show that

$$\left\langle 1/r^3 \right\rangle_{n\ell m} = \frac{Z}{a_0 \ell(\ell+1)} \left\langle 1/r^2 \right\rangle_{n\ell m}$$

and hence

$$\left\langle 1/r^3 \right\rangle_{n\ell m} = \frac{Z^3}{n^3 a_0^3 \ell(\ell+1)(\ell+1/2)}$$

Finally,

$$p_r = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right)$$

Therefore,

$$\begin{aligned} \frac{p_r^2}{2\mu} f(r) &= -\frac{\hbar^2}{2\mu} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) f(r) = -\frac{\hbar^2}{2\mu} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \left(\frac{\partial f}{\partial r} + \frac{f}{r} \right) \\ &= -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2 f}{\partial r^2} - \frac{f}{r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{f}{r^2} \right) = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) f \end{aligned}$$

Now, we also have

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r} \right) = \frac{1}{r^2}\left(2r\frac{\partial f}{\partial r} + r^2 \frac{\partial^2 f}{\partial r^2} \right) = \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) f$$

so that

$$\frac{p_r^2}{2\mu} = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right)$$

Therefore,

$$\hat{H} = \frac{p_r^2}{2\mu} - \frac{Ze^2}{r} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}$$

Now,

$$\langle n\ell m | \left[\hat{H}, \hat{p}_r \right] | n\ell m \rangle = (E_n - E_n) \langle n\ell m | \hat{p}_r | n\ell m \rangle = 0$$

for all states. But

$$\begin{aligned} \langle n\ell m | \left[\hat{H}, \hat{p}_r \right] | n\ell m \rangle &= \langle n\ell m | \left[\left(-\frac{Ze^2}{r} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right), -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \right] | n\ell m \rangle \\ &= \langle n\ell m | \left[\left(-\frac{Ze^2}{r} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right), -i\hbar \left(\frac{\partial}{\partial r} \right) \right] | n\ell m \rangle \, notag \\ &= \frac{\hbar}{i} \langle n\ell m | \left(-\frac{Ze^2}{r^2} + \frac{\hbar^2 \ell(\ell+1)}{\mu r^3} \right) | n\ell m \rangle = 0 \end{aligned}$$

Therefore,

$$\left\langle \frac{Ze^2}{r^2} \right\rangle_{n\ell m} = \left\langle \frac{\hbar^2 \ell(\ell+1)}{\mu r^3} \right\rangle_{n\ell m}$$

or

$$\left\langle \frac{1}{r^3} \right\rangle_{n\ell m} = \frac{Z\mu}{\hbar^2 \ell(\ell+1)} \left\langle \frac{1}{r^2} \right\rangle_{n\ell m} = \frac{Z\mu}{\hbar^2 \ell(\ell+1)} \frac{Z^2}{n^3 a_0^2 (\ell+1/2)} \quad = \frac{Z^3}{n^3 a_0^3 \ell(\ell+1)(\ell+1/2)}$$

12.9.5 Hund's rule

Explain on the basis of Hund's rules why the ground state of carbon is $^3P_0$ and that of oxygen is $^3P_2$. Carbon is $2p^2 \rightarrow S = 0, 1$ *and* $L = 0, 1, 2$. This give the following table of allowed multiplets:

L	S	J	
2	0	2	$^1D_2$
1	1	2	$^3P_2$
1	1	1	$^3P_1$
1	1	0	$^3P_0$
0	0	0	$^1S_2$

Hund's rule then says that

$$\begin{array}{ll} Maximum & S \rightarrow S = 1 \rightarrow {}^3P_2, {}^3P_1, {}^3P_0 \\ Maximum & L \rightarrow L = 1 \rightarrow {}^3P_2, {}^3P_1, {}^3P_0 \\ Maximum & J \rightarrow J = 0 \rightarrow {}^3P_0 \text{ (less than half - filled shell)} \end{array}$$

so that the ground state of carbon is $^3P_0$. Oxygen is $2p^4 \rightarrow S = 0, 1$ *and* $L = 0, 1, 2$. This give the following table of allowed multiplets (same as for carbon):

L	S	J	
2	0	2	$^1D_2$
1	1	2	$^3P_2$
1	1	1	$^3P_1$
1	1	0	$^3P_0$
0	0	0	$^1S_2$

Hund's rule then says that

$$\begin{array}{ll} Maximum & S \to S = 1 \to {}^3P_2, {}^3P_1, {}^3P_0 \\ Maximum & L \to L = 1 \to {}^3P_2, {}^3P_1, {}^3P_0 \\ Maximum & J \to J = 2 \to {}^3P_2 \text{ (more than half - filled shell)} \end{array}$$

so that ground state of oxygen is ${}^3P_2$.

12.9.6 Russell-Saunders Coupling in Multielectron Atoms

Consider a configuration of k equivalent p electrons outside a closed shell, which we denote simply by p^k, i.e., carbon= p^2, nitrogen= p^3 and oxygen= p^4.

(a) Use the implied-terms method to determine all the terms that can arise from p^3. Which of them will have the lowest energy?

Following the methods described in Chapter 12 we have for the p^3 configuration where $\ell_1 = \ell_2 = \ell_3 = 1$ and $s_1 = s_2 = s_3 = 1/2$ we have the state table

Entry	$m_\ell = -1$	$m_\ell = 0$	$m_\ell = +1$	M_L	M_S
1	↑↓	↑		-2	1/2
2	↑↓	↓		-2	-1/2
3	↑↓		↑	-1	1/2
4	↑↓		↓	-1	-1/2
5	↑	↑↓		-1	1/2
6	↓	↑↓		-1	-1/2
7		↑↓	↑	1	1/2
8		↑↓	↓	1	-1/2
9	↑		↑↓	1	1/2
10	↓		↑↓	1	-1/2
11		↑	↑↓	2	1/2
12		↓	↑↓	2	-1/2
13	↑	↑	↑	0	3/2
14	↓	↓	↓	0	-3/2
15	↑	↑	↓	0	1/2
16	↑	↓	↑	0	1/2
17	↓	↑	↑	0	1/2
18	↓	↓	↑	0	-1/2
19	↓	↑	↓	0	-1/2
20	↑	↓	↓	0	-1/2

so that we have the $M_L - M_S$ table:

