PHYS 661 - Quantum Mechanics II

Modern Quantum Mechanics by *J. J. Sakurai*
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Homework 1

Problem 1 - Pauli Matrices
Show that for Pauli matrices

$$\mathrm{e}^{\mathrm{i}\theta\mathbf{n}\cdot\boldsymbol{\sigma}} = \mathbb{I}\cos(\theta) + \mathrm{i}\mathbf{n}\cdot\boldsymbol{\sigma}\sin(\theta), \text{ where } \mathbf{n}^2 = 1$$

and

$$\mathrm{e}^{\mathrm{i}\frac{1}{2}\theta\sigma_y}\left(\sigma_x, \sigma_y, \sigma_z\right)\mathrm{e}^{-\mathrm{i}\frac{1}{2}\theta\sigma_y} = \left(\sigma_x, \sigma_y, \sigma_z\right)\cos(\theta) + \left(\sigma_z, 0, -\sigma_x\right)\sin(\theta) + \left(0, \sigma_y, 0\right)\left(1 - \cos(\theta)\right)$$

Suppose we have a Hamiltonian $H = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}$ with $a, b \in \mathbb{R}$. What are the eigenvalues $E_{\pm}$? Find the unitary transformation U that diagonalizes H, i.e.,

$$U^\dagger H U = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}.$$

Solution. Let $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices. Rotations on spin states with respect to a unit vector $\mathbf{n}$ are given by

$$R_{\mathbf{n}}(\phi) = \mathrm{e}^{\mathrm{i}\frac{\phi}{\hbar}\mathbf{n}\cdot\mathbf{S}} = \mathrm{e}^{\mathrm{i}\frac{\phi}{2}\mathbf{n}\cdot\boldsymbol{\sigma}}.$$

We have the following property of the Pauli matrices

$$\sigma_j\sigma_k = \delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l.$$

We will first show that, for any ordinary vectors in $\mathbb{R}^3$, we have

$$\left(\mathbf{a}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{b}\cdot\boldsymbol{\sigma}\right) = \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\boldsymbol{\sigma}\cdot\left(\mathbf{a}\times\mathbf{b}\right).$$

In fact

$$\begin{aligned}
\left(\mathbf{a}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{b}\cdot\boldsymbol{\sigma}\right) &= \sum_j \sigma_j a_j \sum_k \sigma_k b_k \\
&= \sum_j\sum_k \sigma_j\sigma_k a_j b_k \\
&= \sum_j\sum_k \left(\delta_{jk} + \mathrm{i}\sum_l \epsilon_{jkl}\sigma_l\right) a_j b_k \\
&= \sum_j\sum_k \delta_{jk} a_j b_k + \mathrm{i}\sum_j\sum_k\sum_l \epsilon_{jkl}\sigma_l a_j b_k \\
&= \sum_j a_j b_j + \mathrm{i}\sum_l \sigma_l\left(\sum_j\sum_k \epsilon_{jkl} a_j b_k\right) \\
&= \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\sum_l \sigma_l\left(\mathbf{a}\times\mathbf{b}\right) \\
&= \left(\mathbf{a}\cdot\mathbf{b}\right) + \mathrm{i}\boldsymbol{\sigma}\cdot\left(\mathbf{a}\times\mathbf{b}\right).
\end{aligned}$$

Note that, if we take $\mathbf{a} = \mathbf{b} = \mathbf{n}$, then

$$(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = (\mathbf{n}\cdot\boldsymbol{\sigma})(\mathbf{n}\cdot\boldsymbol{\sigma})^2 = (\mathbf{n}\cdot\mathbf{n}) + \mathrm{i}\boldsymbol{\sigma}\cdot(\mathbf{n}\times\mathbf{n}) = \mathbf{n}^2 + i\boldsymbol{\sigma}\cdot(0) = \mathbb{I}.$$

