PHY4370 ASSIGNMENT 5

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Problem 1. Problem 9.11 from Bransden and Joachain

(a) The original well of $0 \leq x \leq L$ becomes $0 \leq x \leq 2L$.

Let H_0 be the Hamiltonian of the original well and H_1 be the Hamiltonian of the expanded well:

$$\begin{aligned} H_0 &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x) \\ H_1 &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_1(x) \end{aligned}$$

The potentials are given by

$$\begin{aligned} V_0(x) &= \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases} \\ V_1(x) &= \begin{cases} 0 & 0 \leq x \leq 2L \\ \infty & \text{otherwise} \end{cases} \end{aligned}$$

Let ψ_k^0 and ϕ_n^1 be the eigenstates of H_0 and H_1, respectively. These are given by:

$$\begin{aligned} \psi_k^0(x) &= \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{k\pi}{L}x\right) \qquad x \in [0, L],\ k = 1, 2, 3... \\ \phi_n^1(x) &= \left(\frac{1}{L}\right)^{1/2} \sin\left(\frac{n\pi}{2L}x\right) \qquad x \in [0, 2L],\ n = 1, 2, 3... \end{aligned}$$

We know from (9.144) that the probability amplitudes d_n^1 of the particle being in the state ϕ_n^1 are given by

$$d_n^1 = \sum_k c_k^0 \langle \phi_n^1 | \psi_k^0 \rangle$$

Where c_k^0 are the probability amplitudes that the particle is in state ψ_k^0. Since we know the particle was in the ground state before the well expanded, $k = 1$, and $c_1^0 = 1$ and $c_k^0 = 0$ when $k \neq 0$. So

$$\begin{aligned} d_n^1 &= \langle \phi_n^1 | \psi_1^0 \rangle \\ &= \int_{-\infty}^{\infty} \phi_n^{1*} \psi_1^0 dx \\ &= \int_0^L \phi_n^{1*} \psi_1^0 dx \end{aligned}$$

Since $\psi_1^0(x) = 0$ for $x \notin [0, L]$.

$$\begin{aligned} d_n^1 &= \left(\frac{2}{L}\right)^{1/2} \left(\frac{1}{L}\right)^{1/2} \int_0^L \sin\left(\frac{n\pi}{2L}x\right) \sin\left(\frac{\pi}{L}x\right) dx \\ &= \frac{\sqrt{2}}{L} \int_0^L \sin\left(\frac{n\pi}{2L}x\right) \sin\left(\frac{\pi}{L}x\right) dx \end{aligned}$$

Expanding the integrand using the identity $\sin\alpha \sin\beta = \frac{1}{2}(\cos(\alpha - \beta) - \cos(\alpha + \beta))$:

$$\sin\left(\frac{n\pi}{2L}x\right) \sin\left(\frac{\pi}{L}x\right) = \frac{1}{2}\Big(\cos\left(\frac{\pi}{L}\left(\frac{n}{2} - 1\right)x\right) - \cos\left(\frac{\pi}{L}\left(\frac{n}{2} + 1\right)x\right)\Big)$$

So

$$\begin{aligned}
d_n^1 &= \frac{\sqrt{2}}{L}\frac{1}{2}\Big[\int_0^L \cos\left(\frac{\pi}{L}\left(\frac{n}{2}-1\right)x\right)dx - \int_0^L \cos\left(\frac{\pi}{L}\left(\frac{n}{2}+1\right)x\right)dx\Big] \\
&= \frac{\sqrt{2}}{L}\frac{1}{2}\Big[\frac{L}{\pi}\frac{2}{(n-2)}\sin\left(\frac{\pi}{L}\left(\frac{n}{2}-1\right)x\right) - \frac{L}{\pi}\frac{2}{(n+2)}\sin\left(\frac{\pi}{L}\left(\frac{n}{2}+1\right)x\right)\Big]_0^L \\
&= \frac{\sqrt{2}}{\pi}\Big[\frac{1}{n-2}\sin\left(\frac{\pi}{L}\left(\frac{n}{2}-1\right)x\right) - \frac{1}{n+2}\sin\left(\frac{\pi}{L}\left(\frac{n}{2}+1\right)x\right)\Big]_0^L \\
&= \frac{\sqrt{2}}{\pi}\Big[\frac{1}{n-2}\sin\left(\left(\frac{n}{2}-1\right)\pi\right) - \frac{1}{n+2}\sin\left(\left(\frac{n}{2}+1\right)\pi\right)\Big]
\end{aligned}$$

