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Practice for Qualifying Exams

Problem Source: **CMU August 2004 Qualifying Exam**

(a) Solve the energy eigenvalue equation for a particle of mass m in the square-well potential $V(x)$ that vanishes for 0 < x < a and equals $+\infty$ elsewhere. Show that the energy eigenvalues are given by:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}, n = 1,2,3,...$$

with the corresponding normalized energy eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Explicitly discuss the boundary conditions.

The boundary conditions are:

$$\psi(0) = \psi(a) = 0$$

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

Here boundary conditions on the derivative are waived in the case of an infinite-potential barrier. Showing that these solutions are valid by substitution, I take:

$$H\psi_n(x)$$
$$= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right) = \frac{\hbar^2}{2m}\sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)^2 \sin\left(\frac{n\pi x}{a}\right) = \frac{\hbar^2\pi^2 n^2}{2ma^2}\left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right)$$
$$= E_n\psi_n(x)$$

Showing that these solutions are normal by substitution, I take

$$\int_0^a \psi_n^2(x)dx = \frac{2}{a}\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a\left[\frac{1}{2} - \frac{1}{2}\cos\left(\frac{2n\pi x}{a}\right)\right]dx$$
$$= \frac{2}{a}\left[\frac{1}{2}a - \frac{1}{2}\left(\frac{a}{2n\pi}\right)\sin\left(\frac{2n\pi x}{a}\right)\right] \rightarrow boundary \rightarrow \frac{2}{a}\left[\frac{1}{2}a\right] = 1 = normalized$$

(b) Suppose we place two electrons (spin ½) in the infinite square well potential above. Determine the two-particle wave function, whose spatial part is $\psi_{n_1,n_2}(x_1, x_2)$ for the ground state(s) and the first excited state(s), neglecting electron-electron interactions. State the corresponding energies and degeneracies.

The ground state is non-degenerate, of energy $2E_1$:

$$\psi_{1,1}(x_1,x_2)=\frac{1}{\sqrt{2}}\psi_0(x_1)\psi_0(x_2)\left(\chi_-(\sigma_1)\chi_+(\sigma_2)-\chi_-(\sigma_2)\chi_+(\sigma_1)\right)$$

The minus sign comes from the anti-symmetric combination, since identical fermions are anti-symmetric under exchange of particles.

The first excited state has energy E_1+E_2, however, has degeneracy four:

$$\psi_{1,2}(x_1,x_2)=-\psi_{2,1}(x_1,x_2)$$

$$=\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_-(\sigma_2)-\psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_-(\sigma_1)\right)$$

or

$$=\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_+(\sigma_1)\chi_-(\sigma_2)-\psi_1(x_2)\psi_2(x_1)\chi_+(\sigma_2)\chi_-(\sigma_1)\right)$$

or

$$=\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_+(\sigma_2)-\psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_+(\sigma_1)\right)$$

or

$$=\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_-(\sigma_2)-\psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_-(\sigma_1)\right)$$

Four linearly independent solutions (not exactly the ones given, but linear combinations thereof) can be considered to correspond to $S=0, m_S=0; S=1, m_S\in\{-1,0,1\}$.

(c) **Repeat part (b) twice, first for a pair of spinless neutral pions π^0 and then for the case of an electron and a muon (spin-½) in the infinite square well potential ($m_e<m_\mu$). Again, ignore particle-particle interactions.**

In the case of spinless, neutral pions, the ground state $2E_0$ is non-degenerate and the first excited state E_0+E_1 is also non-degenerate:

$$\psi_{1,1}(x_1,x_2)=\psi_1(x_1)\psi_1(x_2)$$

$$\psi_{1,2}(x_1,x_2)=\psi_{2,1}(x_1,x_2)=\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2)+\psi_2(x_1)\psi_1(x_2)\right]$$

In the case of distinguishable spin-half particles, there is a great deal of degeneracy: The ground state has degeneracy four and energy $E_{e,1}+E_{\mu,1}$:

$$x_1 \to e^-$$
$$x_2 \to \mu$$
$$\psi_{1,1}(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)\chi_+(x_1)\chi_+(x_2)$$
$$or$$
$$= \psi_1(x_1)\psi_1(x_2)\chi_+(x_1)\chi_-(x_2)$$
$$or$$
$$= \psi_1(x_1)\psi_1(x_2)\chi_-(x_1)\chi_+(x_2)$$
$$or$$
$$= \psi_1(x_1)\psi_1(x_2)\chi_+(x_1)\chi_+(x_2)$$

The first excited state has energy $E_{e,0} + E_{\mu,1}$ and also has degeneracy four:

$$x_1 \to e^-$$
$$x_2 \to \mu$$
$$\psi_{0,1}(x_1, x_2) = \psi_0(x_1)\psi_1(x_2)\chi_+(x_1)\chi_+(x_2)$$
$$or$$
$$= \psi_0(x_1)\psi_1(x_2)\chi_+(x_1)\chi_-(x_2)$$
$$or$$
$$= \psi_0(x_1)\psi_1(x_2)\chi_-(x_1)\chi_+(x_2)$$
$$or$$
$$= \psi_0(x_1)\psi_1(x_2)\chi_+(x_1)\chi_+(x_2)$$

(d) The two electrons from part (b) interact via a spin-dependent interaction:

$U(r) = V(r) + \frac{\vec{S}_1 \cdot \vec{S}_2}{\hbar^2} W(r)$**, where** $V(r), W(r)$ **are potentials depending on** $r = |x_1 - x_2|$**. Find the lowest-order shifts in the ground state energy caused by U. You may leave your result in terms of clearly defined integrals. The following identities may prove helpful:**

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right) = \frac{1}{2}\left(S_{1+}S_{2-} + S_{1-}S_{2+}\right) + S_{1z}S_{2z}\,.$$

Finding the matrix element for this shift, I have:

$$E_0^{(1)} = \langle \psi_{1,1} | U | \psi_{1,1} \rangle = \langle \psi_{1,1} \| \left(V(r) + \left(\frac{1}{2}\left(S_{1+}S_{2-} + S_{1-}S_{2+}\right) + \frac{1}{4} \right) W(r) \right) \| \psi_{0,0} \rangle$$

$$= \frac{1}{2}\int_0^a\int_0^a \psi_0^2(x_1)\psi_0^2(x_2)\left[V(r) + \left(1+\frac{1}{4}\right)W(r)\right]dx_1dx_2 = \int_0^a\int_0^a \left[V(r)+\frac{5}{4}W(r)\right]\psi_0^2(x_1)\psi_0^2(x_2)dx_1dx_2$$

(e) Find the lowest-order shifts in the first excited energy state caused by U.

In order to find the energy shifts of this degenerate state, I must diagonalize the matrix

$$M_{i,j} = \int_0^a\int_0^a \left[V(r)+\frac{5}{4}W(r)\right]\psi_{1,0}^{i}(x_1,x_2)\psi_{1,0}^{j}(x_1,x_2)dx_1dx_2$$

The easiest way to do this will likely be to take the functions I found in (b) to the $|S, m_S\rangle$ basis, which are eigenstates of $\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right)$. However, to find the more-useful eigenstates of the potential or to integrate anything of the form $\int |x-y|^n \sin(ax)\sin(bx)dx$ is substantially more difficult.

For convenience, eigenstates of $\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right)$ will be given by:

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_-(\sigma_2) - \psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_-(\sigma_1)\right) = |1,-1\rangle$$

$$\frac{1}{2}\begin{bmatrix} \psi_1(x_1)\psi_2(x_2)\chi_+(\sigma_1)\chi_-(\sigma_2) - \psi_1(x_2)\psi_2(x_1)\chi_+(\sigma_2)\chi_-(\sigma_1) \\ -\left(\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_+(\sigma_2) - \psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_+(\sigma_1)\right) \end{bmatrix} = |0,0\rangle$$

$$\frac{1}{2}\begin{bmatrix} \psi_1(x_1)\psi_2(x_2)\chi_+(\sigma_1)\chi_-(\sigma_2) - \psi_1(x_2)\psi_2(x_1)\chi_+(\sigma_2)\chi_-(\sigma_1) \\ +\psi_1(x_1)\psi_2(x_2)\chi_-(\sigma_1)\chi_+(\sigma_2) - \psi_1(x_2)\psi_2(x_1)\chi_-(\sigma_2)\chi_+(\sigma_1) \end{bmatrix} = |1,0\rangle$$

$$\frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2)\chi_+(\sigma_1)\chi_+(\sigma_2) + \psi_1(x_2)\psi_2(x_1)\chi_+(\sigma_2)\chi_+(\sigma_1)\right) = |1,1\rangle$$

This leaves the matrix as (ordered $|0,0\rangle, |1,-1\rangle, |1,0\rangle, |1,1\rangle$)

$$\begin{bmatrix}
\iint\langle 0,0|V(r)-\frac{3}{4}W(r)|0,0\rangle & \iint\langle 1,-1|V(r)+\frac{1}{4}W(r)|0,0\rangle & \iint\langle 1,0|V(r)+\frac{1}{4}W(r)|0,0\rangle & \iint\langle 1,1|V(r)+\frac{1}{4}W(r)|0,0\rangle \\
\iint\langle 0,0|V(r)+\frac{1}{4}W(r)|1,-1\rangle & \iint\langle 1,-1|V(r)+\frac{1}{4}W(r)|1,-1\rangle & \iint\langle 1,0|V(r)+\frac{1}{4}W(r)|1,-1\rangle & \iint\langle 1,1|V(r)+\frac{1}{4}W(r)|1,-1\rangle \\
\iint\langle 0,0|V(r)+\frac{1}{4}W(r)|1,0\rangle & \iint\langle 1,-1|V(r)+\frac{1}{4}W(r)|1,0\rangle & \iint\langle 1,0|V(r)+\frac{1}{4}W(r)|1,0\rangle & \iint\langle 1,1|V(r)+\frac{1}{4}W(r)|1,0\rangle \\
\iint\langle 0,0|V(r)+\frac{1}{4}W(r)|1,1\rangle & \iint\langle 1,-1|V(r)+\frac{1}{4}W(r)|1,1\rangle & \iint\langle 1,0|V(r)+\frac{1}{4}W(r)|1,1\rangle & \iint\langle 1,1|V(r)+\frac{1}{4}W(r)|1,1\rangle
\end{bmatrix}$$

If I could perform these integrals and then diagonalize, I would have both the perturbed states and their energies.