M_L/M_S	3/2	1/2	−1/2	−3/2
2	0	1	1	0
1	0	2	2	0
0	1	3	3	1
-1	0	2	2	0
-2	0	1	1	0

Largest L and S are $L = 2$ and $S = 1/2$ which says that we have a

^2D term
$J = 5/2\,,\, 3/2 \rightarrow 6 + 4 = 10\; levels$

Therefore we get the new(remaining states) $M_L - M_S$ table:

M_L/M_S	3/2	1/2	−1/2	−3/2
2	0	0	0	0
1	0	1	1	0
0	1	2	2	1
-1	0	1	1	0
-2	0	0	0	0

Next largest L and S are $L = 1$ and $S = 1/2$ which says that we have a

^2P term
$J = 3/2\,,\, 1/2 \rightarrow 4 + 2 = 6\; levels$

Therefore we get the new(remaining states) $M_L - M_S$ table:

M_L/M_S	3/2	1/2	−1/2	−3/2
2	0	0	0	0
1	0	0	0	0
0	1	1	1	1
-1	0	0	0	0
-2	0	0	0	0

Next largest L and S are $L = 0$ and $S = 3/2$ which says that we have a

^4S term
$J = 3/2 \rightarrow 4\; levels$

There are no remaining states and thus we are finished.

We therefore have the allowed multiplets

$$^2D_{5/2,3/2} \quad , \quad ^2P_{3/2,1/2} \quad , \quad ^4S_{3/2}$$

The rule for finding the ground state is

maximum S or multiplicity
maximum L
maximum J if $> 1/2-$ full
minimum J if $< 1/2-$ full

In this case, the first part of the rule gives the ground state as ${}^4S_{3/2}$ and we are done since there is only one multiplet satisfying this part of the rule.

(b) Repeat this calculation for p^4 and show that we get the same result as for p^2

For the p^4 configuration we get the state table

Entry	$m_\ell = -1$	$m_\ell = 0$	$m_\ell = +1$	M_L	M_S
1	$\uparrow\downarrow$	$\uparrow\downarrow$		-2	0
2	$\uparrow\downarrow$		$\uparrow\downarrow$	0	0
3	$\uparrow\downarrow$	$\uparrow$	$\uparrow$	-1	1
4	$\uparrow\downarrow$	$\downarrow$	$\downarrow$	-1	-1
5	$\uparrow\downarrow$	$\uparrow$	$\downarrow$	-1	0
6	$\uparrow\downarrow$	$\downarrow$	$\uparrow$	-1	0
7		$\uparrow\downarrow$	$\uparrow$	2	0
8	$\uparrow$	$\uparrow\downarrow$	$\uparrow$	0	1
9	$\downarrow$	$\uparrow\downarrow$	$\downarrow$	0	-1
10	$\downarrow$	$\uparrow\downarrow$	$\uparrow$	0	0
11	$\uparrow$	$\uparrow\downarrow$	$\downarrow$	0	0
12	$\uparrow$	$\uparrow$	$\uparrow\downarrow$	1	1
13	$\downarrow$	$\downarrow$	$\uparrow\downarrow$	1	-1
14	$\uparrow$	$\downarrow$	$\uparrow\downarrow$	1	0
15	$\downarrow$	$\uparrow$	$\uparrow\downarrow$	1	0

which is the same as the state table for the p^2 configuration in Chapter 12. Therefore we get the same $M_L - M_S$ table as for p^2

M_L/M_S	1	0	-1
2	0	1	0
1	1	2	1
0	1	3	1
-1	1	2	1
-2	0	1	0

and we get the allowed multiplets

$${}^1D_2 \quad , \quad {}^3P_{0,1,2} \quad , \quad {}^1S_0$$

$$\begin{array}{l}\text{maximum } S \to {}^3P_{0,1,2}\\ \text{maximum } L \to {}^3P_{0,1,2}\\ \text{maximum } J \text{ if } > 1/2 - \text{ full } \to {}^3P_2\end{array}$$

so that the ground state is ${}^3P_2$

12.9.7 Magnetic moments of proton and neutron

The magnetic dipole moment of the proton is

$$\hat{\mu}_p = g_p \frac{e}{2m_p} \hat{S}_p$$

with a measured magnitude corresponding to a value for the gyromagnetic ratio of

$$g_p = 2 \times (2.792847337 \pm 0.000000029)$$

We have not studied the Dirac equation yet, but the prediction of the Dirac equation for a point spin$-1/2$ particle is $g_p = 2$. We can understand the fact that the proton gyromagnetic ratio is not two as being due its compositeness, i.e., in a simple quark model, the proton is made up of three quarks, two *ups* (u), and a *down* (d). The quarks are supposed to be point spin$-1/2$, hence, their gyromagnetic ratios should be $g_u = g_d = 2$ (up to higher order corrections, as in the case of the electron). Let us see if we can make sense out of the proton magnetic moment.

The proton magnetic moment should be the sum of the magnetic moments of its constituents, and any moments due to their orbital motion in the proton. The proton is the ground state baryon, so we assume that the three quarks are bound together (by the strong interaction) in a state with no orbital angular momentum. The Pauli principle says that the two identical up quarks must have an overall odd wave function under interchange of all quantum numbers. We must apply this rule with some care since we will be including *color* as one of these quantum numbers.

Let us look at some properties of *color*. It is the strong interaction analog of electric charge in the electromagnetic interaction. However, instead of one fundamental dimension in charge, there are three color directions, labeled as *red* (r), *blue* (b), and *green* (g). Unitary transformations in this color space(up to overall phases) are described by elements of the group $SU(3)$, the group of unimodular 3×3 matrices (electromagnetic charge corresponds to the group $U(1)$ whose elements are local phase changes). Just like combining spins, we can combine these three colors according to a Clebsch-Gordon series, with the result

$$3 \otimes 3 \otimes 3 = 10 \oplus 8 \oplus 8 \oplus 1$$

These are different rules than for the addition of spin case because that case uses the rotation group instead. We do not need to understand all aspects of

the $SU(3)$ group for this problem. The essential aspect here is that there is a singlet in the decomposition, i.e., it is possible to combine three colors in a way as to get a color singlet state or a state with no net color charge. These turn out to be the states of physical interest for the observed baryons according to a postulate of the quark model.

(a) The singlet state in the decomposition above must be antisymmetric under the interchange of any two colors. Assuming this is the case, write down the color portion of the proton wave function.