The probability is given by the square of the amplitude

$$P(n) = |d_n^1|^2 = \frac{2}{\pi^2}\Big[\frac{1}{n-2}\sin\left(\left(\frac{n}{2}-1\right)\pi\right) - \frac{1}{n+2}\sin\left(\left(\frac{n}{2}+1\right)\pi\right)\Big]^2$$

The case for $n=2$ can be evaluated by taking the limit of $P(n=x)$ as $x \to 2$ where x is real.

(b) Original well of $-L/2 \leq x \leq L/2$, expanded well of $-L \leq x \leq L$.

The Hamiltonians are the same but the potentials are now

$$\begin{aligned}
V_0(x) &= \begin{cases} 0 & -L/2 \leq x \leq L/2 \\ \infty & \text{otherwise} \end{cases} \\
V_1(x) &= \begin{cases} 0 & -L \leq x \leq L \\ \infty & \text{otherwise} \end{cases}
\end{aligned}$$

The states are split into even and odd principal quantum numbers. That is

$$\begin{aligned}
\psi_k^0(x) &= \begin{cases} \frac{\sqrt{2}}{\sqrt{L}}\cos\left(\frac{k\pi}{L}x\right) & k = 1,3,5... \\ \frac{\sqrt{2}}{\sqrt{L}}\sin\left(\frac{k\pi}{L}x\right) & k = 2,4,6... \end{cases} \qquad x \in [-L/2, L/2] \\
\phi_n^1(x) &= \begin{cases} \frac{1}{\sqrt{L}}\cos\left(\frac{n\pi}{2L}x\right) & n = 1,3,5... \\ \frac{1}{\sqrt{L}}\sin\left(\frac{n\pi}{2L}x\right) & n = 2,4,6... \end{cases} \qquad x \in [-L, L]
\end{aligned}$$

As before, the probability amplitudes are given by

$$d_n^1 = \langle \phi_n^1 | \psi_1^0 \rangle = \int_{-\infty}^{\infty} \phi_n^{1*}\psi_1^0 dx$$

The integrals are over the range $-L/2$ to $L/2$. To find the probability amplitudes for odd n, we do

$$d_{n_{\text{odd}}}^1 = \frac{1}{\sqrt{L}}\frac{\sqrt{2}}{\sqrt{L}}\int_{-L/2}^{L/2}\cos\left(\frac{n\pi}{2L}x\right)\cos\left(\frac{\pi}{L}x\right)dx$$

Expand with the identity $\cos\alpha\cos\beta = \frac{1}{2}(\cos(\alpha-\beta)+\cos(\alpha+\beta))$:

$$\begin{aligned}
d^1_{n_{\text{odd}}} &= \frac{\sqrt{2}}{L}\frac{1}{2}\Big[\int_{-L/2}^{L/2}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big)dx + \int_{-L/2}^{L/2}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big)dx\Big] \\
&= \frac{\sqrt{2}}{L}\frac{1}{2}\Big[\frac{L}{\pi}\frac{2}{(n-2)}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big) + \frac{L}{\pi}\frac{2}{(n+2)}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big)\Big]_{-L/2}^{L/2} \\
&= \frac{\sqrt{2}}{\pi}\Big[\frac{1}{n-2}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big) + \frac{1}{n+2}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big)\Big]_{-L/2}^{L/2} \\
&= \frac{\sqrt{2}}{\pi}\Big[\frac{1}{n-2}\Big(\sin\Big(\Big(\frac{n}{2}-1\Big)\frac{\pi}{2}\Big) - \sin\Big(-\Big(\frac{n}{2}-1\Big)\frac{\pi}{2}\Big)\Big) + \frac{1}{n+2}\Big(\sin\Big(\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big) - \sin\Big(-\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big)\Big)\Big] \\
&= \frac{\sqrt{2}}{\pi}\Big[\frac{2}{n-2}\sin\Big(\Big(\frac{n}{2}-1\Big)\frac{\pi}{2}\Big) + \frac{2}{n+2}\sin\Big(\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big)\Big]
\end{aligned}$$

