Poggensee
P564

Homework #8

1A

In class, we showed that a potential

$$H' = \varepsilon xy$$

could be solved exactly by a coordinate transformation $(x,y) \to (u,v)$ where (u,v) were rotated $45°$ counter clockwise from (x,y).

Solve this same problem using perturbation theory to first order and show that the results are the same as the exact result expanded to first order in ε.

The first order perturbative energy correction is

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

However, due to the degeneracy of the first excited state, $E_{10} = E_{01}$, we need degenerate perturbation theory.

We found the "good states" in class by observing that under the symmetry $D\psi(x,y) = \psi(y,x)$

1) Both H_0 & H' exhibit this symmetry
2) However, $|10\rangle$ and $|01\rangle$ are <u>NOT</u> eigenstates of this symmetry
3) However, we <u>CAN</u> construct linear combinations which are
   a) Not only eigenstates
   b) But also have different eigenvalues under D

These states are, as found in class,

$$\psi_+ = \frac{1}{\sqrt{2}}\left(|10\rangle + |01\rangle\right), \text{ with D eigenvalue } +1$$

$$\psi_- = \frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right), \text{ with D eigenvalue } -1$$

Thus, these are the states we should use.

$$E_{\pm}^{(1)} = \langle \psi_{\pm}^{(0)} | H' | \psi_{\pm}^{(0)} \rangle \leftarrow \text{The first-order correction to the } \psi_\pm \text{ energy}$$

$$E_{\pm}^{(1)} = \left[\frac{1}{\sqrt{2}}\left(\langle 10| \pm \langle 01|\right) \middle| \epsilon xy \middle| \frac{1}{\sqrt{2}}\left(|10\rangle \pm |01\rangle\right)\right]$$

$$= \frac{\epsilon}{2}\left[\left(\langle 10| \pm \langle 01|\right) \middle| xy \middle| \left(|10\rangle \pm |01\rangle\right)\right]$$

Now, this can be done with integrals, but the easier way is, as usual, to write x and y in terms of rasing & lowering operators:

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(a_x^+ + a_x\right) \qquad y = \sqrt{\frac{\hbar}{2m\omega}}\left(a_y^+ + a_y\right)$$

$$\therefore \; xy = \frac{\hbar}{2m\omega}\left(a_x^+ + a_x\right)\left(a_y^+ + a_y\right)$$

$$= \frac{\hbar}{2m\omega}\left(a_x^+ a_y^+ + a_x^+ a_y + a_x a_y^+ + a_x a_y\right)$$

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$$\therefore E_{\pm}^{(1)} = \frac{\hbar\varepsilon}{4m\omega}\Big[\big(\langle 10| \pm \langle 01|\big)\big(\underbrace{\cancel{a_x^+ a_y^+}}_{\text{zero by orthogonality}} + a_x^+ a_y + a_y^+ a_x + \cancel{a_x a_y}\big)\big(|10\rangle \pm |01\rangle\big)$$

$$E_{\pm}^{(1)} = \frac{\hbar\varepsilon}{4m\omega}\Big[\cancel{\langle 10|(a_x^+ a_y + a_y^+ a_x)|10\rangle} \pm \langle 10|(a_x^+ a_y + \cancel{a_y^+ a_x})|01\rangle$$
$$\pm \langle 01|(\cancel{a_x^+ a_y} + a_y^+ a_x)|10\rangle + \cancel{\langle 01|(a_x^+ a_y + a_y^+ a_x)|01\rangle}\Big]$$

$$E_{\pm}^{(1)} = \frac{\hbar\varepsilon}{4m\omega}\Big[\pm\sqrt{1}\sqrt{1} \pm \sqrt{1}\sqrt{1}\Big]$$

$$E_{\pm}^{(1)} = \pm\frac{\hbar\varepsilon}{2m\omega}$$

$$E_{\pm}^{(0)} + E_{\pm}^{(1)} = \hbar\omega \pm \frac{\hbar\varepsilon}{2m\omega}$$ ← The total energy to first order in ε.