Note that there are 6 permutations of the 3 colors among the 3 quarks, if no 2 quarks have the same color. The completely antisymmetric combination of 3 colors is:

$$\frac{1}{\sqrt{6}}(|rgb\rangle - |rbg\rangle + |brg\rangle - |bgr\rangle + |gbr\rangle - |grb\rangle)$$

(b) Now that you know the color wave function of the quarks in the proton, write down the spin wave function. You must construct a total spin state $|1/2, 1/2\rangle$ total spin angular momentum state from three spin$-1/2$ states where the two up quarks must be in a symmetric state.

To construct the spin wave function, we first note that the 3 spin$-1/2$ quarks must combine in such a way as to give an overall spin$-1/2$ for the proton. Second, since the space wave function is symmetric and the color wave function is antisymmetric, the spin wave function of the 2 up quarks must be symmetric. Thus, the 2 up quarks are in a spin-1 state. To give the spin wave function of the proton, we pick the $z-$axis to be along the spin direction. Then the spin state is:

$$|1/2, 1/2\rangle = \sqrt{\frac{2}{3}}\,|11; 1/2, -1/2\rangle - \sqrt{\frac{1}{3}}\,|10; 1/2, 1/2\rangle$$

(c) Since the proton is uud and its partner the neutron (the are just two states of the same particle) is ddu and $m_p \simeq m_n$, we can make the simplifying assumption that $m_u \simeq m_d$. Given the measured value of g_p, what does you model give for m_u? Remember that the up quark has electric charge $2/3$ and the down quark has electric charge $-1/3$, in units of positron charge.

The magnetic moment of the proton in this model is thus:

$$\mu_p = \frac{2}{3}(2\mu_u - \mu_d) + \frac{1}{3}\mu_d = \frac{4}{3}\mu_u - \frac{2}{3}\mu_d$$

Hence,

$$g_p \frac{e}{2m_p} = \frac{4}{3}2\frac{2}{3}\frac{e}{2m_u} - \frac{1}{3}2\left(-\frac{1}{3}\right)\frac{e}{2m_d}$$

With $g_p = 5.58$,$m_p = 938\,MeV$, and $m_u = m_d$, we obtain

$$m_u = \frac{2m_p}{g_p} = 336\,MeV$$

(d) Finally, use your results to predict the gyromagnetic moment of the neutron(neutron results follows from proton results by interchanging u and d labels) and compare with observation.

The neutron wave function may be obtained from the proton wave function by interchanging the u and d quark labels. Thus

$$\mu_n = \frac{2}{3}(2\mu_d - \mu_u) + \frac{1}{3}\mu_u = \frac{4}{3}\mu_d - \frac{2}{3}\mu_u$$

We predict the gyromagnetic moment of the neutron to be:

$$\begin{aligned}\frac{\mu_n}{\mu_p} &= \frac{\frac{4}{3}\mu_d - \frac{2}{3}\mu_u}{\frac{4}{3}\mu_u - \frac{2}{3}\mu_d} \\ &= \frac{\frac{4}{3}\left(-\frac{1}{3}\right) - \frac{1}{3}\frac{2}{3}}{\frac{4}{3}\frac{2}{3} - \frac{1}{3}\left(-\frac{1}{3}\right)} = -\frac{2}{3}\end{aligned}$$

that is, we predict (neglecting the mass difference), $g_n = -3.72$. This may be compared with the observed value of -3.83.

12.9.8 Particles in a 3-D harmonic potential

A particle of mass m moves in a 3−dimensional harmonic oscillator well. The Hamiltonian is

$$\hat{H} = \frac{\vec{p}^2}{2m} + \frac{1}{2}kr^2$$

(a) Find the energy and orbital angular momentum of the ground state and the first three excited states.

A three-dimensional harmonic oscillator (Chapter 9) has energy levels

$$E_{n_r,\ell} = \hbar\omega(2n_r + \ell + \frac{3}{2}) \quad , \quad \omega = \sqrt{\frac{k}{m}}$$

with

$$\begin{aligned}&N = 2n_r + \ell \quad , \quad N, n_r = 0, 1, 2, ... \\ &\psi_{n_r,\ell,m}(y,\theta,\varphi) = y^\ell e^{-\frac{y^2}{2}} L_{n_r}^{\ell+\frac{1}{2}}(y^2) Y_{\ell m}(\theta,\varphi) \\ &r = \rho y, \rho^2 = \tfrac{\hbar^2}{M\omega}\end{aligned}$$

such that
The degeneracy is given by

$$\frac{(N+1)(N+2)}{2}$$

$E/\hbar\omega$	n_r	ℓ	n	*degeneracy*
3/2	0	0	0	1
5/2	0	1	1	$3 : m = \pm 1, 0$
7/2	1,0	0,2	2	$6 : m = \pm 2, \pm 1, 0, 0$

For the ground state, $N = 0$, $\ell = 0$ and the energy is

$$E_0 = E_{00} = \frac{3}{2}\hbar\omega$$

This level is non-degenerate ($2\ell + 1 = 1$). For the 1st excited state, $N = 1$, $\ell = 1$ and the energy is

$$E_1 = E_{01} = \frac{5}{2}\hbar\omega$$

This level is 3-fold degenerate ($2\ell + 1 = 3$).

(b) If eight identical non-interacting (spin 1/2) particles are placed in such a harmonic potential, find the ground state energy for the eight-particle system.

For spin = 1/2 particles, two particles will fill up a state. Thus, when completely full, the ground state contain 2 particles and the 1^{st} excited states contain a total of 6 particles.

Therefore, the ground state energy of the 8-particle system is

$$E_0 = 2 \times \frac{3}{2}\hbar\omega + 6 \times \frac{5}{2}\hbar\omega = 18\hbar\omega$$

(c) Assume that these particles have a magnetic moment of magnitude μ. If a magnetic field B is applied, what is the approximate ground state energy of the eight-particle system as a function of B (what is the effect of a closed shell?). Determine the magnetization $-\partial E/\partial B$ for the ground state as a function of B. What is the susceptibility? Don't do any integrals.