The square of which is

$$P(n_{\text{odd}}) = \frac{2}{\pi^2}\Big[\frac{2}{n-2}\sin\Big(\Big(\frac{n}{2}-1\Big)\frac{\pi}{2}\Big) + \frac{2}{n+2}\sin\Big(\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big)\Big]^2$$

To find the probability amplitudes for even n we do

$$d^1_{n_{\text{even}}} = \frac{1}{\sqrt{L}}\frac{\sqrt{2}}{\sqrt{L}}\int_{-L/2}^{L/2}\sin\Big(\frac{n\pi}{2L}x\Big)\cos\Big(\frac{\pi}{L}x\Big)dx$$

and we use the identity $\sin\alpha\cos\beta = \frac{1}{2}(\sin(\alpha+\beta)+\sin(\alpha-\beta))$:

$$\begin{aligned}
d^1_{n_{\text{even}}} &= \frac{\sqrt{2}}{L}\Big[\int_{-L/2}^{L/2}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big)dx + \int_{-L/2}^{L/2}\sin\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big)dx\Big] \\
&= \frac{\sqrt{2}}{L}\frac{1}{2}\Big[-\frac{L}{\pi}\frac{2}{(n+2)}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big) - \frac{L}{\pi}\frac{2}{(n-2)}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big)\Big]_{-L/2}^{L/2} \\
&= \frac{\sqrt{2}}{\pi}\Big[-\frac{1}{(n+2)}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}+1\Big)x\Big) - \frac{1}{(n-2)}\cos\Big(\frac{\pi}{L}\Big(\frac{n}{2}-1\Big)x\Big)\Big]_{-L/2}^{L/2} \\
&= \frac{\sqrt{2}}{\pi}\Big[-\frac{1}{(n+2)}\Big(\cos\Big(\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big) - \cos\Big(-\frac{\pi}{2}\Big(\frac{n}{2}+1\Big)\Big)\Big) - \frac{1}{(n-2)}\Big(\cos\Big(\frac{\pi}{2}\Big(\frac{n}{2}-1\Big)\Big) - \cos\Big(-\frac{\pi}{2}\Big(\frac{n}{2}-1\Big)\Big) \\
&= \frac{\sqrt{2}}{\pi}[0-0] \\
&= 0
\end{aligned}$$

The square of which is $P(n_{\text{even}}) = 0$.

In part (a) we also found that the even states have a zero probability of being occupied. The numerical values for the odd states are different from part (a).

Problem 2. Problem 9.12 from Bransden and Joachain

Take the fourier transform of Ψ to get the wavefunction in momentum space.

Problem 3. Explore the symmetric gauge vector potential $\mathbf{A}_S = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ in the presence of a uniform magnetic field $\mathbf{B} = B\hat{z}$. The Hamiltonian is $H = \frac{1}{2m}(\mathbf{P} - q\mathbf{A}_S)^2$.

(a) Prove $\mathbf{B} = \nabla\times\mathbf{A}_S$.

$\mathbf{B} = B\hat{z}$ and $\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z}$. Then

$$\begin{aligned}\mathbf{A}_S &= \frac{1}{2}\mathbf{B}\times\mathbf{r} \\ &= \frac{1}{2}(-By, Bx, 0) \\ &= \frac{1}{2}B(-y, x, 0)\end{aligned}$$

Now take the curl where $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$:

$$\begin{aligned}\nabla\times\mathbf{A}_S &= \frac{1}{2}B\Big(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\Big)\times(-y, x, 0) \\ &= \frac{1}{2}B\Big(\frac{\partial x}{\partial z}, -\frac{\partial y}{\partial z}, \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y}\Big) \\ &= \frac{1}{2}B(0, 0, 2) \\ &= B\hat{z} \\ &= \mathbf{B}\end{aligned}$$

as needed.

