PHSX 462: HW02

William Jardee

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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 $V_{aa} = V_{bb} = 0$

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

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

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

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

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

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:

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

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

Bingo!

Now, checking for the second order:

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

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

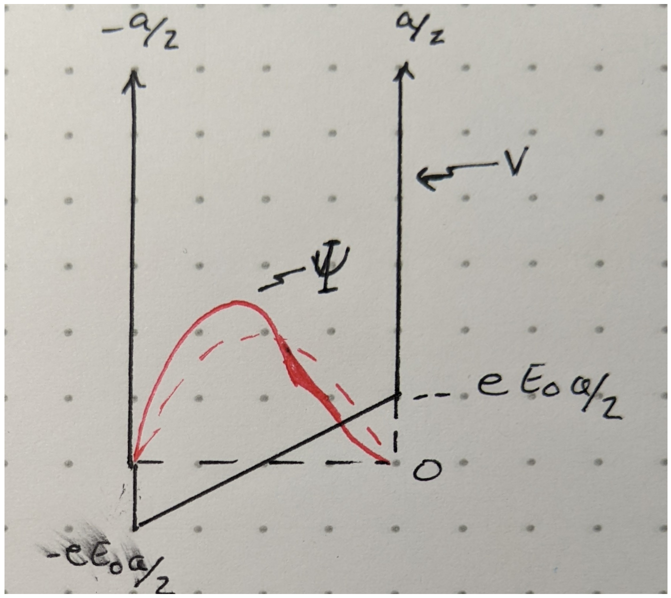

Figure 1: The image diagram for both part's **a)** and f). The dashed lines are the unperturbed system and the solid is the perturbed system.

a) See Fig. 1

b) Let's start with the unperturbed system:

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

Now, let's find the first solution.

$$\begin{aligned}
E_n^{(1)} &= \left\langle \Psi_n^0 \middle| H^1 \middle| \Psi_n^0 \right\rangle \\
&= \int_{-a/2}^{a/2} \frac{2}{a}\sin^2\left(\frac{n\pi}{a}x + \frac{n\pi}{2}\right) eE_0 \,\mathrm{d}x \\
&= \frac{2}{a}eE_0 \int_{-a/2}^{a/2} \left[\frac{1-\cos\left(\frac{2n\pi}{a}x + n\pi\right)}{2}\right] x \,\mathrm{d}x \\
&= \frac{1}{a}eE_0 \int_{-a/2}^{a/2} x - \cos\left(\frac{2n\pi}{a}x + n\pi\right) x \,\mathrm{d}x \\
&= \frac{1}{a}eE_0 \left[0 - \left(\frac{a}{2n\pi}\sin\left(\frac{2n\pi}{a}x + n\pi\right)\right) x \Big|_{-a/2}^{a/2} - \int_{-a/2}^{a/2} \frac{a}{2n\pi}\sin\left(\frac{2n\pi}{a}x + n\pi\right) \mathrm{d}x\right] \\
&= \frac{1}{a}eE_0 \left[-\left(\frac{a}{2n\pi}\right)^2 \cos\left(\frac{2n\pi}{a}x + n\pi\right) \Big|_{-a/2}^{a/2}\right] = 0 \qquad \checkmark
\end{aligned}$$

c) We need to invoke the second order approximation to the energy:

$$E_n^{(2)} = \sum_{m\neq n} \frac{\left|\left\langle \Psi_m^0 \middle| H_1 \middle| \Psi_n^0 \right\rangle\right|^2}{E_n^0 - E_m^0}$$

First looking at the numerator:

$$\langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle = \frac{2}{a}\int_{-a/2}^{a/2} \sin\left(\frac{m\pi}{a}x + \frac{m\pi}{2}\right) eE_0\, x \sin\left(\frac{n\pi}{a}x + \frac{n\pi}{2}\right) \mathrm{d}x$$

Through some IBP and actually pretty fun algebra:

$$= eE_0 \frac{a}{\pi^2}\left[\frac{\cos((m-n)\pi)}{(m-n)^2} - \frac{\cos((m+n)\pi)}{(m+n)^2} - \frac{1}{(m-n)^2} + \frac{1}{(m+n)^2}\right]$$

Setting $m = 2$ and $n = 1$

$$\longrightarrow eE_0 \frac{a}{\pi^2}\left[\frac{\cos(\pi)}{1^2} - \frac{\cos(3\pi)}{3^2} - \frac{1}{1^2} + \frac{1}{3^2}\right]$$

$$= eE_0 \frac{a}{\pi^2}\left[-1 + \frac{1}{9} - 1 + \frac{1}{9}\right]$$

$$= -eE_0 \frac{a}{\pi^2}\frac{16}{9}$$

Dealing with the denominator:

$$\left(E_n^0 - E_m^0\right) \to \left(E_1^0 - E_2^0\right)$$

$$= \frac{\pi^2\hbar^2}{a^2 2m} - \frac{\pi^2\hbar^2 4}{a^2 2m}$$

$$= \frac{\pi^2\hbar^2}{a^2 m}\left[\frac{1}{2} - \frac{4}{2}\right]$$

$$= \frac{3\pi^2\hbar^2}{2a^2 m}$$

Putting both of these together:

$$E_n^{(2)} = \left(-eE_0 \frac{a}{\pi^2}\frac{16}{9}\right)\frac{3\pi^2\hbar^2}{2a^2 m}$$

$$= -\frac{a^4}{\pi^6}\frac{2^9}{3^5}\frac{m}{\hbar^2}$$

$$\boxed{= -24\left(\frac{2}{3\pi}\right)^6 \frac{e^2 a^4 m}{\hbar^2}\left(E_0\right)^2} \quad \checkmark$$

d) To find the largest term in the $E_2^{(2)}$ we can just recognize that

$$\left|\langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle\right|^2 = \left|\langle \Psi_n^0 | H_1 | \Psi_m^0 \rangle\right|^2$$

So, the numerator of the previous calculation can just be reused. The denominator will just gain a negative. So:

$$\boxed{E_2^{(2)} = 24\left(\frac{2}{3\pi}\right)^6 \frac{e^2 a^4 m}{\hbar^2}\left(E_0\right)^2}$$

e)

$$\Delta E = E_2 - E_1 = \frac{\pi^2\hbar^2 4}{a^2 2m} + 24\left(\frac{2}{3\pi}\right)^6 \frac{e^2 a^4 m}{\hbar^2}\left(E_0\right)^2 - \frac{\pi^2\hbar^2}{a^2 2m} + 24\left(\frac{2}{3\pi}\right)^6 \frac{e^2 a^4 m}{\hbar^2}\left(E_0\right)^2$$

$$\boxed{= \frac{3\pi^2\hbar^2}{2a^2 m} + 48\left(\frac{2}{3\pi}\right)^6 \frac{e^2 a^4 m}{\hbar^2}\left(E_0\right)^2}$$

f) See Fig. 1