The Hamiltonian of the system is

$$\hat{H} = \sum_{i=1}^{8}\left(\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}kr_i^2\right) - \sum_{i=1}^{8}\vec{\mu}_i \cdot \vec{B} - \frac{e}{2mc}\sum_{i=1}^{8}\vec{L}_i \cdot \vec{B}$$
$$+ \frac{e^2}{2mc^2}\sum_{i=1}^{8}\vec{A}_i^{\,2} + \frac{1}{2mc^2}\sum_{i=1}^{8}\frac{1}{r_i^2}\frac{dV(r_i)}{dr_i}\vec{L}_i \cdot \vec{S}_i$$

where

$$V(r_i) = \frac{1}{2}kr_i^2$$

and

$$\nabla \times \vec{A} = \vec{B} \rightarrow \vec{A} = \frac{1}{2}\vec{B} \times \vec{r}$$

is the vector potential. Since the eight particles occupy 2 shells, all shells are full. This says that

$$S = 0 \ , \ L = 0 \ , \ J = 0 \text{ (total values)}$$

or that

$$\sum_{i=1}^{8} \vec{\mu}_i \cdot \vec{B} = 0 = \sum_{i=1}^{8} \vec{L}_i \cdot \vec{B}$$

We also have that

$$\sum_{i=1}^{8} \frac{1}{r_i^2} \frac{dV(r_i)}{dr_i} \vec{L}_i \cdot \vec{S}_i = 0$$

as is shown below:

The wave functions of the system are the products of the following functions (excluding radial parts)

$$\begin{array}{l} Y_{00}(\hat{e}_1)Y_{00}(\hat{e}_2)\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1\right) \\ Y_{11}(\hat{e}_3)Y_{11}(\hat{e}_2)\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_3 |\downarrow\rangle_4 - |\uparrow\rangle_4 |\downarrow\rangle_3\right) \\ Y_{10}(\hat{e}_5)Y_{10}(\hat{e}_4)\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_5 |\downarrow\rangle_6 - |\uparrow\rangle_6 |\downarrow\rangle_5\right) \\ Y_{1,-1}(\hat{e}_7)Y_{1,-1}(\hat{e}_8)\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_7 |\downarrow\rangle_8 - |\uparrow\rangle_8 |\downarrow\rangle_7\right) \end{array}$$

where

$$\hat{e}_i = \frac{\vec{r}_i}{r_i}$$

This implies that all individual ℓ_z-values are paired and each pair has $S = 0$ (singlet spin state).

The total space wavefunction is symmetric so that the total spin vector must be antisymmetric.

Since

$$\begin{array}{l} \sigma_{1x}\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1\right) = \frac{1}{\sqrt{2}}\left(|\downarrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\uparrow\rangle_1\right) \\ \sigma_{2x}\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1\right) = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\uparrow\rangle_2 - |\downarrow\rangle_2 |\downarrow\rangle_1\right) \end{array}$$

and so on .....

Then taking the scalar product with

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1\right)^+$$

we get

$$\langle\sigma_{1x}\rangle = \langle\sigma_{2x}\rangle = \langle\sigma_{1y}\rangle = \langle\sigma_{2y}\rangle = \langle\sigma_{1z}\rangle = \langle\sigma_{2z}\rangle = 0$$

Therefore,

$$\langle\sigma_{1z}L_{1z} + \sigma_{2z}L_{2z}\rangle \to \langle L_{1z}\rangle\langle\sigma_{1z}\rangle + \langle L_{2z}\rangle\langle\sigma_{2z}\rangle = 0$$

and so on.... Thus, the indicated term is zero. We then have

$$\hat{H} = \sum_{i=1}^{8}\left(\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}kr_i^2\right) + \frac{e^2}{2mc^2}\sum_{i=1}^{8}(\vec{B}\times\vec{r}_i)^2$$

which corresponds to 8 free oscillators + an extra term. The ground state energy is then

$$E_0 = 18\hbar\omega + \frac{e^2}{8mc^2}\sum_{i=1}^{8}\left\langle(\vec{B}\times\vec{r}_i)^2\right\rangle = 18\hbar\omega + \frac{e^2B^2}{8mc^2}\sum_{i=1}^{8}\left\langle r_i^2\sin^2\theta_i\right\rangle$$

and the magnetization is

$$-\frac{\partial E_0}{\partial B} = \frac{e^2B}{4mc^2}\sum_{i=1}^{8}\left\langle r_i^2\sin^2\theta_i\right\rangle = \chi B \quad ,\ \chi = \text{ susceptibility(diamagnetic)}$$

and

$$\chi = -\frac{e^2}{4mc^2}\sum_{i=1}^{8}\left\langle r_i^2\sin^2\theta_i\right\rangle$$

12.9.9 2 interacting particles

Consider two particles of masses $m_1 \neq m_2$ interacting via the Hamiltonian

$$\hat{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m_1\omega^2x_1^2 + \frac{1}{2}m_2\omega^2x_2^2 + \frac{1}{2}K(x_1-x_2)^2$$

(a) Find the exact solutions.

We let

$$R = \frac{m_1x_1 + m_2x_2}{m_1+m_2} \quad , \quad r = x_1 - x_2$$

We then have

$$\begin{aligned}\tfrac{d}{dx_1} &= \tfrac{\partial R}{\partial x_1}\tfrac{d}{dR} + \tfrac{\partial r}{\partial x_1}\tfrac{d}{dr} = \tfrac{m_1}{m_1+m_2}\tfrac{d}{dR} + \tfrac{d}{dr}\\ \tfrac{d^2}{dx_1^2} &= \left(\tfrac{m_1}{m_1+m_2}\right)^2\tfrac{d^2}{dR^2} + \tfrac{2m_1}{m_1+m_2}\tfrac{d^2}{drdR} + \tfrac{d^2}{dr^2}\end{aligned}$$

and similarly,

$$\frac{d^2}{dx_2^2} = \left(\frac{m_2}{m_1+m_2}\right)^2\frac{d^2}{dR^2} - \frac{2m_2}{m_1+m_2}\frac{d^2}{drdR} + \frac{d^2}{dr^2}$$

In addition,

$$x_1^2 = R^2 + \tfrac{2m_2}{m_1+m_2} Rr + \left(\tfrac{m_2}{m_1+m_2}\right)^2 r^2$$
$$x_2^2 = R^2 - \tfrac{2m_1}{m_1+m_2} Rr + \left(\tfrac{m_1}{m_1+m_2}\right)^2 r^2$$

Therefore, the Hamiltonian becomes

$$H = \left(-\frac{\hbar^2}{2M}\frac{d^2}{dR^2} + \frac{1}{2}M\omega^2 R^2\right) + \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{1}{2}\mu\left(1 + \frac{K}{\mu\omega^2}\right)\omega^2 2^2\right)$$

where

$$M = m_1 + m_2 = \text{ total mass} \quad , \quad \mu = \frac{m_1 m_2}{m_1 + m_2} = \text{ reduced mass}$$