We have

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}\theta\mathbf{n}\cdot\boldsymbol{\sigma}} &= \sum_{k=0}^{\infty}(\mathrm{i})^k\frac{[\theta(\mathbf{n}\cdot\boldsymbol{\sigma})]^k}{k!} \\
&= \sum_{k=0}^{\infty}(\mathrm{i})^{2k}\frac{[\theta(\mathbf{n}\cdot\boldsymbol{\sigma})]^{2k}}{(2k)!} + \sum_{k=0}^{\infty}(\mathrm{i})^{2k+1}\frac{[\theta(\mathbf{n}\cdot\boldsymbol{\sigma})]^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty}(-1)^k\frac{[\theta(\mathbf{n}\cdot\boldsymbol{\sigma})]^{2k}}{(2k)!} + \mathrm{i}\sum_{k=0}^{\infty}(-1)^k\frac{[\theta(\mathbf{n}\cdot\boldsymbol{\sigma})]^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty}(-1)^k\frac{\theta^{2k}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2k}}{(2k)!} + \mathrm{i}\sum_{k=0}^{\infty}(-1)^k\frac{\theta^{2k+1}(\mathbf{n}\cdot\boldsymbol{\sigma})^{2k+1}}{(2k+1)!} \\
&= \sum_{k=0}^{\infty}(-1)^k\frac{\theta^{2k}}{(2k)!}\mathbb{I} + \mathrm{i}\sum_{k=0}^{\infty}(-1)^k\frac{\theta^{2k+1}}{(2k+1)!}(\mathbf{n}\cdot\boldsymbol{\sigma}) \\
&= \mathbb{I}\cos(\theta) + \mathrm{i}\sin(\theta)(\mathbf{n}\cdot\boldsymbol{\sigma})
\end{aligned}$$

Now that we calculated that, we can solve the following

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}\frac{1}{2}\theta\sigma_y}(\sigma_x,\sigma_y,\sigma_z)\mathrm{e}^{-\mathrm{i}\frac{1}{2}\theta\sigma_y} &= \left[\mathbb{I}\cos\left(\frac{\theta}{2}\right) + \mathrm{i}\sin\left(\frac{\theta}{2}\right)\sigma_y\right](\sigma_x,\sigma_y,\sigma_z)\left[\mathbb{I}\cos\left(\frac{\theta}{2}\right) - \mathrm{i}\sin\left(\frac{\theta}{2}\right)\sigma_y\right] \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) - \mathrm{i}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z)\sigma_y \\
&\quad + \mathrm{i}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\sigma_y(\sigma_x,\sigma_y,\sigma_z) + \sin^2\left(\frac{\theta}{2}\right)\sigma_y(\sigma_x,\sigma_y,\sigma_z)\sigma_y \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) - \mathrm{i}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(\mathrm{i}\sigma_z,1,-\mathrm{i}\sigma_x) \\
&\quad + \mathrm{i}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(-\mathrm{i}\sigma_z,1,\mathrm{i}\sigma_x) + \sin^2\left(\frac{\theta}{2}\right)(-\sigma_x,\sigma_y,-\sigma_z) \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(-\sigma_z,1,\sigma_x) \\
&\quad + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(\sigma_z,1,-\sigma_x) + \sin^2\left(\frac{\theta}{2}\right)(-\sigma_x,\sigma_y,-\sigma_z) \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) + \sin^2\left(\frac{\theta}{2}\right)(-\sigma_x,\sigma_y,-\sigma_z) \\
&\quad + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)[(\sigma_z,-1,-\sigma_x) + (\sigma_z,1,-\sigma_x)] \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) - \sin^2\left(\frac{\theta}{2}\right)(\sigma_x,-\sigma_y,\sigma_z) \\
&\quad + 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)(\sigma_z,0,-\sigma_x) \\
&= \cos^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) - \sin^2\left(\frac{\theta}{2}\right)(\sigma_x,\sigma_y,\sigma_z) \\
&\quad + 2\sin^2\left(\frac{\theta}{2}\right)(0,\sigma_y,0) + \sin(\theta)(\sigma_z,0,-\sigma_x) \\
&= \cos(\theta)(\sigma_x,\sigma_y,\sigma_z) + (1-\cos(\theta))(0,\sigma_y,0) + \sin(\theta)(\sigma_z,0,-\sigma_x).
\end{aligned}$$

