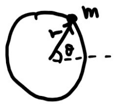
5. *Quantum Mechanics* (Spring 2006)

A particle with mass m is confined to move on a circle of radius r. It is perturbed by a potential $V(\theta) = a(1+\cos(2\theta))$.

(a) What are the unperturbed energy levels?



(b) Find the shift in the energy levels to first order in a.

(c) Find the second order energy shift for all the states.

Hint: Beware of the special care needed for some of the states.

(a) Step 1 : Find unperturbed Hamiltonian

Starting w/ Lagrangian: $\mathcal{L} = T - V$

$T = \sum_i \frac{1}{2} m v_i^2 = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2) \rightarrow$ using polar coords

$\dot{x} = \frac{d}{dt}(r\cos\theta) = -r\sin\theta\,\dot{\theta}$

$\dot{y} = \frac{d}{dt}(r\sin\theta) = r\cos\theta\,\dot{\theta}$

$= \frac{1}{2} m r^2 \dot{\theta}^2$

$\mathcal{L}(\theta,\dot{\theta},t) = \frac{1}{2} m r^2 \dot{\theta}^2 + V(\theta)$ (polar)

the conjugate momenta to the ang coor θ:

$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m r^2 \dot{\theta} - \frac{[\text{mass}][\text{dist}]^2}{[\text{time}]} \equiv L_z$

$|L| = |\vec{r} \times \vec{p}| = r p_\theta |\hat{r} \times \hat{\theta}| = r p_\theta |\hat{z}|$

$L_z = r p_\theta \equiv p_\theta$

$\therefore H(\theta, p_\theta, t) = \dot{\theta} p_\theta - \mathcal{L} = \dot{\theta} L_z - \mathcal{L}$

$= \frac{L_z^2}{mr^2} - \frac{1}{2} m r^2 \dot{\theta}^2 - V(\theta)$

$= \frac{L_z^2}{mr^2} - \frac{1}{2}\frac{L_z^2}{mr^2} - V(\theta) = \frac{L_z^2}{2mr^2} - V(\theta)$

notice that this is $\frac{L^2}{2I}$ for $I = mr^2$ (ring)

$\Rightarrow$ compare to rigid-rotor for rotating molecule!

Step 2: Quantize

$H_0 = \frac{L_z^2}{2mr^2} \Rightarrow \hat{H}_0 = \frac{\hat{L}_z^2}{2mr^2}$

$V(\theta) = a(1+\cos(2\theta)) \Rightarrow \hat{V}(\theta) = a(1+\cos(2\hat{\theta}))$

Simple b/c factors commute!

Review: How to find Hamiltonian from Lagrangian:

$dH = \left(\frac{\partial H}{\partial q_i}\right) dq_i + \left(\frac{\partial H}{\partial p_i}\right) dp_i + \left(\frac{\partial H}{\partial t}\right) dt$

from Hamilton's Eqns $-\dot{p}_i$; $\dot{q}_i$; $-\frac{\partial \mathcal{L}}{\partial t}$ Total differentiation $H(q_i, p_i, t)$

Rewritten, $dH = \left[-\dot{p}_i \, dq_i + \dot{q}_i \, dp_i \right] - \left(\frac{d\mathcal{L}}{dt}\right) dt$

Using Lagrange Eqn: $\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \dot{p}_i = \frac{\partial \mathcal{L}}{\partial q_i}$ $F = ma = \dot{p}$

$dH = \left[-\left(\frac{\partial \mathcal{L}}{\partial q_i}\right) dq_i + \dot{q}_i \, d\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) \right] - \left(\frac{d\mathcal{L}}{dt}\right) dt$

$= \dot{q}_i \, d\left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right) - \left(\frac{\partial \mathcal{L}}{dq_i}\right) dq_i - \left(\frac{\partial \mathcal{L}}{\partial t}\right) dt$

using exact diff of

$d\mathcal{L}(q_i, \dot{q}_i, t) = \frac{d\mathcal{L}}{dq_i} dq_i + \frac{d\mathcal{L}}{d\dot{q}_i} d\dot{q}_i + \frac{d\mathcal{L}}{dt} dt$

$= \dot{q}_i \, d\left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right) + \left(\frac{d\mathcal{L}}{d\dot{q}_i}\right) d\dot{q}_i - d\mathcal{L}$