We thus have two independent harmonic oscillators and we can write

$$E_{pq} = (p + 1/2)\,\hbar\omega + (q + 1/2)\,\hbar\omega\sqrt{1 + \frac{K}{\mu\omega^2}} \quad , \quad p, q = 0, 1, 2, 3, ...$$

and

$$\psi_{pq}(R, r) = \psi_p(R)\psi_q(r) = N_p N_q e^{-\alpha_1^2 R^2/2} H_p(\alpha_1 R) e^{-\alpha_2^2 r^2/2} H_q(\alpha_2 r)$$

where

$$N_p = \left(\tfrac{\alpha_1}{\sqrt{\pi} 2^p p!}\right)^{1/2} \quad , \quad \alpha_1 = \left(\tfrac{M\omega}{\hbar}\right)^{1/2}$$
$$N_q = \left(\tfrac{\alpha_2}{\sqrt{\pi} 2^q q!}\right)^{1/2} \quad , \quad \alpha_2 = \left(\tfrac{\mu\omega}{\hbar}\right)^{1/2} \left(1 + \tfrac{K}{\mu\omega^2}\right)^{1/4}$$

(b) Sketch the spectrum in weak coupling limit $K << \mu\omega^2$ where μ = reduced mass.

For $K << \mu\omega^2$ we have

$$\left(1 + \frac{K}{\mu\omega^2}\right)^{1/4} \approx 1$$

so that

$$E_{pq} = (p + q + 1)\,\hbar\omega = (N + 1)\hbar\omega = E_N \quad , \quad N = 0, 1, 2, 3, ...$$

The energy level(degeneracy) structure looks like:

degeneracy	N				
4	3	$p=3, q=0$	$p=2, q=1$	$p=1, q=2$	$p=0, q=3$
3	2	$p=2, q=0$	$p=1, q=1$	$p=0, q=2$	
2	1	$p=1, q=0$	$p=0, q=1$		
1	0	$p=0, q=0$			

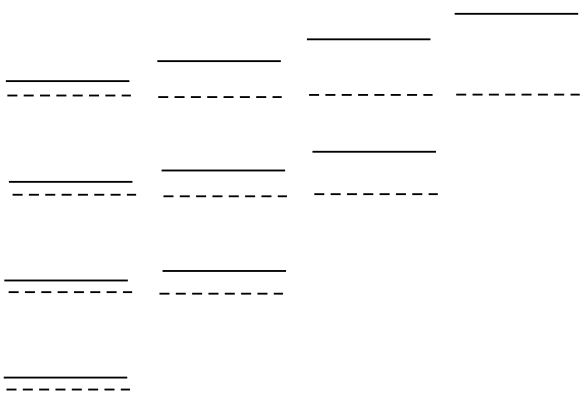
If $K < \mu\omega^2$ we have

$$\left(1+\frac{K}{\mu\omega^2}\right)^{1/4} \approx 1+\frac{K}{2\mu\omega^2}$$

so that energy levels with the same q value will move upwards by

$$(q+1/2)\hbar\omega\left(\frac{K}{2\mu\omega^2}\right)$$

as we show schematically below.



Clearly, the degeneracies are broken!

12.9.10 LS versus JJ coupling

Consider a multielectron atom whose electron configuration is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p 4d$$

(a) To what element does this configuration belong? Is it the ground state or an excited state? Explain.

We have $Z = 32$ which is Germanium. It is an excited state of Germanium. The ground state is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$$

(b) Suppose that we apply the Russell-Saunders coupling scheme to this atom. Draw and energy level diagram roughly to scale for the atom, beginning with the single unperturbed configuration energy and taking into account the various interactions one at a time in the correct order. Be sure to label each level at each stage of your diagram with the appropriate term designation, quantum numbers and so on.

We consider two electrons in a $4p4d$ configuration. Following Chapter 12, in the LS-Coupling scheme we have:

$$\begin{aligned}
&\ell_1 = 1, \ell_2 = 2 \rightarrow L = 1, 2, 3 \\
&s_1 = s_2 = \tfrac{1}{2} \rightarrow S = 0, 1 \\
&3 \otimes 1 \rightarrow J = 4, 3, 2 \\
&3 \otimes 0 \rightarrow J = 3 \rightarrow 7 \text{ states} \\
&2 \otimes 1 \rightarrow J = 3, 2, 1 \rightarrow 16 \text{ states} \\
&2 \otimes 0 \rightarrow J = 2 \rightarrow 5 \text{ states} \\
&1 \otimes 1 \rightarrow J = 2, 1, 0 \rightarrow 9 \text{ states} \\
&1 \otimes 0 \rightarrow J = 1 \rightarrow 3 \text{ states}
\end{aligned}$$

or

$J = 4$ in 1 level

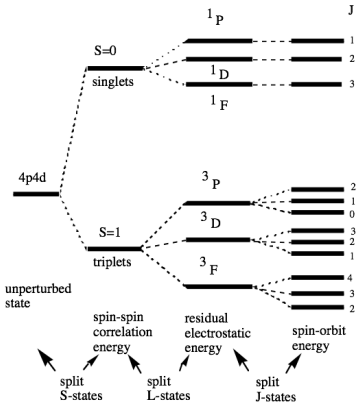
$J = 3$ in 3 levels

$J = 2$ in 4 levels

$J = 1$ in 3 levels

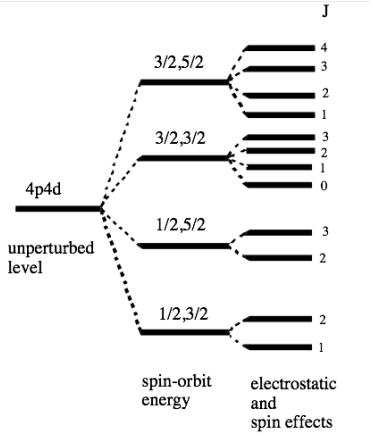
$J = 0$ in 1 level

We have 12 total levels. The energy diagram looks like:



(c) Suppose instead we apply pure $jj-$coupling to the atom. Starting again from the unperturbed $n = 4$ level, draw a second energy level diagram. [HINT: Assume that for a given level (j_1, j_2), the state with the lowest J lies lowest in energy]

In the $jj-$coupling scheme this looks like:



Notice that the final J values are identical, but their arrangement in energy is very different.

