Quantum Mechanics 3 2001/2002

Solution set 8

(1) For the single-particle states,

$$E = n^2 \frac{\pi^2 \hbar^2}{8ma^2} \equiv \epsilon n^2.$$

Because this well is not centred on zero, the single-particle eigenstates are all just proportional to $\sin(n\pi x/2a) \equiv |n\rangle$. If we write the two-particle states as $|n_1, n_2\rangle$, the ground state is $|1,1\rangle$ ($E = 2\epsilon$). The first excited states are $|2,1\rangle$ and $|1,2\rangle$ ($E = 5\epsilon$). The second excited state is $|2,2\rangle$ ($E = 8\epsilon$). 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: $(\,|2,1\rangle \pm |1,2\rangle\,)/\sqrt{2}$; these would need to pair with spin wavefunctions that are respectively symmetric and antisymmetric. If $s > 0$, both are possible; if $s = 0$, only the symmetric space state is allowed.

The (normalized) ground-state wavefunction is

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

According to first-order perturbation theory, the change in the ground-state energy caused by H' is just $\delta E = \langle H' \rangle$, where the expectation value uses the unperturbed eigenfunctions:

$$\delta E = \iint \psi(x_1, x_2)^* \; H' \psi(x_1, x_2) \; dx_1 \, dx_2.$$

Now, H' contains $\delta(x_1 - x_2)$, and $\iint f(x_1, x_2)\,\delta(x_1 - x_2)\; dx_1\, dx_2 = \int f(x_1, x_1)\; dx_1$, for any function f. Therefore,

$$\delta E = -2aV_0 \int |\psi(x,x)|^2 \; dx = (-2/a)V_0 \int_0^{2a} \sin^4(\pi x/2a)\; dx = -4V_0 \int_0^1 \sin^4 \pi y \; dy.$$

The $\sin^4 \pi y$ looks nasty, but write it as $\sin^2 \pi y \times \sin^2 \pi y$ and use $\sin^2 \pi y = (1 - \cos 2\pi y)/2$. The integral then gives $3/8$, so $\delta E = -3V_0/2$.

(2)

(a) The allowed values of j range between $s_1 + s_2$ and $|s_1 - s_2|$ in integral steps. $s_1 = 1/2$ and $s_2 = 1/2$ therefore only permit the values $j = 1$ and 0. $j = 1$ allows $m = -1, 0, 1$; $j = 0$ is $m = 0$ only, so there are only three allowed values of m.

(b) Symmetric ('triplet') states are $u(1)u(2)$, $d(1)d(2)$ and $[u(1)d(2) + d(1)u(2)]/\sqrt{2}$. The antisymmetric ('singlet') state is $[u(1)d(2) - d(1)u(2)]/\sqrt{2}$. The $\sqrt{2}$ is there to keep the states normalized.

(c) The $m = 1$ state requires both particles to be spin up (so it must be $j = 1$ also). We therefore need the symmetric state $u(1)u(2)$. The $j = 0$ state is antisymmetric (although a proper proof of this requires Q3).

(d) 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 $\psi = u(\text{space}) \times v(\text{spin})$, then the symmetries of u & v must be opposite. Therefore, if $j = 0$ (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: $u(1,2) = [u_1(1)u_2(2) - u_2(1)u_1(2)]/\sqrt{2}$. The single-particle energies are $E = p^2/2m = (\hbar k)^2/2m$, 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 $E = 2 \times (\hbar\pi/L)^2/2m$, whereas the antisymmetric ground-state energy is a factor 5/2 larger.

(3) The commutation relations are $[J_x, J_y] = i\hbar J_z$, $[J_z, J_x] = i\hbar J_y$, and $[J_y, J_z] = i\hbar J_x$.

(a) First define the eigenstates ψ_m: $J_z\psi_m = m\hbar\psi_m$. To see if $J_\pm\psi_m$ is an eigenstate of J_z, we need to look at $J_zJ_\pm\psi_m$, which is equal to $J_\pm J_z\psi_m - [J_\pm, J_z]\psi_m$. The required commutator is $[J_\pm, J_z] = [J_x, J_z] \pm i[J_y, J_z]$, from the definition of $J_\pm$. From the basic commutators given at the start, this is $[J_\pm, J_z] = \hbar(-iJ_y \pm -J_x) = - \pm \hbar J_\pm$ (if treating $\pm$ like a number is confusing, do this separately for J_+ and J_-). Going back to $J_zJ_\pm\psi_m$, we can now write this as $J_\pm J_z\psi_m + \pm\hbar J_\pm\psi_m$. The first term is just $J_\pm m\hbar\psi_m$, so this is $(m \pm 1)\hbar(J_\pm\psi_m)$. Thus, $J_\pm\psi_m$ is an eigenstate of J_z, with eigenvalue $(m \pm 1)\hbar$. This establishes the raising and lowering property of $J_\pm$.