$d\left(\dot{q}_i \frac{\partial \mathcal{L}}{d\dot{q}_i}\right) = \dot{q}_i \, d\left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right) + \left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right) d\dot{q}_i$

$= d\left(\dot{q}_i \frac{\partial \mathcal{L}}{d\dot{q}_i}\right) - \cancel{\left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right)} d\dot{q}_i + \cancel{\left(\frac{d\mathcal{L}}{d\dot{q}_i}\right)} d\dot{q}_i - d\mathcal{L}$

$\therefore \left\{ H = \sum_i \dot{q}_i \left(\frac{\partial \mathcal{L}}{d\dot{q}_i}\right) - \mathcal{L} \right\}$

Step 3: Find unperturbed energies

$H_0 |\psi\rangle = \frac{\hat{L}_z^2}{2mr^2} |\psi\rangle$ and $\hat{\vec{L}} = \hat{r} \times \hat{p} = [\hat{x} + \hat{y}] \times [\hat{p}_x + \hat{p}_y]$

$= \hat{x} \times \hat{p}_y + \hat{y} \times \hat{p}_x$

$= -\frac{\hbar^2}{2mr^2} \frac{\partial^2}{\partial \theta^2} |\psi\rangle$ $\quad \vec{L} = \hat{x}\hat{p}_y \hat{e}_z - \hat{y}\hat{p}_x \hat{e}_z$

$H_0 \langle \theta' | \psi \rangle = -\frac{\hbar^2}{2mr^2} \frac{\partial^2}{\partial \theta'^2} \langle \theta' | \psi \rangle$ $\quad L_z = -i\hbar \left[\hat{x}\frac{d}{dy} - \hat{y}\frac{d}{dx} \right]$

$H_0 \psi(\theta') = -\frac{\hbar^2}{2mr^2} \partial_{\theta'}^2 \psi(\theta')$ $\quad L_z = -i\hbar \frac{\partial}{\partial \theta}$

note that $\frac{d}{d\theta} = \left(\frac{dx}{d\theta}\right)\left(\frac{d}{dx}\right) + \left(\frac{dy}{d\theta}\right)\left(\frac{d}{dy}\right)$

$= -r\sin\theta \frac{d}{dx} + r\cos\theta \frac{d}{dy}$

$= x\frac{d}{dy} - y\frac{d}{dx}$

$\partial_{\theta'}^2 \psi = -\frac{2mr^2}{\hbar^2} E \psi \Rightarrow \psi = C_\pm e^{\pm i\gamma\theta} \Rightarrow$ and normalize wrt θ-coord

$\gamma = \sqrt{\frac{2mr^2}{\hbar^2} E}$ (unitless)

$\psi_\pm(\theta) = \frac{1}{\sqrt{2\pi}} e^{\pm i\gamma\theta} = \langle \pm | \psi \rangle$

B.C. $\psi(\theta) = \psi(\theta + 2\pi) \Rightarrow e^{i\gamma\theta} = e^{i(\theta+2\pi)\gamma} \Rightarrow 1 = e^{i2\pi\gamma}$

$2\pi\gamma = 2\pi m$ w/ $m \in$ all $\mathbb{Z}$

$\gamma_m = m$

s.t. $\langle \theta | \gamma_m \rangle = \frac{1}{\sqrt{2\pi}} e^{im\theta}$ and $\gamma_m \Rightarrow \boxed{E_m = \frac{m^2\hbar^2}{2m_0 r^2} \text{ for } m \in \mathbb{Z} \text{ (pos and neg)}}$

$\langle \theta | \psi_{-m} \rangle = \frac{1}{\sqrt{2\pi}} e^{-im\theta}$

Degenerate

(b) Find the shift in E_m to $\mathcal{O}(a')$

TIDPT: $\Delta_\ell^{(1)} = \langle \ell^{(0)} | \hat{V}(\theta) | \ell^{(0)} \rangle$; $|\ell^{(0)}\rangle = \sum_{m \in D} \langle m^{(0)} | \ell^{(0)} \rangle |m^{(0)}\rangle$