(b) Prove the Hamiltonian is $H = \frac{1}{2m}\Big(\mathbf{P}^2 + \frac{q^2}{4}(B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2) - q\mathbf{B}\cdot\mathbf{L}\Big)$

$$\begin{aligned}H &= \frac{1}{2m}(\mathbf{P} - q\mathbf{A}_S)^2 \\ &= \frac{1}{2m}(\mathbf{P}^2 + q^2\mathbf{A}_S^2 - 2q\mathbf{P}\cdot\mathbf{A}_S)\end{aligned}$$

Notice

$$\mathbf{A}_S^2 = \frac{1}{4}(\mathbf{B}\times\mathbf{r})\cdot(\mathbf{B}\times\mathbf{r})$$

Use the vector identity $(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{C}\times\mathbf{D}) = (\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) - (\mathbf{B}\cdot\mathbf{C})(\mathbf{A}\cdot\mathbf{D})$:

$$\begin{aligned}\mathbf{A}_S^2 &= \frac{1}{4}((\mathbf{B}\cdot\mathbf{B})(\mathbf{r}\cdot\mathbf{r}) - (\mathbf{r}\cdot\mathbf{B})(\mathbf{B}\cdot\mathbf{r})) \\ &= \frac{1}{4}(B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2)\end{aligned}$$

Now

$$\begin{aligned}\mathbf{P}\cdot\mathbf{A}_S &= \frac{1}{2}\mathbf{P}\cdot(\mathbf{B}\times\mathbf{r}) \\ &= \frac{1}{2}\mathbf{B}\cdot(\mathbf{r}\times\mathbf{P}) \qquad (\text{by } \mathbf{A}\cdot(\mathbf{B}\times\mathbf{C}) = \mathbf{B}\cdot(\mathbf{C}\times\mathbf{A})) \\ &= \frac{1}{2}\mathbf{B}\cdot\mathbf{L}\end{aligned}$$

Substituting these results back in

$$\begin{aligned}H &= \frac{1}{2m}(\mathbf{P}^2 + q^2\mathbf{A}_S^2 - 2q\mathbf{P}\cdot\mathbf{A}_S) \\ &= \frac{1}{2m}\Big(\mathbf{P}^2 + q^2(\frac{1}{4}(B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2)) - 2q(\frac{1}{2}\mathbf{B}\cdot\mathbf{L})\Big) \\ &= \frac{1}{2m}\Big(\mathbf{P}^2 + \frac{q^2}{4}(B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2) - q\mathbf{B}\cdot\mathbf{L}\Big)\end{aligned}$$

If you substitute $\mathbf{B} = B\hat{z}$ you get

$$\begin{aligned} H &= \frac{1}{2m}\Big(\mathbf{P}^2 + \frac{q^2}{4}(B^2r^2 - (B^2z^2)) - qBL_z\Big) \\ &= \frac{1}{2m}\Big(\mathbf{P}^2 + \frac{q^2}{4}(B^2(r^2 - z^2)) - qBL_z\Big) \\ &= \frac{1}{2m}\Big(\mathbf{P}^2 + \frac{q^2B^2}{4}(x^2 + y^2) - qBL_z\Big) \end{aligned}$$

Problem 4. A hydrogen atom is placed in a time dependent electric field given by

$$\mathbf{E}(t) = \begin{cases} 0 & t < 0 \\ E_0 e^{-\gamma t}\hat{z} & t > 0 \end{cases}$$

What is the probability to first order as $t \to \infty$ the atom has made a transition from the ground state to the $2p$ state?

The transition probability to first order from a to b is

$$P_{ba}^{(1)}(\infty) = \frac{1}{\hbar^2}\Big| \int_0^\infty H'_{ba}(t)\exp(i\omega_{ba}t)dt \Big|^2$$

where

$$\omega_{ba} = \frac{E_b^{(0)} - E_a^{(0)}}{\hbar}$$

and

$$H'_{ba}(t) = \langle \psi_b^{(0)} | H'(t) | \psi_a^{(0)} \rangle$$

The position vector in spherical polar coordinates is $\mathbf{r} = r\sin\theta\cos\phi\hat{x} + r\sin\theta\sin\phi\hat{y} + r\cos\theta\hat{z}$. So the perturbed Hamiltonian is

$$\begin{aligned} H'(t) &= e\mathbf{r}\cdot\mathbf{E}(t) \\ &= eE_0 r\cos\theta\exp(-\gamma t) \end{aligned}$$

Now the ground state corresponds to the quantum numbers $(n, l, m) = (1, 0, 0)$. The $2p$ state can be either $(n, l, m) = (2, 1, -1)$, $(2, 1, 0)$, or $(2, 1, 1)$.