12.9.11 In a harmonic potential

Two identical, noninteracting spin= 1/2 particles of mass m are in a one dimensional harmonic oscillator potential for which the Hamiltonian is

$$H = \frac{p_{1x}^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{p_{2x}^2}{2m} + \frac{1}{2}m\omega^2 x_2^2$$

(a) Determine the ground-state and first-excited state kets and the corresponding energies when the two particles are in a total spin= 0 state. What are the lowest energy states and the corresponding kets for the particles if they are in a total spin= 1 state?

We decompose the Hamiltonian into two parts

$$\hat{H} = \left(\frac{\hat{p}_{1x}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_1^2\right) + \left(\frac{\hat{p}_{2x}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_2^2\right) = \hat{H}_1 + \hat{H}_2$$

where

$$\left[\hat{H}_1, \hat{H}_2\right] = 0$$

This means that we can the simultaneous eigenvectors of $\hat{H}_1$ and $\hat{H}_2$ by

$$|n_1 n_2\rangle\,|s, m_s\rangle$$

where

$$|n_1 n_2\rangle = 2- \text{ particle total spatial state}$$
$$|s, m_s\rangle = 2- \text{ particle total spin state}$$

and

$$E = (n_1 + n_2 + 1)\,\hbar\omega$$

The ground state is

$$|00\rangle\,|s = 0, m_s = 0\rangle$$

with energy

$$E_0 = \hbar\omega$$

The 1^{st} excited state has $E_1 = 2\hbar\omega$ and is 4-fold degenerate. The state vectors are

$$\frac{1}{\sqrt{2}}\left(|10\rangle + |01\rangle\right)|s = 0, m_s = 0\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle + |01\rangle\right)\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$
$$= (symmetric)(antisymmetric) = antisymmetric$$

$$\frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)|s = 1, m_s = 1\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)\left(|\uparrow\uparrow\rangle\right)$$
$$= (antisymmetric)(symmetric) = antisymmetric$$

$$\frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)|s = 1, m_s = 0\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$
$$= (antisymmetric)(symmetric) = antisymmetric$$

$$\frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)|s = 1, m_s = -1\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)\left(|\downarrow\downarrow\rangle\right)$$
$$= (antisymmetric)(symmetric) = antisymmetric$$

(b) Suppose that the two particles interact with a potential energy of interaction

$$V(|x_1 - x_2|) = \begin{cases} -V_0 & |x_1 - x_2| < a \\ 0 & \text{elsewhere} \end{cases}$$

Argue what the effect will be on the energies that you determined in (a), that is, whether the energy of each state moves up, moves down, or remains unchanged.

If the 2 particles interact with the potential energy function above, then the energy of the 2 particles will be lowered when the two particles are within a distance a of each other.

The spatial wave function will have a larger amplitude for particles to

be close together ($x_1 \approx x_2$) when the spatial wave function is symmetric rather than in the antisymmetric case, which vanishes when $x_1 \approx x_2$.

Since a symmetric spatial state means we must have an antisymmetric spin state, that is, $|s = 0, m_s = 0\rangle$, the total spin = 0 state will have lower energy than the $|s = 1, m_s = 0, \pm 1\rangle$ states.

This effect is solely due to the Pauli exclusion principle and antisymmetry of the total wavefunction since there is no spin dependent interaction that could lower the energy.

12.9.12 2 particles interacting via delta function

Two particles of mass m are placed in a rectangular box of sides $a > b > c$ in the lowest energy state of the system compatible with the conditions below. The particles interact with each other according to the potential $V = A\delta(\vec{r}_1 - \vec{r}_2)$. Using first order perturbation theory calculate the energy of the system under the following conditions:

(a) particles are not identical

The unperturbed system can be treated as consisting of 2 separate single-particle systems and the wave functions as a product of the 2 single-particle wave functions.

$$\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1)\psi(\vec{r}_2)$$

The lowest energy state wave function is thus (particles are not identical)

$$\psi_0(\vec{r}_1, \vec{r}_2) = \begin{cases} \frac{8}{abc} \sin\frac{\pi x_1}{a} \sin\frac{\pi x_2}{a} \sin\frac{\pi y_1}{b} \sin\frac{\pi y_2}{b} \sin\frac{\pi z_1}{c} \sin\frac{\pi z_2}{c} \\ \qquad\qquad 0 < x_i < a\,, 0 < y_i < b\,,\ 0 < z_i < c \\ 0 \qquad\qquad \text{otherwise} \end{cases}$$

corresponding to energy

$$E_0 = \frac{\hbar^2\pi^2}{2m}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)$$

First-order perturbation theory gives an energy correction

$$\Delta E = \int \psi_0^*(\vec{r}_1, \vec{r}_2) A\delta(\vec{r}_1 - \vec{r}_2)\psi_0(\vec{r}_1, \vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2 = A\int |\psi_0(\vec{r}_1, \vec{r}_1)|^2 d^3\vec{r}_1$$

$$= \left(\frac{8}{abc}\right)^2 \int_0^a \int_0^b \int_0^c \sin^4\frac{\pi x_1}{a} \sin^4\frac{\pi y_1}{b} \sin^4\frac{\pi z_1}{c} dx_1 dy_1 dz_1 = \frac{27A}{8abc}$$

so that (to 1^{st} order)

$$E_0 = \frac{\hbar^2\pi^2}{2m}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right) + \frac{27A}{8abc}$$

(b) identical particles of spin= 0

For a system of identical spin = 0 particles, the total wavefunction must be symmetric under interchange of any pair of particles. Therefore the lowest energy state is

$$\psi_{symmetric}(\vec{r}_1, \vec{r}_2) = \psi_0(\vec{r}_1, \vec{r}_2) = \psi_{111}(\vec{r}_1)\psi_{111}(\vec{r}_2)$$

where $\psi_{111}(\vec{r}_1)$ is the ground-state (single particle) wave function.

So the calculation is identical to (a) and we have

$$E_{0,symmetric} = \frac{\hbar^2\pi^2}{2m}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right) + \frac{27A}{8abc}$$

(c) identical particles of spin= 1/2 with spins parallel

For a system of identical spin = 1/2 particles the total wave function must be antisymmetric. Since the spins are parallel (a symmetric spin state) the spatial wave function must be antisymmetric.