For simplicity, I pulled the sign out of m across the entire problem s.t. $m \geq 0$

in degenerate subspace

$$\hat{V}_{|m|} \doteq \begin{pmatrix} \langle +m^{(0)}|V|+m^{(0)}\rangle & \langle +m^{(0)}|V|-m^{(0)}\rangle \\ \langle -m^{(0)}|V|+m^{(0)}\rangle & \langle -m^{(0)}|V|-m^{(0)}\rangle \end{pmatrix} |\ell^{(0)}\rangle = \Delta_\ell^{(1)} \mathbb{1} |\ell^{(0)}\rangle$$

two-fold degenerate for each $|m|$ value

Step 1: Find matrix elements

$$V_{mm} = \int d\theta' \langle +m^{(0)}|\theta'\rangle \hat{V}(\theta') \langle \theta' | +m^{(0)}\rangle$$

$$= \frac{1}{2\pi} \int d\theta' \, \cancel{e^{im\theta'}} \, a(1+\cos(2\theta')) \, \cancel{e^{-im\theta'}} \Rightarrow V_{mm} = V_{-m-m} = a$$

$$= \frac{1}{2\pi} a \left(2\pi + \cancel{\int d\theta' \cos 2\theta'}^{\,0}\right) = a$$

$u = \sin 2\theta' \Rightarrow u_1 = u_2 = 0$

$du = \cos 2\theta' (2 d\theta') = d \sin 2\theta'$

$$V_{m-m} = \frac{1}{2\pi} \int d\theta' \, e^{-im\theta'} a (1+\cos(2\theta')) e^{-im\theta'} \quad \text{for } m>0$$

$$= \frac{a}{2\pi} \left[\int d\theta' \, e^{-2im\theta'} (1+\cos(2\theta')) \right] = \frac{a}{2\pi} g(\theta')$$

$$\Rightarrow g(\theta') = \frac{1}{-i2m} \left(e^{-i4\pi m} - 1\right) + \int d\theta' e^{-2im\theta'} \cos(2\theta')$$

only care about $m>0$

for $m=0$ though,

$$g(\theta) = \lim_{m\to 0} \frac{i}{2m} \left(e^{-i4\pi m} - 1\right) = \frac{i(-i4\pi)e^{\cdots}}{2} = 2\pi \quad \text{used in (c)}$$

$$= \frac{1}{2} \int d\theta' \left[e^{-2im\theta'} e^{i2\theta'} + e^{-2im\theta'} e^{-i2\theta'} \right] + \cancel{\frac{i}{2m} \left(e^{-i4\pi m} - 1\right)}$$

$$= \frac{1}{2} \left[\frac{1}{i2(1-m)} \left(e^{-i4\pi m} \cancel{e^{i4\pi}}^{\,1} - 1\right) + \frac{1}{-i2(1+m)} \left(e^{-i4\pi m} \cancel{e^{-i4\pi}}^{\,1} - 1\right) \right]$$

$$= \frac{1}{2} \left[\frac{-i(1+m)}{2(1-m^2)} \left(e^{-i4\pi m} - 1\right) + \frac{i(1-m)}{2(1-m^2)} \left(e^{-i4\pi m} - 1\right) \right]$$

$$= \frac{im}{2(1-m^2)} \left(1 - e^{-i4\pi m}\right) \quad \text{and} \quad g(\theta') = \begin{cases} 0 & m \neq 1, 0 \\ \pi & m = 1 \end{cases}$$

$$\Rightarrow \lim_{m\to 1} \frac{i\cancel{m}(+i4\pi)\cancel{e}^{\,1} + (1-\cancel{e})^{\,0} i}{-4\cancel{m}}$$

only non-zero crossterm m

Degenerate space

$V_{mm} = V_{-m-m} = a \quad m \neq 1, m>0$ (degenerate) note $V_{00} = a$ too

$V_{1-1} = V_{-11} = a/2$ and zero for other deg non-diagonal terms

$V_{m-m} = V_{-mm} = 0$ for $m \neq 1, m>0$

$$\begin{pmatrix} \ddots & 0 & 0 & 0 \\ 0 & V_{mm} & V_{1-1} & 0 \\ 0 & V_{-11} & V_{-m-m} & 0 \\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