Does this match the exact result $E_{\pm} = \hbar\sqrt{\frac{k\pm\varepsilon}{m}}$?

$$E_{\pm} = \hbar\sqrt{\frac{k}{m} \pm \frac{\varepsilon}{m}}$$

$$= \hbar\sqrt{\frac{k}{m}\left(1 \pm \frac{\varepsilon}{\cancel{m}}\cdot\frac{\cancel{m}}{k}\right)}$$

$$= \hbar\omega\sqrt{1 \pm \frac{\varepsilon}{k}} \approx \hbar\omega\left(1 + \frac{1}{2}\frac{\varepsilon}{k} + \mathcal{O}\left(\frac{\varepsilon^2}{k^2}\right)\right)$$

To see if they match, we need to massage $E_{\pm}^{(0)} + E_{\pm}^{(1)}$:

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$$E_{\pm}^{(0)} + E_{\pm}^{(1)} = \hbar\omega \pm \frac{\varepsilon\hbar}{2m\omega}$$

$$= \hbar\omega\left[1 + \frac{\varepsilon}{2m\omega^2}\right] \qquad \text{but } m\omega^2 = k$$

$$\therefore E_{\pm}^{(0)} + E_{\pm}^{(1)} = \hbar\omega\left[1 + \frac{\varepsilon}{2k}\right]$$

which agrees with the exact solution to 1st order!

Q.E.D

Problem 3 (Griffiths 7.4)

Start by stating global assumptions for this notebook: that both energies are real and positive while $0 < \lambda < 1$.

In[1]:=
```
$Assumptions = Ea ∈ Reals && Ea > 0 && Eb ∈ Reals && Eb > 0 && λ ∈ Reals && λ > 0 && λ < 1
```
Out[1]= $\text{Ea} \in \mathbb{R} \,\&\&\, \text{Ea} > 0 \,\&\&\, \text{Eb} \in \mathbb{R} \,\&\&\, \text{Eb} > 0 \,\&\&\, \lambda \in \mathbb{R} \,\&\&\, \lambda > 0 \,\&\&\, \lambda < 1$

Apply perturbation theory to the most general two-state system with unperturbed energies:

In[2]:=
```
MatrixForm[H0 = {{Ea, 0}, {0, Eb}}]
```
Out[2]//MatrixForm=

$$\begin{pmatrix} \text{Ea} & 0 \\ 0 & \text{Eb} \end{pmatrix}$$

and perturbation

In[3]:=
```
MatrixForm[H1 = λ {{Vaa, Vab}, {Vab, Vbb}}]
```
Out[3]//MatrixForm=

$$\begin{pmatrix} \text{Vaa}\,\lambda & \text{Vab}\,\lambda \\ \text{Vab}\,\lambda & \text{Vbb}\,\lambda \end{pmatrix}$$

(Note, I am using Vab = Vba. What is really true, however, Vba* = Vab. However, this is simpler for Mathematica)

In[4]:=
```
MatrixForm[H1]
```
Out[4]//MatrixForm=

$$\begin{pmatrix} \text{Vaa}\,\lambda & \text{Vab}\,\lambda \\ \text{Vab}\,\lambda & \text{Vbb}\,\lambda \end{pmatrix}$$

a) Find the exact energies

In[5]:=
```
MatrixForm[H = H0 + H1]
```
Out[5]//MatrixForm=

$$\begin{pmatrix} \text{Ea} + \text{Vaa}\,\lambda & \text{Vab}\,\lambda \\ \text{Vab}\,\lambda & \text{Eb} + \text{Vbb}\,\lambda \end{pmatrix}$$

In[6]:=
```
Emp = Eigenvalues[H]
```

Out[6]=
$$\left\{\frac{1}{2}\left(\text{Ea}+\text{Eb}+\text{Vaa}\,\lambda+\text{Vbb}\,\lambda-\sqrt{\left((-\text{Ea}-\text{Eb}-\text{Vaa}\,\lambda-\text{Vbb}\,\lambda)^2-4\left(\text{Ea}\,\text{Eb}+\text{Eb}\,\text{Vaa}\,\lambda+\text{Ea}\,\text{Vbb}\,\lambda-\text{Vab}^2\,\lambda^2+\text{Vaa}\,\text{Vbb}\,\lambda^2\right)\right)}\right),\right.$$
$$\left.\frac{1}{2}\left(\text{Ea}+\text{Eb}+\text{Vaa}\,\lambda+\text{Vbb}\,\lambda+\sqrt{\left((-\text{Ea}-\text{Eb}-\text{Vaa}\,\lambda-\text{Vbb}\,\lambda)^2-4\left(\text{Ea}\,\text{Eb}+\text{Eb}\,\text{Vaa}\,\lambda+\text{Ea}\,\text{Vbb}\,\lambda-\text{Vab}^2\,\lambda^2+\text{Vaa}\,\text{Vbb}\,\lambda^2\right)\right)}\right)\right\}$$

Which simplifies into E- (Em) and E+ (Ep) via

In[7]:=
```
Simplify[(a + b)^2 - 4 a * b]
```

Out[7]=
$$(a-b)^2$$

In[8]:=
```
Em = 1 / 2 * ((Ea + Eb + Vaa * λ + Vbb * λ) - Sqrt[(Ea + λ * Vaa - Eb - λ * Vbb)^2 + 4 * λ^2 * Vab^2])
```