Since

$$\frac{1}{a^2} < \frac{1}{b^2} < \frac{1}{c^2}$$

the lowest energy (antisymmetric) state is

$$\psi_{antisymmetric}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_{211}(\vec{r}_1)\psi_{111}(\vec{r}_2) - \psi_{211}(\vec{r}_2)\psi_{111}(\vec{r}_1)\right)$$

where we only need to change index corresponding to the $x-$direction where $|x| < a$ and where $\psi_{211}(\vec{r}_1)$ is the 1^{st} excited-state (single particle) wave function.

Therefore, the unperturbed energy is

$$E_{0,antisymmetric} = \frac{\hbar^2\pi^2}{2m}\left(\frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)$$

The first-order energy correction is

$$\Delta E = \int \psi^*_{anti}(\vec{r}_1, \vec{r}_2) A\delta(\vec{r}_1 - \vec{r}_2)\psi_{anti}(\vec{r}_1, \vec{r}_2) d^3\vec{r}_1 d^3\vec{r}_2 = 0$$

since it is the antisymmetric wave function is zero if $\vec{r}_1 = \vec{r}_2$ as required by the delta-function.

Therefore, to 1^{st} order

$$E_{0,antisymmetric} = \frac{\hbar^2\pi^2}{2m}\left(\frac{4}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)$$

12.9.13 2 particles in a square well

Two identical nonrelativistic fermions of mass m, spin$= 1/2$ are in a $1-$dimensional square well of length L with V infinitely large outside the well. The fermions are subject to a repulsive potential $V(x_1 - x_2)$, which may be treated as a perturbation.

(a) Classify the three lowest-energy states in terms of the states of the individual particles and state the spin of each.

For the unperturbed potential energy

$$V(x) = \begin{cases} 0 & x \in [0, L] \\ \infty & otherwise \end{cases}$$

the single particle wave functions are

$$\psi_n(x) = \begin{cases} \sqrt{2/L} \sin n\pi x/L & x \in [0, L] \\ 0 & \text{otherwise} \end{cases} \quad , \quad n = \text{ integer}$$

The spin vector of a single particle has the form

$$\begin{pmatrix} a \\ b \end{pmatrix}$$

Since we do not consider spin-dependent forces, the wave function of the two particles can be written as the product of the spatial part and the spin part.

The spin part $\chi_{SM} = \chi_S(M)$ is chosen as an eigenstate of $\vec{S} = \vec{S}_1 + \vec{S}_2$ and $S_z = S_{1z} + S_{2z}$, that is,

$$\vec{S}^2 \chi_{SM} = S(S+1)\hbar^2 \chi_{SM} \quad , \quad S_z \chi_{SM} = M\hbar \chi_{SM}$$

Now,

$$S = 0 \rightarrow \text{ spin singlet state}$$
$$\rightarrow \text{ antisymmetric under interchange of particles}$$

$$S = 1 \rightarrow \text{ spin triplet state}$$
$$\rightarrow \text{ symmetric under interchange of particles}$$

Symmetrizing and antisymmetrizing the spatial wave functions of the 2-particle system, we have

$$\psi^S_{nm}(x_1, x_2) = \begin{cases} \frac{1}{\sqrt{2}} \left(\psi_n(x_1)\psi_m(x_2) + \psi_n(x_2)\psi_m(x_1)\right) & n \neq m \\ \psi_n(x_1)\psi_n(x_2) & n = m \end{cases} \quad , \quad n = \text{ integer}$$

$$\psi^A_{nm}(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\psi_n(x_1)\psi_m(x_2) - \psi_n(x_2)\psi_m(x_1)\right)$$

The corresponding energies are

$$E_{nm} = \frac{\pi^2\hbar^2}{2mL^2}\left(n^2+m^2\right) \qquad n,m = 1,2,3,.....$$

The total wavefunctions, which must be antisymmetric (fermions), are

$$\begin{array}{l}\psi^A_{nm}(x_1,x_2)\chi^S_{SM} = \psi^A_{nm}(x_1,x_2)\chi_{00} \\ \psi^S_{nm}(x_1,x_2)\chi^A_{SM} = \psi^S_{nm}(x_1,x_2)\chi_{1M} \quad M = 0,\pm 1\end{array}$$

The three lowest energy states are the following:

1. the ground state has $n = m = 1$, which has a symmetric spatial state, and therefore is a spin singlet

$$\psi_0 = \psi^S_{11}(x_1,x_2)\chi_{00} \rightarrow \text{ non-degenerate}$$

2. the first excited state has $n = 1, m = 2$ so that

$$\psi_1 = \begin{cases}\psi^A_{12}(x_1,x_2)\chi_{1M} & M = 0,\pm 1 \\ \psi^S_{12}(x_1,x_2)\chi_{00}\end{cases} \quad , \quad n = \text{ integer}$$

   which is 4-fold degenerate.

3. the second excited state has $n = 2, m = 2$, which has a symmetric spatial state, and therefore is a spin singlet

$$\psi_2 = \psi^S_{22}(x_1,x_2)\chi_{00} \rightarrow \text{ non-degenerate}$$

(b) Calculate to first-order the energies of the second- and third- lowest states; leave your result in the form of an integral. Neglect spin-dependent forces throughout.

Because the perturbation is independent of spin, the calculation of the 1st-order energy correction can be treated as all non-degenerate cases (there are no nonzero off-diagonal matrix elements).

The corrections are

$$\begin{array}{l}\Delta E^A_1 = \int\int dx_1 dx_2 \left|\psi^A_{12}(x_1,x_2)\right|^2 V(x_1-x_2) \\ \Delta E^S_1 = \int\int dx_1 dx_2 \left|\psi^S_{12}(x_1,x_2)\right|^2 V(x_1-x_2) \\ \Delta E_2 = \int\int dx_1 dx_2 \left|\psi^S_{22}(x_1,x_2)\right|^2 V(x_1-x_2)\end{array}$$

12.9.14 2 particles interacting via a harmonic potential

Two particles, each of mass M are bound in a $1-$dimensional harmonic oscillator potential

$$V = \frac{1}{2}kx^2$$

and interact with each other through an attractive harmonic force $F_{12} = -K(x_1 - x_2)$. Assume that K is very small.

We have the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{1}{2}k\left(x_1^2 + x_2^2\right) + \frac{1}{2}K\left(x_1 - x_2\right)^2$$

(a) What are the energies of the three lowest states of this system?