Step 2: Diagonalize in degenerate basis

$$\text{for } m=1: \quad \hat{V} \doteq \begin{array}{cc} & \\ \begin{pmatrix} a & a/2 \\ a/2 & a \end{pmatrix} & \begin{array}{l} m=1 \\ m=-1 \end{array} \\ \begin{array}{cc} m=1 & m=-1 \end{array} & \end{array} \xRightarrow{\text{diagonalizing}} (a - \Delta_\ell^{(1)})(a - \Delta_\ell^{(1)}) - a^2/4 = 0$$

$$a^2 + \Delta_\ell^{(1)2} - 2a\Delta_\ell^{(1)} - a^2/4 = 0$$

Denote $\ell = |m|_\pm$

$$\Delta_\ell^{(1)} = \frac{-(-2a) \pm \sqrt{(-2a)^2 - 4(1)(3a^2/4)}}{2} = \frac{2a \pm \sqrt{4a^2 - 3a^2}}{2} = \left(\frac{2 \pm 1}{2}\right) a$$

for $m=1$

$$|1_\pm^{(0)}\rangle = \begin{pmatrix} \langle +m^{(0)}|1_\pm^{(0)}\rangle \\ \langle -m^{(0)}|1_\pm^{(0)}\rangle \end{pmatrix} \qquad \begin{pmatrix} a - \Delta_{1\pm}^{(1)} & a/2 \\ a/2 & a - \Delta_{1\pm}^{(1)} \end{pmatrix} |1_\pm^{(0)}\rangle = 0$$

diagonal elements of $\langle \ell^{(0)}|V|\ell^{(0)}\rangle$ matrix

$$\ell = 1_+: \quad a/2 \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} |1_+^{(0)}\rangle = \frac{a}{2}\left[\sigma_x - \mathbb{1}\right] |1_+^{(0)}\rangle$$

$|S_x; +\rangle$

$$\ell = 1_-: \quad \frac{a}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} |1_-^{(0)}\rangle = \frac{a}{2}\left[\sigma_x + \mathbb{1}\right] |1_-^{(0)}\rangle$$

$|S_x; -\rangle$

$$|1_+^{(0)}\rangle = \frac{1}{\sqrt{2}}\left[|m=1\rangle + |m=-1\rangle\right] \quad \text{w/} \quad \boxed{\begin{aligned} E_{1+} &= E_1^{(0)} + \tfrac{3}{2}a \\ E_{1-} &= E_1^{(0)} + \tfrac{1}{2}a \end{aligned}}$$

$$|1_-^{(0)}\rangle = \frac{1}{\sqrt{2}}\left[|m=1\rangle - |m=-1\rangle\right]$$

since $E_1^{(0)} = E_{-1}^{(0)}$

Degeneracy lifted!

for $m \neq 1$ & $m>0$

$V \doteq a\mathbb{1}$ which is diagonal, just like non-deg case

$V|\pm m^{(0)}\rangle = a|\pm m^{(0)}\rangle$

$$\Delta_m^{(1)} = a \Rightarrow \boxed{E_m = E_m^{(0)} + a \quad \text{for } m \neq \pm 1}$$

still degenerate; still don't know what is a "good" basis → cont. (c)

(c) Now, we can see what the hint is trying to tell us.

Case 1: $m=1$ (non-degenerate in "good" basis $l = 1_\pm$)

Step 1: Find $\Delta_l^{(2)}$ eqn

We can now use non-deg pert theory w/ "good states"

$$\Delta_l = \lambda \langle l^{(0)} | V | l \rangle \quad \text{and w/} \quad \langle l^{(0)} | l \rangle = 1$$

$$\Delta_l^{(2)} = \langle l^{(0)} | V | l^{(1)} \rangle = \langle l^{(0)} | V \sum_{k \notin D} \frac{|k^{(0)}\rangle\langle k^{(0)} | V | l^{(0)}\rangle}{E_D^{(0)} - E_k^{(0)}}$$

$$= \sum_{k \notin D} \frac{|V_{kl}|^2}{E_D^{(0)} - E_k^{(0)}}$$

(just good ol' TIPT w/ $|l^{(0)}\rangle$ instead!)