Out[8]=
$$\frac{1}{2}\left(\text{Ea}+\text{Eb}+\text{Vaa}\,\lambda+\text{Vbb}\,\lambda-\sqrt{4\,\text{Vab}^2\,\lambda^2+(\text{Ea}-\text{Eb}+\text{Vaa}\,\lambda-\text{Vbb}\,\lambda)^2}\right)$$

In[9]:=
```
Ep = 1 / 2 * ((Ea + Eb + Vaa * λ + Vbb * λ) + Sqrt[(Ea + λ * Vaa - Eb - λ * Vbb)^2 + 4 * λ^2 * Vab^2])
```

Out[9]=
$$\frac{1}{2}\left(\text{Ea}+\text{Eb}+\text{Vaa}\,\lambda+\text{Vbb}\,\lambda+\sqrt{4\,\text{Vab}^2\,\lambda^2+(\text{Ea}-\text{Eb}+\text{Vaa}\,\lambda-\text{Vbb}\,\lambda)^2}\right)$$

b) Expand your results from (a) to second order in λ. Show that the results are the same as what we obtained in perturbation theory.

In[10]:=
```
Series[Em, {λ, 0, 2}]
```

Out[10]=
$$\frac{1}{2}\left(\text{Ea}+\text{Eb}-\text{Abs}[\text{Ea}-\text{Eb}]\right)+\frac{1}{2}\left(\text{Vaa}+\text{Vbb}-\frac{(\text{Vaa}-\text{Vbb})\,\text{Abs}[\text{Ea}-\text{Eb}]}{\text{Ea}-\text{Eb}}\right)\lambda-\frac{\text{Vab}^2\,\text{Abs}[\text{Ea}-\text{Eb}]\,\lambda^2}{(\text{Ea}-\text{Eb})^2}+O[\lambda]^3$$

This, of course, simplifies to (Ea-Eb)^2 = (Eb - Ea)^2

In[11]:=
```
Em = 1 / 2 (2 * Eb - Ea + Ea) + 1 / 2 (Vaa + Vbb - Vaa + Vbb) * λ + (Vab^2 * λ^2) / (Eb - Ea)
```

Out[11]=
$$\text{Eb}+\text{Vbb}\,\lambda+\frac{\text{Vab}^2\,\lambda^2}{-\text{Ea}+\text{Eb}}$$

Similarly for Ep

In[12]:=
```
Series[Ep, {λ, 0, 2}]
```

Out[12]=
$$\frac{1}{2}\left(\text{Ea}+\text{Eb}+\text{Abs}[\text{Ea}-\text{Eb}]\right)+\frac{1}{2}\left(\text{Vaa}+\text{Vbb}+\frac{(\text{Vaa}-\text{Vbb})\,\text{Abs}[\text{Ea}-\text{Eb}]}{\text{Ea}-\text{Eb}}\right)\lambda+\frac{\text{Vab}^2\,\text{Abs}[\text{Ea}-\text{Eb}]\,\lambda^2}{(\text{Ea}-\text{Eb})^2}+O[\lambda]^3$$

Simplifies to

In[13]:= `Ep = 1 / 2 (2 * Ea - Eb + Eb) + 1 / 2 (Vaa + Vaa - Vbb + Vbb) λ + (Vab^2 * λ^2) / (Eb - Ea)`

Out[13]=

$$\text{Ea} + \text{Vaa}\,\lambda + \frac{\text{Vab}^2\,\lambda^2}{-\text{Ea} + \text{Eb}}$$

Both of which match our results from perturbation theory!

c) Setting Vaa = Vbb = 0, show that the series only converges if | Vab / (Eb - Ea) | < 1/2

The series only converge if

In[14]:=

`4 Vab^2 / (Eb - Ea)^2 < 1`

Out[14]=

$$\frac{4\,\text{Vab}^2}{(-\text{Ea} + \text{Eb})^2} < 1$$

or equivalently

In[15]:= `| Vab / (Eb - Ea) | < 1 / 2`

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HW #8 2A

2. (Griffiths 7.9) Consider a particle of mass m that is free to move on a circular wire of length L.

a) Show that the stationary states can be written as

$$\psi_n = \frac{1}{\sqrt{L}} e^{2\pi i n x/L} \quad \Big| \quad x \in (-L/2, L/2)$$

This is pretty straightforward, the wave must "fit around the ring"

$$\therefore \psi_n = C e^{2\pi i n x/L} \quad \Big| \quad n \in \{0, \pm 1, \pm 2, \pm 3, \ldots\}$$

with C being some normalization constant which turns out to be $C = 1/\sqrt{L}$

$$\therefore \psi_n = \frac{1}{\sqrt{L}} e^{2\pi i n x/L}$$

The fact that $n \in \{\pm 1, \pm 2, \ldots\}$ is the fact that the particle can go either direction around the ring.

b) Now add the perturbation $H' = -V_0 e^{-x^2/a^2}$ with $a \ll L$ and solve $E_\pm^{(1)}$ by brute force.