The eigenvalues of the Hamiltonian H are found by solving

$$\det(H-\lambda I)=0.$$

We have

$$\begin{aligned}
\det(H-\lambda I) &= \begin{vmatrix} a-\lambda & b \\ b & -a-\lambda \end{vmatrix} \\
&= -(a-\lambda)(a+\lambda)-b^2 \\
&= \lambda^2-(a^2+b^2) \\
&= 0 \\
\implies \lambda^2 &= a^2+b^2 \\
\implies \lambda_\pm \equiv E_\pm &= \pm\sqrt{a^2+b^2}.
\end{aligned}$$

The eigenvectors $e_\pm$ are given by solving the following set of equations

$$\begin{pmatrix} a-\lambda & b \\ b & -a-\lambda \end{pmatrix}\begin{pmatrix} e_1 \\ e_2 \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\implies \begin{cases} (a-\lambda)e_1+be_2 &= 0 \\ be_1+(-a-\lambda)e_2 &= 0 \end{cases}$$

$\boxed{\text{For } \lambda = E_+\text{:}}$

$$\begin{pmatrix} a-E_\pm & b \\ b & -a-E_\pm \end{pmatrix}\begin{pmatrix} e_{\pm,1} \\ e_{\pm,2} \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\begin{cases} (a-E_\pm)e_{\pm,1}+be_{\pm,2} &= 0 \\ be_{\pm,1}+(-a-E_\pm)e_{\pm,2} &= 0 \end{cases}$$

The two eigenvector equations are redundant, so considering the first, we have

$$\begin{aligned}
(a-E_\pm)e_{\pm,1}+be_{\pm,2} &= 0 \\
be_{\pm,2} &= (E_\pm-a)e_{\pm,1} \\
e_{\pm,2} &= \frac{E_\pm-a}{b}e_{\pm,1}.
\end{aligned}$$

Since $e_{\pm,1}$ is arbitrary, we will set $e_{\pm,1}=1$, then $e_{\pm,2}=\frac{E_\pm-a}{b}$. Thus, the two eigenvectors $e_\pm$ corresponding to $E_\pm$ are

$$e_\pm=\begin{pmatrix} e_{\pm,1} \\ e_{\pm,2} \end{pmatrix}=\begin{pmatrix} 1 \\ \frac{E_\pm-a}{b} \end{pmatrix}=\begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix}.$$

Finally, we now normalize the eigenvectors

$$\begin{aligned}
e_\pm &= \frac{1}{\sqrt{\langle e_\pm|e_\pm\rangle}}\begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{1+\frac{(\sqrt{a^2+b^2}\mp a)^2}{b^2}}}\begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{1+\frac{(a^2+b^2\mp 2a\sqrt{a^2+b^2}+a^2)}{b^2}}}\begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix} \\
&= \frac{1}{\sqrt{2+\frac{2a(a\mp\sqrt{a^2+b^2})}{b^2}}}\begin{pmatrix} 1 \\ \frac{\pm\sqrt{a^2+b^2}-a}{b} \end{pmatrix}.
\end{aligned}$$

Let $c_\pm = \frac{1}{\sqrt{2+\frac{2a(a\mp\sqrt{a^2+b^2})}{b^2}}}$. The unitary transformation U that diagonalizes H is given by

$$U = (e_-, e_+) = \begin{pmatrix} c_- & c_+ \\ \frac{-\sqrt{a^2+b^2}-a}{b}c_- & \frac{\sqrt{a^2+b^2}-a}{b}c_+ \end{pmatrix}.$$

■

Problem 2 - 1D Harmonic Oscillator (Sakurai 5.1)
A simple harmonic oscillator in 1D is subjected to a perturbation

$$V = bx.$$

where $b \in \mathbb{R}$ is a constant.

(a) Calculate the energy shift of the ground state to the *lowest non-vanishing order*.

(b) Solve the problem *exactly* and compare your answer to (a).