Step 2: Calculate the matrix element for $k=0$ (only non-deg) ← $\frac{1}{\sqrt{2}}(|+1\rangle \pm |-1\rangle)$

Since $l = 1_\pm$: $\langle 0^{(0)} | V | 1_\pm^{(0)} \rangle = \int d\theta \, \langle + l^{(0)} | \theta' \rangle \, a(1 + \cos 2\theta') \langle \theta' | 1_\pm^{(0)} \rangle$

$$= \frac{1}{2\sqrt{2}\pi} \int d\theta \; (1) \; a(1 + \cos 2\theta') \left[e^{i\theta'} \pm e^{-i\theta'} \right]$$

If you exchange $\pm i\theta \to -2is\theta'$

you'll notice that this is just $g(\theta)$

for this transformation, $|s| = 1/2$

but $g(\theta') = 0$ for $|s| \neq 0, 1$

$$\langle 0^{(0)} | V | 1_\pm^{(0)} \rangle = 0 \quad \text{and} \quad \boxed{\Delta_{1_\pm}^{(2)} = 0}$$

Case 2: $m \neq 1$ (still degenerate)

Here, we must use second-order deg pert

Answer: $\Delta_{m,\beta}^{(2)} = \sum_{k \notin D} \frac{\langle \beta | V | k \rangle \langle k | V | m \rangle}{E_D^{(0)} - E_k^{(0)}}$, but Sakurai doesn't cover...

need $\langle 0 | V | \pm m \rangle \Big|_{m \neq 1} = a \int_0^{2\pi} d\theta' \frac{1}{\sqrt{2\pi}} (1)(1 + \cos(2\theta')) \frac{1}{\sqrt{2\pi}} e^{\pm i m \theta'} = \frac{a}{2\pi} g(\theta; \pm m = -2s) = \begin{cases} 0 & s \notin \{0,1\} \\ 1 & s = 0 \quad (\cancel{m} = 0) \\ 1/2 & s = 1 \quad (|m| = 2) \end{cases}$

$m \neq 2$ — ignore non-deg

$\langle 0 | V | \pm 2 \rangle = a/2$

$$\Rightarrow \boxed{\begin{array}{l} \Delta_{+2,+2}^{(2)} = \Delta_{-2,-2}^{(2)} = \Delta_{+2,-2}^{(2)} = \Delta_{-2,+2}^{(2)} = \frac{a^2}{4} \left(\frac{1}{E_1^{(0)} - E_0^{(0)}} \right) \\ 0 \text{ for any other } m, \beta \end{array}}$$

Explanation: $|\psi\rangle = \sum_{k \notin D} c_k |k\rangle + \sum_{m \in D} d_m |m\rangle$

$H|\psi\rangle = E|\psi\rangle \to (H - E)|\psi\rangle = (H_0 + \lambda V - E)|\psi\rangle = 0$

By expansion: $0 = \sum_{k \notin D} c_k (H - E_\psi)|k\rangle + \sum_{m \in D} d_m (H - E_\psi)|m\rangle$

$$= \sum_k c_k (E_k - E + \lambda V)|k\rangle + \sum_m d_m (E_m - E + \lambda V)|m\rangle$$

multiply by $\langle \beta|$ for $\beta \in D$ and $\langle \alpha|$ for $\alpha \notin D$

Get 2 eqns: $0 = \sum_k c_k \langle \beta | \lambda V | k \rangle + d_\beta (E_\beta - E) + \sum_m d_m \langle \beta | \lambda V | m \rangle$

$0 = c_\alpha (E_\alpha - E) + \cancel{\sum_k c_k \langle \alpha | \lambda V | k \rangle} + \sum_m d_m \langle \alpha | \lambda V | m \rangle$

(1) we argue that $|\psi\rangle$ is mostly linear comb of degenerate states (doesn't really contribute)
(2) limit $\lambda \to 0$, this term would disappear

Solving for c_α

$$c_\alpha = -\lambda \sum_{m \in D} \frac{d_m \langle \alpha | V | m \rangle}{(E_\alpha - E)}$$

⇒ sub into top eqn w/ $\alpha \to k$: $0 = d_\beta (E_\beta - E) + \sum_m d_m \left[\lambda \langle \alpha | V | m \rangle + \lambda^2 \sum_{k \notin D} \frac{\langle \beta | V | k \rangle \langle k | V | m \rangle}{(E - E_k)} \right]$

If $E_\beta \equiv E_D = E$, we get an eigenvalue eqn

$$\Delta_{\beta,m}^{\text{eff}} = \lambda \langle \alpha | V | m \rangle + \lambda^2 \sum_{k \notin D} \frac{\langle \beta | V | k \rangle \langle k | V | m \rangle}{E_D - E_k}$$

$$\Delta_{\beta,m}^{\text{eff}\,(2)} = \sum_{k \notin D} \frac{\langle \beta | V | k \rangle \langle k | V | m \rangle}{E_D - E_k}$$