PHSX 462: HW02

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Question 1

Show that $\Psi = e^{ig}\Psi'$ is a solution to

$$\left[\frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

where

$$g(\vec{r}) = \frac{q}{h}\int_{\mathcal{O}}^{\vec{r}} \vec{A}(\vec{r}')\cdot \mathrm{d}\vec{r} \qquad\qquad -\frac{\hbar^2}{2m}\nabla^2\Psi' = i\hbar\frac{\partial\Psi'}{\partial t}$$

In the hints is also provided that $g = \frac{q}{\hbar}\alpha\Big|_{\mathcal{O}}^{\vec{r}}$, since the $\boldsymbol{\nabla}\times A = 0$. So, $\boldsymbol{\nabla} g = \frac{q}{\hbar}A\Big|_{\mathcal{O}}^{\vec{r}} = \frac{q}{\hbar}A(\vec{r})$. The only other thing that needs to be noticed is that g is independent of t, thus it can be moved inside a partial derivative with respect to t.

$$\begin{aligned}
\left[\frac{1}{2m}\left(-i\hbar\nabla - qA\right)^2\right]\Psi &= \left[\frac{1}{2m}\left(-i\hbar\nabla - qA\right)\left(-i\hbar\nabla - qA\right)\right]e^{ig}\Psi' \\
&= \frac{1}{2m}\left(-i\hbar\nabla - qA\right)\left[-i\hbar\left(\boldsymbol{\nabla}e^{ig}\right)\Psi' - i\hbar e^{ig}\boldsymbol{\nabla}\Psi' - qAe^{ig}\Psi'\right] \\
&= \frac{1}{2m}\left(-i\hbar\nabla - qA\right)\left[-i\hbar e^{ig}\left(\boldsymbol{\nabla}ig\right)\Psi' - i\hbar e^{ig}\boldsymbol{\nabla}\Psi' - qAe^{ig}\Psi'\right] \\
&= \frac{1}{2m}\left(-i\hbar\nabla - qA\right)\left[-i\hbar e^{ig}i\frac{q}{\hbar}A\Psi' - i\hbar e^{ig}\boldsymbol{\nabla}\Psi' - qAe^{ig}\psi'\right] \\
&= \frac{1}{2m}\left(-i\hbar\nabla - qA\right)\left[-i\hbar e^{ig}\boldsymbol{\nabla}\Psi'\right] \\
&= \frac{1}{2m}\left[\hbar e^{ig}i\boldsymbol{\nabla}g\boldsymbol{\nabla}\Psi' - \hbar e^{ig}\nabla^2\Psi' + qAi\hbar e^{ig}\boldsymbol{\nabla}\Psi'\right] \\
&= \frac{1}{2m}\left[\hbar e^{ig}i\frac{q}{\hbar}A\boldsymbol{\nabla}\Psi' - \hbar e^{ig}\nabla^2\Psi' + qAi\hbar e^{ig}\boldsymbol{\nabla}\Psi'\right] \\
&= -\frac{1}{2m}\hbar e^{ig}\nabla^2\Psi' \\
&= -\frac{\hbar}{2m}e^{ig}\nabla^2\Psi' \\
&= e^{ig}\frac{\partial\Psi'}{\partial t} = \frac{\partial e^{ig}\Psi'}{\partial t} = \frac{\partial\Psi}{\partial t}
\end{aligned}$$

Griffiths 7.1

Find the first-order correction to the allowed energies and the first three terms of the first order correction to the ground state, Ψ_1^1.

$$H' = \alpha\delta(x - a/2)$$

Before we get started, let's remind ourselves of the general solutions to an infinite potential well:

$$E_n^0 = \hbar^2 \frac{n^2\pi^2}{2a^2 m} \qquad\qquad \left|\psi_m^0\right\rangle \to \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

a)

$$\begin{aligned}
E_n^1 &= \left\langle\Psi_n^0\middle|H_1\middle|\Psi_n^0\right\rangle \\
&= \left\langle\Psi_n^0\middle|\alpha\delta\left(x - \frac{a}{2}\right)\middle|\Psi_n^0\right\rangle \\
&= \alpha\frac{2}{a}\sin^2\left(\frac{n\pi}{a}\frac{a}{2}\right)
\end{aligned}$$

Using the properties of the sin function, if n is even then $\sin(k\pi) = 0$ such that $k \in \mathbb{N}$. So, the even energies are not changed, but the odd ones are. This is a nature of what the probability distribution looks like. If the n is odd, then a node is located at the center of the well and the delta function will not have an impact.