From equation 7.33, the brute force method is

$$E_\pm^{(1)} = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right.$$

HW #8 2B

Where $W_{ij} = \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle$

with i and j being degenerate states. In our case:
- 'a' are the $+n$ states.
- 'b' are the $-n$ degenerate states.

Start with W_{aa}

$$W_{aa} = \langle \psi_a^{(0)} | H' | \psi_a^{(0)} \rangle$$
$$= \int_{-L/2}^{L/2} dx \left(\frac{1}{\sqrt{L}} \cancel{e^{-2\pi i n x/L}}\right)\left(-V_0 e^{-x^2/a^2}\right)\left(\frac{1}{\sqrt{L}} \cancel{e^{+2\pi i n x/L}}\right)$$
$$= -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-x^2/a^2} dx$$

Using Griffiths' trick of sending $L/2 \to \infty$ as $a \ll L$, we get

$$W_{aa} = -\frac{V_0}{L} \int_{-\infty}^{\infty} e^{-x^2/a^2} dx = \frac{-V_0 a\sqrt{\pi}}{L}$$

W_{bb} will be the same. All that is left is W_{ab}:

$$W_{ab} = \langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle$$
$$= \int_{-L/2}^{L/2} dx \left(\frac{1}{\sqrt{L}} e^{-2\pi i n x/L}\right)\left(-V_0 e^{-x^2/a^2}\right)\left(\frac{1}{\sqrt{L}} e^{-2\pi i n x/L}\right)$$

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$$W_{ab} = -\frac{V_0}{L}\int_{-L/2}^{L/2} dx \; \exp\left[-\frac{4\pi i n x}{L} - \frac{x^2}{a^2}\right]$$

$$W_{ab} = -\frac{V_0 a\sqrt{\pi}}{L} e^{-(2\pi n a/L)^2}$$

Putting back into 7.33, we get

$$E_{\pm}^{(1)} = \frac{1}{2}\left[\frac{-2V_0 a\sqrt{\pi}}{L} \pm \sqrt{(0)^2 + 4|W_{ab}|^2}\right]$$

Since $W_{ab} \in \mathbb{R}$

$$E_{\pm}^{(1)} = -\frac{V_0 a\sqrt{\pi}}{L} \pm W_{ab} = -\frac{V_0 a\sqrt{\pi}}{L}\left(1 \mp e^{-(2\pi n a/L)^2}\right)$$

c & d) (Note, I'm doing them together!) What are the "good states" for perturbation theory here? What is the symmetry you could use to find the good states?

As before the "trick" to finding "good states" is to find a symmetry shared by H_0 & H' but one where the degenerate states are <u>NOT</u> eigenstates of that symmetry, but linear combinations <u>can</u> be contructed which have different eigenvalues.

Both H_0 & H' have a 2π rotational symmetry, but our eigenstates also have this symmetry, and all have the <u>same</u> eigenvalue, so that doesn't work.

HW #8 2D

Looking at our degenerate states again:

$$\psi_{+n} = \frac{1}{\sqrt{L}} \exp\left[+\frac{2\pi i n x}{L}\right] \qquad \psi_{-n} = \frac{1}{\sqrt{L}} \exp\left[-\frac{2\pi i n x}{L}\right]$$

I could build eigenstates of parity with different eigenvalues:

$$\psi_+ = \frac{\psi_{+n} + \psi_{-n}}{2} = \frac{1}{\sqrt{L}} \cos\left(\frac{2\pi i n x}{L}\right), \quad \Pi \psi_+ = +1\,\psi_+$$

$$\psi_- = \frac{\psi_{+n} - \psi_{-n}}{2i} = \frac{1}{\sqrt{L}} \sin\left(\frac{2\pi i n x}{L}\right), \quad \Pi \psi_- = -1\,\psi_-$$

Which are "good states" as both H_0 & H' are symmetric under parity manifestly.

