408 Final Solution Spring 15

Problem 1

Solution:

(a) A CSCO would be $\{H_x, H_y, H_z\}$ with $H_x = \frac{p_x^2}{2m} + V(x)$ etc. If we write out the energy spectrum, it's $E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$, you notice that the combination (n_x, n_y, n_z) uniquely defines each individual state (or lifts all the degeneracy).

(b) Once again, the energy levels are $E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$, with $n_x, n_y, n_z = 1, 2, 3....$ The possible values of each quantum number count for credits. For the 1-D case, take x as our spatial coordinate. We know the parity of the wavefunction alternates based on n_x is even or odd. Parity is even if n_x is odd and vise versa. Therefore, the 1-D parity operator is going to be

$$\mathcal{P} = e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}(H_x)^{\frac{1}{2}}} = e^{i\pi n_x}$$

However, for even n_x that operator gives eigenvalue $+1$, which means we get even parity. It's easy to fix just by multiplying (-1). Therefore, the parity for 1-D case is

$$\mathcal{P} = (-1)e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}(H_x)^{\frac{1}{2}}}$$

Now let's go back to the 3-D case, the parity is

$$\mathcal{P} = (-1)e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}(H_x)^{\frac{1}{2}}}(-1)e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}(H_y)^{\frac{1}{2}}}(-1)e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}(H_z)^{\frac{1}{2}}} = (-1)e^{i\pi(\frac{2mL^2}{\hbar^2\pi^2})^{\frac{1}{2}}\{(H_x)^{\frac{1}{2}}+(H_y)^{\frac{1}{2}}+(H_z)^{\frac{1}{2}}\}}$$

Each time the quantum number of any spatial dimension is increased by one, the parity of the overall wavefunction changes.

Someone asked a question in lecture, should we always have the sqrt of the Hamiltonian. The answer is no. Take the 1-D SHO as an example. We know the parity of the wavefunction alternates as n increases. The energy levels are $E_n = \hbar\omega(n + \frac{1}{2})$ for $n = 0, 1, 2...$ The parity operator including H in this case is

$$\mathcal{P} = e^{i\pi(\frac{H}{\hbar\omega} - \frac{1}{2})} = e^{i\pi n}$$

Here we don't need to fix anything since ground state is $n = 0$ with even parity.

(c) For ground state, $n_x = n_y = n_z = 0$, 1st order is trivially zero, since

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} xcos^2(\frac{\pi x}{L})dx \int_{-\frac{L}{2}}^{\frac{L}{2}} ycos^2(\frac{\pi y}{L})dy \int_{-\frac{L}{2}}^{\frac{L}{2}} dz = 0 \quad \text{for xy term, and same for the others}$$

(d) The wavefunction for the 1-D infinite square well located between $-\frac{L}{2}$ to $\frac{L}{2}$ is

$$\phi_n(x) = \sqrt{\frac{2}{L}}\begin{cases} cos(\frac{n\pi x}{L}) & n = 1, 3, 5, 7... \\ sin(\frac{n\pi x}{L}) & n = 2, 4, 6, 8... \end{cases}$$

For 3-D case, the 1st excited states are denoted as $|2,1,1\rangle$, $|1,2,1\rangle$, and $|1,1,2\rangle$ as from the notation $|n_x,n_y,n_z\rangle$. These are all degenerate in energy. Therefore, we need degenerate perturbation theory for this part. Corresponding wavefunctions are

$$\phi_{211} = (\sqrt{\frac{2}{L}})^3 sin(\frac{2\pi x}{L})cos(\frac{\pi y}{L})cos(\frac{\pi z}{L})$$

$$\phi_{121} = (\sqrt{\frac{2}{L}})^3 cos(\frac{\pi x}{L})sin(\frac{2\pi y}{L})cos(\frac{\pi z}{L})$$

$$\phi_{112} = (\sqrt{\frac{2}{L}})^3 cos(\frac{\pi x}{L})cos(\frac{\pi y}{L})sin(\frac{2\pi z}{L})$$

Our perturbation term is $V = \lambda(xy + yz + xz)$. Let's calculate the matrix element

$$\langle 211\,|V|\,121\rangle = \lambda \iiint \phi^*_{211}(xy + yz + xz)\phi_{121}dxdydz$$