We let

$$\xi = \frac{1}{\sqrt{2}}\left(x_1 + x_2\right) \quad , \quad \eta = \frac{1}{\sqrt{2}}\left(x_1 - x_2\right)$$

and the Hamiltonian becomes

$$\hat{H} = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2}\right) + \frac{1}{2}k\xi^2 + \frac{1}{2}\left(k + 2K\right)\eta^2$$

which corresponds to 2 independent harmonic oscillators with angular frequencies

$$\omega_1 = \sqrt{\frac{k}{M}} \quad , \quad \omega_2 = \sqrt{\frac{k + 2K}{M}}$$

The total energy of the system is

$$E_{nm} = (n + 1/2)\hbar\omega_1 + (m + 1/2)\hbar\omega_2$$

and the corresponding eigenfunctions are

$$|nm\rangle \rightarrow \psi_{nm} = \varphi_n^{(k)}\left(\xi\right)\varphi_m^{(k+2K)}\left(\eta\right)$$

where $n, m = 0, 1, 2, ...$ and $\varphi_n^{(k)}$ is the n^{th} eigenfunction of a harmonic oscillator with spring constant k.

Thus, the energies of the 3 lowest states of the system are

$$E_{00} = \frac{1}{2}\hbar(\omega_1 + \omega_2)\ ,\ E_{10} = \frac{1}{2}\hbar(\omega_1 + \omega_2) + \hbar\omega_1\ ,\ E_{01} = \frac{1}{2}\hbar(\omega_1 + \omega_2) + \hbar\omega_2$$

(b) If the particles are identical and spinless, which of the states of (a) are allowed?

If the two particles are identical and spinless, the wave function must be symmetric with respect to interchange of the two particles. Thus, the allowed states are

$$|1\rangle = |00\rangle \quad , \quad |2\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right)$$

which are symmetric.

(c) If the particles are identical and have spin= 1/2, which of the states of (a) are allowed?

If the particles are fermions, then the wave functions must be antisymmetric. Thus, the allowed states are

$$|1\rangle = |00\rangle\,|spin\ singlet\rangle \rightarrow \text{ non-degenerate}$$
$$|2\rangle = \tfrac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right)|spin\ singlet\rangle \rightarrow \text{ non-degenerate}$$
$$|3\rangle = \tfrac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)|spin\ triplet\rangle \rightarrow \text{ 3-fold degenerate}$$

12.9.15 The Structure of helium

Consider a Helium atom in the $1s2p$ configuration. The total angular momentum is $L = 1$ (a $P-$state). Due to the Fermi-Pauli symmetry this state splits into singlet and triplet multiplets as shown below.

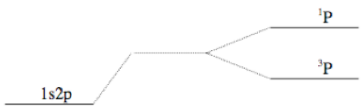


Figure 12.1: Fermi-Pauli Splittings

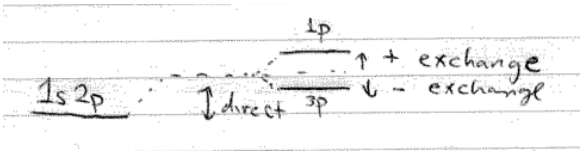
where the superscripts 1 and 3 represent the spin degeneracy for the singlet/triplet respectively.

(a) Explain qualitatively why the triplet state has lower energy.

Given the electron configuration $1s2p$, the total orbital angular momentum is

$$L = \ell_{1s} + \ell_{2p} = 0 + 1 = 1$$

so we have a $P-$state. We have the energy level diagram



The two-electron state is

$$|\Psi\rangle = (\text{spatial wave function}) \otimes (\text{spin state})$$
$$= \frac{1}{\sqrt{2}}(|\phi_{1s}\rangle\,|\phi_{2p}\rangle \pm |\phi_{2p}\rangle\,|\phi_{1s}\rangle) \otimes \left|\chi^{\mp}_{spin}\right\rangle$$

This is the Fermi symmetry, i.e., symmetric space function with antisymmetric spin state and antisymmetric space function with symmetric spin

state.

Now we have

$$\left|\chi^{-}_{spin}\right\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \text{singlet}$$

$$\left|\chi^{+}_{spin}\right\rangle \left\{ \begin{array}{ll} |\uparrow\uparrow\rangle & or \\ |\downarrow\downarrow\rangle & or \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & \end{array} \right\} \quad \text{triplet}$$

With a symmetric spatial wave function electrons are (on average) closer to together $\rightarrow$ more repulsion $\rightarrow$ higher energy. Thus, the singlet is higher energy than the triplet.

Now include spin-orbit coupling described by the Hamiltonian $\hat{H}_{SO} = f(r)\hat{L}\cdot\hat{S}$, where $\hat{L}$ and $\hat{S}$ are the total orbital and spin angular momentum respectively.

(b) Without the spin-orbit interaction, good quantum numbers for the angular momentum degrees of freedom are $|LM_LSM_S\rangle$. What are the good quantum numbers with spin-orbit present?

LS Coupling: We have $\hat{H}_{SO} = f(r)\hat{L}\cdot\hat{S}$. The good quantum numbers correspond to the coupled representation of $\vec{L}$ and $\vec{S}$, namely,

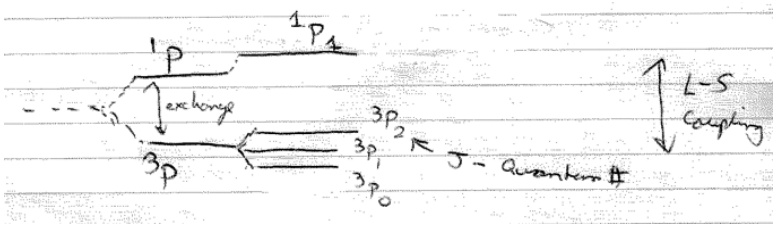
$$|JM_JLS\rangle$$

(c) The energy level diagram including spin-orbit corrections is sketched below.

Figure 12.2: Including Spin-Orbit

Label the states with appropriate quantum numbers. NOTE: Some of the levels are degenerate; the sublevels are not shown.

The possible J values are $|L-S| \leq J \leq L+S$. Therefore for the singlet $S=0$, we have $J=L=1$ and for the triplet $S=1$ we have $J=2,1,0$. The labelled energy diagram looks like:


$^1P_1$
^1P
exchange
$^3P_2$
$^3P_1$
$^3P_0$
^3P
J - quantum #
L-S
coupling