$$E_n^1 = \begin{cases} \frac{2}{a} & n \text{ is odd} \\ 0 & n \text{ is even} \end{cases}$$

b) For this part we need to recall:

$$\left|\Psi_n^1\right\rangle = \sum_{m \neq n} \frac{\left\langle\Psi_m^0\middle|H'\middle|\Psi_n^0\right\rangle}{E_n^0 - E_m^0}\left|\Psi_m^0\right\rangle$$

now, simply doing the calculation we get that:

$$\begin{aligned}
\left|\Psi_1^1\right\rangle &= \sum_{m \neq 1} \frac{\left\langle\Psi_m^0\middle|H'\middle|\Psi_1^0\right\rangle}{E_1^0 - E_m^0}\left|\Psi_m^0\right\rangle \\
&= \sum_{m \neq 1} \frac{1}{E_1^0 - E_m^0}\frac{2}{a}\int \sin\left(\frac{n\pi}{a}x\right)\delta\left(x - \frac{a}{2}\right)\sin\left(\frac{\pi}{a}x\right)\mathrm{d}x\left|\Psi_m^0\right\rangle \\
&= \sum_{m \neq 1} \frac{1}{E_1^0 - E_m^0}\frac{2}{a}\sin\left(\frac{n\pi}{a}\frac{a}{2}\right)\left|\Psi_m^0\right\rangle \\
&= \sum_{m \neq 1} \frac{1}{E_1^0 - E_m^0}\frac{2}{a}\sin\left(\frac{n\pi}{2}\right)\left|\Psi_m^0\right\rangle \\
&= \frac{4ma}{\hbar^2\pi^2}\left(\frac{1}{1-3^2}\sin\left(\frac{3\pi}{2}\right)\sin\left(\frac{3\pi}{2}x\right) + \frac{1}{1-5^2}\sin\left(\frac{5\pi}{2}\right)\sin\left(\frac{5\pi}{2}x\right)\right. \\
&\qquad \left. + \frac{1}{1-7^2}\sin\left(\frac{7\pi}{2}\right)\sin\left(\frac{7\pi}{2}x\right) + \cdots\right) \\
&= \frac{4ma}{\hbar^2\pi^2}\left(\frac{1}{8}\sin\left(\frac{3\pi}{2}x\right) - \frac{1}{24}\sin\left(\frac{5\pi}{2}x\right) + \frac{1}{48}\sin\left(\frac{7\pi}{2}x\right) + \cdots\right)
\end{aligned}$$

So, the first three terms in the first order correction is:

$$\boxed{\left|\Psi_1^1\right\rangle = \frac{4ma}{\hbar^2\pi^2}\left(\frac{1}{8}\sin\left(\frac{3\pi}{2}x\right) - \frac{1}{24}\sin\left(\frac{5\pi}{2}x\right) + \frac{1}{48}\sin\left(\frac{7\pi}{2}x\right)\right)}$$

Griffiths 7.2

Find the exact solution to the permutated system, then find the first-order perturbation in the energy and compare the two.

$$V(x) = \frac{1}{2}kx^2 \,;\; k \to (1+\varepsilon)k$$

a) This part is pretty straight forward, so let's just do it.

$$\begin{aligned}
E_n &= \left(n+\frac{1}{2}\right)\hbar\omega \\
&= \left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}} \\
&\to \left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{(1+\varepsilon)k}{m}} && \text{(Changing } k \to (1+\varepsilon)k\text{)} \\
&= \left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\sqrt{1+\varepsilon} \\
&= \left[\left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\right]\left[1+\frac{\varepsilon}{2}-\frac{\varepsilon^2}{8}+\frac{\varepsilon^3}{16}-\frac{5\varepsilon^4}{128}+\cdots\right] && \text{(Assuming that } \varepsilon < 1\text{)} \\
&\to \left[\left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}\right]\left[1+\frac{\varepsilon}{2}-\frac{\varepsilon^2}{8}\right]
\end{aligned}$$

b) We are p

$$\begin{aligned}
E_n' &= \langle \Psi_n^0 | H' | \Psi_n^0 \rangle \\
&= \langle \Psi_n^0 | \varepsilon\frac{1}{2}kx^2 | \Psi_n^0 \rangle \\
&= \varepsilon\,\langle \Psi_n^0 | \frac{1}{2}kx^2 | \Psi_n^0 \rangle \\
&= \varepsilon\hbar\sqrt{\frac{k}{m}}\left(n+\frac{1}{2}\right)\langle \Psi_n^0 | \Psi_n^0 \rangle \\
&= \varepsilon\sqrt{\frac{k}{m}}\left(n+\frac{1}{2}\right)
\end{aligned}$$

We have to recognize that the permutation is on the potential energy, not the total energy. Using the Vivial Theorem to draw a parallel to the classical system: $E = \langle V \rangle + \langle T \rangle$ and $\langle V \rangle = \langle T \rangle$. So, $\langle V \rangle = \frac{1}{2}E$

Using this, the first order correction is: $\boxed{E_n^1 = \left[\sqrt{\frac{k}{m}}\left(n+\frac{1}{2}\right)\right]\frac{\varepsilon}{2}}$; which is exactly what we got for part **a)**.