The only term gets non-zero contribution is xy term based on parity argument. ie. in z spatial dimension, $\langle 211|$ and $|121\rangle$ are both even parity, therefore $\langle 211\,|z|\,121\rangle$ has odd parity and results in zero after integration. Thus

$$\begin{aligned}\langle 211\,|V|\,121\rangle &= \lambda \iiint \phi^*_{211} xy \phi_{121} dxdydz \\ &= (\frac{2}{L})^3\lambda \int_{-\frac{L}{2}}^{\frac{L}{2}} xcos(\frac{\pi x}{L})sin(\frac{2\pi x}{L})dx \int_{-\frac{L}{2}}^{\frac{L}{2}} ycos(\frac{\pi y}{L})sin(\frac{2\pi y}{L})dy \int_{-\frac{L}{2}}^{\frac{L}{2}} cos^2(\frac{\pi z}{L})dz \\ &= (\frac{2}{L})^3\lambda \Big[\int_{-\frac{L}{2}}^{\frac{L}{2}} xcos(\frac{\pi x}{L})sin(\frac{2\pi x}{L})dx\Big]^2 \frac{L}{2}\end{aligned}$$

The square comes from integrations over dx and dy being the same, $\frac{L}{2}$ comes from integration over dz. This results in the matrix

$$\langle V\rangle = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} (\frac{2}{L})^3\lambda \Big[\int_{-\frac{L}{2}}^{\frac{L}{2}} xcos(\frac{\pi x}{L})sin(\frac{2\pi x}{L})dx\Big]^2 \frac{L}{2}$$

You should be able to connect Prof. Hagen's solutions from here.

Problem 2

Before we do anything, let's back up a little bit. When we coupled two spin particles, we mentioned that our CSCO choice could be $\{S_1^2, S_2^2, S_{1z}, S_{2z}\}$ in the uncoupled basis, or $\{(\vec{S_1}+\vec{S_2})^2, S_1^2, S_2^2, (\vec{S_1}+\vec{S_2})_z\}$ in the coupled basis. In the CSCO, there isn't any particular reason that we choose the z-component, instead of choosing x or y component. Therefore, I could write my CSCO as $\{S_1^2, S_2^2, S_{1x}, S_{2y}\}$ in the uncoupled basis or $\{(\vec{S_1}+\vec{S_2})^2, S_1^2, S_2^2, (\vec{S_1}+\vec{S_2})_x\}$ in the coupled basis.

When we add 3 spin particles, the number of operators in the CSCO is at least 6, since each particle needs its total spin and one of its component and we have 3 particles. In the uncoupled basis, one CSCO choice would be $\{S_1^2, S_2^2, S_3^2, S_{1z}, S_{2z}, S_{3z}\}$, while in the coupled basis a CSCO is $\{(\vec{S_1} + \vec{S_2} + \vec{S_3})^2, S_1^2, S_2^2, S_3^2, (\vec{S_1} + \vec{S_2})^2, (\vec{S_1} + \vec{S_2} + \vec{S_3})_z\}$. For the coupled one, recall that we add the first two spins together, and add the third one to the result we get from coupling the first two. Once again, we could choose any component of the spin in our CSCO.

Now we are adding four spins together. CSCO in uncoupled basis is $\{S_1^2, S_2^2, S_3^2, S_4^2, S_{1z}, S_{2z}, S_{3z}, S_{4z}\}$. In the coupled basis, we could add the 1st and 2nd together, 3rd and 4th together. Therefore, a CSCO choice would be $\{(\vec{S_1} + \vec{S_2})^2, S_1^2, S_2^2, (\vec{S_1} + \vec{S_2})_z, (\vec{S_3} + \vec{S_4})^2, S_3^2, S_4^2, (\vec{S_3} + \vec{S_4})_z\}$. You could change the component if you'd like to.

(a)(b) Let's get back to the problem. If you are only asked to give a CSCO, both ones up there would work. However, here you want H to be diagonal in your CSCO basis. The reason that $\{(\vec{S_1} + \vec{S_2})^2, S_1^2, S_2^2, (\vec{S_1} + \vec{S_2})_z, (\vec{S_3} + \vec{S_4})^2, S_3^2, S_4^2, (\vec{S_3} + \vec{S_4})_z\}$ doesn't work is $(\vec{S_1} + \vec{S_2})_z, (\vec{S_3} + \vec{S_4})_z$ don't diagonalize H. Recall in the Pauli Spin matrices, if $H = AS_x$, H is only diagonalized in S_x eigenbasis, but not in S_z eigenbasis. Same situation here, based on the Hamiltonian given in this problem, we choose our CSCO to be $\{(\vec{S_1} + \vec{S_2})^2, S_1^2, S_2^2, (\vec{S_1} + \vec{S_2})_x, (\vec{S_3} + \vec{S_4})^2, S_3^2, S_4^2, (\vec{S_3} + \vec{S_4})_y\}$ so that H is diagonal. You also need to mention that they trivially commute to each other to get full credits.

The rest of parts are pretty clear based on the solutions.