(Griffiths 7.12) Consider a 3-state quantum system with the Hamiltonian

$$H = V_0 \begin{pmatrix} (1-\varepsilon) & 0 & 0 \\ 0 & 1 & \varepsilon \\ 0 & \varepsilon & 2 \end{pmatrix}$$

with V_0 a constant & $\varepsilon \ll 1$.

a) What are the eigenvalues & eigenstates for the unperturbed Hamiltonian ($\varepsilon \to 0$)?

$$H_0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

by this point, you can probably just write the eigenvalues & eigenvectors down for this Hamiltonian by inspection:

$|1\rangle : \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ w/ $E_1 = V_0$

$|2\rangle : \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ w/ $E_2 = V_0$

degenerate

$|3\rangle : \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ w/ $E_3 = 2V_0$

b) Solve the exact eigenvalues for H and expand to order ε^2.

$$\det(H - \lambda \mathbb{1}) = 0$$

$$\begin{vmatrix} V_0(1-\varepsilon) - \lambda & 0 & 0 \\ 0 & V_0 - \lambda & V_0 \varepsilon \\ 0 & V_0 \varepsilon & 2V_0 - \lambda \end{vmatrix} = 0$$

$$[V_0(1-\varepsilon) - \lambda] \cdot [(V_0 - \lambda)(2V_0 - \lambda) - (V_0 \varepsilon)^2] = 0$$

$$V_0(1-\varepsilon) - \lambda = 0 \rightarrow \boxed{\lambda_1 = V_0(1-\varepsilon)}$$

$$(V_0 - \lambda)(2V_0 - \lambda) - (V_0 \varepsilon)^2 = 0$$

$$2V_0^2 - \lambda V_0 - 2\lambda V_0 + \lambda^2 - (V_0 \varepsilon)^2 = 0$$

$$\lambda^2 - 3V_0 \lambda + (2V_0^2 - \varepsilon^2 V_0^2) = 0$$

$$\lambda = \frac{V_0}{2}\left[3 \pm \sqrt{1 + 4\varepsilon^2}\right]$$

$$\approx \frac{V_0}{2}\left[3 \pm \left(1 + \frac{1}{2}(4\varepsilon^2) + \mathcal{O}(\varepsilon^4)\right)\right]$$

$$\approx \frac{V_0}{2}\left[3 \pm 1 \pm 2\varepsilon^2\right]$$

$$\boxed{\lambda_2 \approx V_0(2 + \varepsilon^2) \qquad \lambda_3 \approx V_0(1 - \varepsilon^2)}$$

c) Use 1^{st} and 2^{nd} order T.I.P.T. for the non-degenerate state.

$$|3\rangle : \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{with } E_3 = 2V_0 \text{ is}$$

the state which is not degenerate at zeroth order

$$E_3^{(1)} = \langle 3 | H' | 3 \rangle = (0\,0\,1)\left[V_0 \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} \right] \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$E_3^{(1)} = 0 \leftarrow \text{No correction at first order}$$

At second order:

$$E_3^{(2)} = \sum_{n \neq 3} \frac{|\langle 3 | H' | n \rangle|^2}{E_3^{(0)} - E_n^{(0)}}$$

$$E_3^{(2)} = \frac{V_0^2}{2V_0 - V_0} \cdot \left[(0\,0\,1) \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right]^2$$

$$+ \frac{V_0^2}{2V_0 - V_0} \cdot \left[(0\,0\,1) \begin{pmatrix} -\varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon \\ 0 & \varepsilon & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right]^2$$

$$E_3^{(2)} = V_0 \cdot \left\{ \cancel{\left[(0\,0\,1) \begin{pmatrix} -\varepsilon \\ 0 \\ 0 \end{pmatrix} \right]^2}^{\,0} + \left[(0\,0\,1) \begin{pmatrix} 0 \\ 0 \\ \varepsilon \end{pmatrix} \right]^2 \right\}$$

$$E_3^{(2)} = V_0 \varepsilon^2$$

With this in hand, we can proceed as usual!

$$E_1^{(1)} = \langle 1 | H' | 1 \rangle$$

$$= (1\ 0)\, V_0 \begin{pmatrix} -\varepsilon & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$E_1^{(1)} = (1\ 0) \begin{pmatrix} -V_0\varepsilon \\ 0 \end{pmatrix} = -V_0\varepsilon$$

$$E_1 \approx E_1^{(0)} + E_1^{(1)} \approx V_0 - V_0\varepsilon \approx V_0(1-\varepsilon)$$

which agrees with the λ_1 we found in part (b)!

For E_2:

$$E_2^{(1)} = (0\ 1)\, V_0 \begin{pmatrix} -\varepsilon & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$$E_2 \approx E_2^{(0)} + E_2^{(1)} \approx V_0$$

which agrees (to first order) with λ_3 from part b!