If it wasn't clear earlier:

$$\boxed{H_n' = \varepsilon\frac{1}{2}kx^2}$$

Griffiths 7.4

Find the exact energies of a permutated two-level system. Then take the second order expansion of λ and set $\lambda = 1$. Verify that this is consistent with the perturbation theory that we derived. When does this converge if $V_{aa} = V_{bb} = 0$

$$H^0 = \begin{pmatrix} E_a^0 & 0 \\ 0 & E_b^0 \end{pmatrix} \qquad H' = \lambda \begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix}$$

$$V_{ba} = V_{ab}^*$$

a)

$$H = H_0 + H_1 = \begin{bmatrix} E_a^0 + \lambda v_{aa} & \lambda v_{ab} \\ \lambda v_{ba} & E_b^0 + \lambda v_{bb} \end{bmatrix} \to \begin{bmatrix} A & \lambda v_{ab} \\ \lambda v_{ab}^* & B \end{bmatrix} \qquad \text{s.t.} \quad \begin{aligned} A &= E_a^0 + \lambda v_{aa} \\ B &= E_b^0 + \lambda v_{bb} \end{aligned}$$

Looking for the eigenvalues of H

$$\begin{aligned} \begin{vmatrix} A - E & \lambda v_{ab} \\ \lambda v_{ab}^* & B - E \end{vmatrix} &= AB - E(A+B) + E^2 + \lambda^2 |v_{ab}|^2 \\ &= E^2 - E(A+B) + AB + C \qquad \text{s.t. } C = \lambda^2 |v_{ab}|^2 \end{aligned}$$

$$\begin{aligned} E &= \frac{(A+B) \pm \sqrt{(A+B)^2 - 4(AB+C)}}{2} \\ &= \frac{(A+B) \pm \sqrt{(A-B)^2 - 4C}}{2} \\ &= \frac{1}{2}\left[(A+B) \pm (A-B)\left(1 - \frac{4C}{2(A-B)^2} - \left(\frac{4C}{(A-B)^2}\right)^2 \frac{1}{8} + \cdots\right)\right] \\ &\boxed{= \frac{1}{2}\left[(A+B) \pm \left((A-B) - \frac{2C}{A_B}\right) - \frac{2C^2}{(A-B)^3} + \cdots\right]} \end{aligned}$$

b) Assuming that $E_a^0 \,\&\, E_b^0 \gg \lambda v_{aa} \,\&\, \lambda v_{bb} \longrightarrow [A - B] \approx [E_a^0 - E_b^0]$:

$$\begin{aligned} E &\approx \frac{1}{2}\left[(A+B) \pm \left((A-B) - \frac{2C}{E_a^0 - E_b^0}\right)\right] \\ &= \frac{1}{2}\left[E_a^0 + E_b^0 + \lambda(v_{aa} + v_{bb}) \pm \left(E_a^0 - E_b^0 + \lambda(v_{aa} - v_{bb}) - \frac{2\lambda^2 |v_{ab}|^2}{E_a^0 - E_b^0}\right)\right] \\ &\to \frac{1}{2}\left[E_a^0 + E_b^0 + v_{aa} + v_{bb} \pm \left(E_a^0 - E_b^0 + v_{aa} - v_{bb} - \frac{2|v_{ab}|^2}{E_a^0 - E_b^0}\right)\right] \qquad \text{by setting } \lambda = 1 \end{aligned}$$

$$\boxed{\begin{aligned} E_+ &= E_a^0 + v_{aa} + \tfrac{|v_{ab}|^2}{E_b^0 - E_a^0} \\ E_- &= E_b^0 + v_{bb} + \tfrac{|v_{ab}|^2}{E_a^0 - E_b^0} \end{aligned}}$$

Checking this against our equation for the first order correction:

$$\begin{aligned} E^1 &= \langle + | H^1 | + \rangle \\ &= \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \begin{bmatrix} v_{aa} & v_{ab} \\ v_{ab}^* & v_{bb} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} v_{aa} \\ v_{ab}^* \end{bmatrix} = v_{aa} \end{aligned}$$

$$E^1 = \langle - | H^1 | - \rangle$$
$$= \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} v_{aa} & v_{ab} \\ v_{ab}^* & v_{bb} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} v_{ab} \\ v_{bb} \end{bmatrix} = v_{bb}$$

Bingo!

Now, checking for the second order:

$$E_a^2 = \frac{\left| \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} v_{aa} & v_{ab} \\ v_{ab}^* & v_{bb} \end{bmatrix} \right|^2}{E_- - E_+}$$
$$= \frac{\left| \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} v_{ab} \\ v_{bb} \end{bmatrix} \right|^2}{E_a - E_b} = \frac{|v_{ab}|^2}{E_a - E_b}$$

And, by a symmetric calculation:
$E_b^2 = \frac{|v_{ab}|^2}{E_b - E_a}$
This is the same second order correction that we have! ✓

c) In the exact solution, we used the binomial expansion on $\sqrt{1 - \frac{4C}{(A-B)^2}}$. So, we need

$$1 > \frac{4C}{(A-B)^2} = \frac{4\lambda^2 |v_{ab}|^2}{(E_a^0 + \lambda v_{aa} - E_b^0 - \lambda v_{bb})^2} > \frac{4\lambda^2 |v_{ab}|^2}{(E_a^0 - E_b^0)^2}$$

By setting $\lambda = 1$ and some algebra:
$$\boxed{\left| \frac{v_{ab}}{E_a^0 - E_b^0} \right| < \frac{1}{2}}$$

Question 5