For the case $m = 1$:

$$\begin{aligned} H'_{1s2p1} &= \langle \psi_{1,0,0} | eE_0 r\cos\theta\exp(-\gamma t) | \psi_{2,1,1} \rangle \\ &= eE_0 \int \psi^*_{1,0,0} r\cos\theta\exp(-\gamma t)\psi_{2,1,1} d\mathbf{r} \\ &= eE_0 \frac{1}{\sqrt{\pi a_0^3}} \frac{1}{8\sqrt{\pi a_0^5}} \int e^{-r/a_0} r\cos\theta e^{-\gamma t} r e^{-r/2a_0}\sin\theta e^{i\phi} d\mathbf{r} \\ &= eE_0 \frac{1}{8\pi a_0^4} e^{-\gamma t} \int e^{-3r/2a_0} r^2 \cos\theta\sin\theta e^{i\phi} d\mathbf{r} \\ &= eE_0 \frac{1}{8\pi a_0^4} e^{-\gamma t} \int_0^\infty e^{-3r/2a_0} r^4 dr \int_0^\pi \cos\theta\sin^2\theta d\theta \int_0^{2\pi} e^{i\phi} d\phi \\ &= 0 \end{aligned}$$

Because $\int_0^{2\pi} e^{i\phi d\phi} = \frac{1}{i}(e^{2i\pi} - e^0) = \frac{1}{i}(1-1) = 0$. This is also true for $m = -1$.

For the case $m = 0$:

$$\begin{aligned}
H'_{1s2p} &= eE_0 \int \psi^*_{1,0,0} r \cos\theta \exp(-\gamma t) \psi_{2,1,1} d\mathbf{r} \\
&= eE_0 \frac{1}{\sqrt{\pi a_0^3}} \frac{1}{\sqrt{32\pi a_0^5}} e^{-\gamma t} \int e^{-r/a_0} r^2 \cos^2\theta e^{-r/2a_0} d\mathbf{r} \\
&= eE_0 \frac{1}{\pi a_0^4 \sqrt{32}} e^{-\gamma t} \int_0^\infty e^{-3r/2a_0} r^4 dr \int_0^\pi \cos^2\theta \sin\theta d\theta \int_0^{2\pi} d\phi \\
&= eE_0 \frac{1}{\pi a_0^4 \sqrt{32}} e^{-\gamma t} \Big(\frac{24(2^5)a_0^5}{3^5}\Big)\Big(\frac{2}{3}\Big)(2\pi) \\
&= eE_0 \frac{4}{3\sqrt{32}} \frac{768 a_0}{243} e^{-\gamma t}
\end{aligned}$$

The transition probability is

$$\begin{aligned}
P^{(1)}_{1s2p} &= \frac{1}{\hbar^2} \Big| \int_0^\infty H'_{ba}(t) \exp(i\omega_{ba} t) dt \Big|^2 \\
&= \frac{1}{\hbar^2} \Big| \int_0^\infty eE_0 \frac{4}{3\sqrt{32}} \frac{768 a_0}{243} e^{-\gamma t} e^{i\omega_{1s2p} t} dt \Big|^2 \\
&= \frac{16 e^2 E_0^2 a_0^2}{9(32)\hbar^2} \Big(\frac{768 a_0}{243}\Big)^2 \Big| \int_0^\infty e^{-\gamma t} e^{i\omega_{1s2p} t} dt \Big|^2
\end{aligned}$$

Now, the energy levels are given by $E_n = -\frac{e^2}{4\pi\epsilon_0 a_0} \frac{1}{2n^2}$. So

$$\begin{aligned}
\omega_{1s2p} &= \frac{E_2 - E_1}{\hbar} \\
&= -\frac{e^2}{4\pi\epsilon_0 a_0 \hbar} (\frac{1}{32} - \frac{1}{2}) \\
&= \frac{63}{64} \frac{e^2}{4\pi\epsilon_0 a_0 \hbar}
\end{aligned}$$

unfinished.