(b) Two electrons would have a total spin of $s = 1$ or 0, by the rule given in question 1. Adding a third spin-half particle creates total $s = 3/2$ or $1/2$ from the $s = 1$ two-particle state. The $s = 0$ two-particle state becomes $s = 1/2$ only on adding the third particle, so total $s = 3/2$ or $1/2$ are the only possibilities.

(c) The states with well-defined values of m_1, m_2 and m_3 for the z-spin components of all particles are the 'uncoupled basis'. Where all particles are 'spin up', this state may be written as $|\uparrow\uparrow\uparrow\rangle$. This state is also the $m = 3/2$ state of total $s = 3/2$ (there is no other way to get $m_1 + m_2 + m_3 = 3/2$ in the uncoupled basis). We can therefore write $|s = 3/2, m = 3/2\rangle = |\uparrow\uparrow\uparrow\rangle$. To get from here to $|s = 3/2, m = 1/2\rangle$, we need to apply $J_- = S_-^{(1)} + S_-^{(2)} + S_-^{(3)}$. In other words, the total lowering operator is the sum of the lowering operator for each separate spin (reasonably enough); this follows from the definition of J_- and $J_x = S_x^{(1)} + S_x^{(2)} + S_x^{(3)}$ etc. Now, we need to use the given normalization result. This says that

$$J_- \,|s=3/2, m=3/2\rangle = \sqrt{15/4 - 3/4}\,\hbar\,|s=3/2, m=1/2\rangle = \sqrt{3}\,\hbar\,|s=3/2, m=1/2\rangle.$$

Notice that the total quantum number, j, is the same as the overall spin quantum number, s, in this case. Therefore $|s=3/2, m=1/2\rangle = (1/\sqrt{3})J_-|s=3/2, m=3/2\rangle$. Using the given normalization result again for a single state, $S_-\,|1/2, 1/2\rangle = \sqrt{3/4+1/4}\,\hbar\,|1/2, -1/2\rangle$. This establishes the required result.

(d) When adding two spins, we get total $j = 1$ or 0. The $m = 1$ state can only arise in one way, so $|j=1, m=1\rangle = |\uparrow\uparrow\rangle$. To get to $|j=1, m=0\rangle$, we need to use $J_-\,|j=1, m=1\rangle = \sqrt{2}\,|j=1, m=0\rangle$, by the given normalization result. As before, J_- is the sum of the two individual lowering operators, so

$$|j=1, m=0\rangle = \frac{1}{\sqrt{2}}\big(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\big).$$

To find $|j=0, m=0\rangle$, we must have a combination similar to $|j=1, m=0\rangle$, with one spin up and one down (these are the only two ways to get $m = 0$). So, write

$$|j=0, m=0\rangle = a|\downarrow\uparrow\rangle + b|\uparrow\downarrow\rangle,$$

where a and b are unknown constants. We know that this state cannot be raised or lowered, unlike $|j=1, m=0\rangle$, so the effect of $J_\pm$ is zero. Consider the effect of $J_+ = S_+^{(1)} + S_+^{(2)}$ on $|j=0, m=0\rangle$: $S_+^{(1)}|\downarrow\uparrow\rangle = |\uparrow\uparrow\rangle$ and $S_+^{(1)}|\uparrow\downarrow\rangle = 0$, since the first spin cannot be raised if it is already up. Similar reasoning applies for the effect of $S_+^{(2)}$, leading to $J_+|j=0, m=0\rangle = (a+b)|\uparrow\uparrow\rangle = 0$. So, $a = -b$, and $|j=0, m=0\rangle$ is antisymmetric. Normalization gives $a = 1/\sqrt{2}$, since

$$\langle j=0, m=0|j=0, m=0\rangle = |a|^2\langle\downarrow\uparrow|\downarrow\uparrow\rangle + |b|^2\langle\uparrow\downarrow|\uparrow\downarrow\rangle + ab^*\langle\uparrow\downarrow|\downarrow\uparrow\rangle + ba^*\langle\downarrow\uparrow|\uparrow\downarrow\rangle.$$

The first two brackets are 1, the latter two vanish, though orthonormality. The sum is just $|a|^2 + |b|^2 = 2|a|^2$; this must be unity, through orthonormality for the bracket on the lhs. Therefore, $|a|^2 = 1/2$, and we can choose the phase so that a is real.