Solution. (a) The energy shift in an unperturbed nth state can be calculated as

$$\Delta_n = \underset{\text{in energy}}{\text{first order correction}} + \underset{\text{in energy}}{\text{second order correction}} + \cdots + \underset{\text{in energy}}{n\text{th order correction}}.$$

The first-order correction to the energy is

$$\begin{aligned} E_n^{(1)} &= \langle n|V|n\rangle \\ &= b\,\langle n|\hat{x}|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\hat{a}+\hat{a}^\dagger|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\langle n|\hat{a}|n\rangle + \langle n|\hat{a}^\dagger|n\rangle\right] \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\,\langle n|n-1\rangle + \sqrt{n+1}\,\langle n|n+1\rangle\right] \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}\right]. \end{aligned}$$

For the ground state ($n=0$), we have

$$E_n^{(1)} = b\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{0}\delta_{0,-1} + \sqrt{1}\delta_{0,1}\right] = 0.$$

The second-order correction to the energy is

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle m|V|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}.$$

We have that

$$\begin{aligned} \langle m|V|n\rangle &= b\,\langle m|\hat{x}|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|\hat{a}+\hat{a}^\dagger|n\rangle \\ &= b\sqrt{\frac{\hbar}{2m\omega}}\left[\langle m|\hat{a}|n\rangle + \langle m|\hat{a}^\dagger|n\rangle\right]. \end{aligned}$$

If we replace in the sum, all the terms will be null, except for those where $m = n-1$ or $m = n+1$. Then, we have

$$\begin{aligned}
E_n^{(2)} &= \sum_{m\neq n} \frac{|\langle m|V|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\langle n-1|\hat{a}|n\rangle + \langle n-1|\hat{a}^\dagger|n\rangle\right|^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{\left|\langle n+1|\hat{a}|n\rangle + \langle n+1|\hat{a}^\dagger|n\rangle\right|^2}{E_n^{(0)} - E_{n+1}^{(0)}}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\sqrt{n}\,\langle n-1|n-1\rangle + \sqrt{n+1}\,\langle n-1|n+1\rangle\right|^2}{\hbar\omega} + \frac{\left|\sqrt{n}\,\langle n+1|n-1\rangle + \sqrt{n+1}\,\langle n+1|n+1\rangle\right|^2}{-\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{\left|\sqrt{n}\delta_{n-1,n-1} + \sqrt{n+1}\delta_{n-1,n+1}\right|^2}{\hbar\omega} - \frac{\left|\sqrt{n}\delta_{n-1,n+1} + \sqrt{n+1}\delta_{n+1,n+1}\right|^2}{\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{|\sqrt{n}|^2}{\hbar\omega} - \frac{\left|\sqrt{n+1}\right|^2}{\hbar\omega}\right] \\
&= \frac{\hbar b^2}{2m\omega}\left[\frac{n}{\hbar\omega} - \frac{n+1}{\hbar\omega}\right] \\
&= -\frac{b^2}{2m\omega^2}.
\end{aligned}$$

The energy correction to the lowest non-vanishing order is

$$E = E_n^{(0)} + E_n^{(2)} = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{b^2}{2m\omega^2}.$$

The energy correction of the ground state ($n = 0$) is

$$E = E_0^{(0)} + E_0^{(2)} = \frac{\hbar\omega}{2} - \frac{b^2}{2m\omega^2}.$$

Thus, the energy shift of the ground state is $-\frac{b^2}{2m\omega^2}$.

(b) The Hamiltonian of the harmonic oscillator is given by

$$\hat{\mathcal{H}}_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2.$$

The Hamiltonian of our perturbed system is

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_p = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx.$$

To solve this problem exactly, we complete the square, getting

$$\begin{aligned}
\hat{\mathcal{H}} &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + bx \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2bx}{m\omega^2}\right) \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + 2x\frac{b}{m\omega^2} + \left(\frac{b}{m\omega^2}\right)^2 - \left(\frac{b}{m\omega^2}\right)^2\right) \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x + \frac{b}{m\omega^2}\right)^2 - \frac{1}{2}m\omega^2\left(\frac{b}{m\omega^2}\right)^2 \\
&= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x + \frac{b}{m\omega^2}\right)^2 - \frac{b^2}{2m\omega^2},
\end{aligned}$$

Let $x' \equiv x + \frac{b}{m\omega^2}$, then we still obtain a simple harmonic oscillator, but with the equilibrium point shifted and with an overall energy shift of $-\frac{b^2}{2m\omega^2}$, which is the same energy shift calculated in (a). Thus, the second-order perturbation theory will give us the exact answer in this case.

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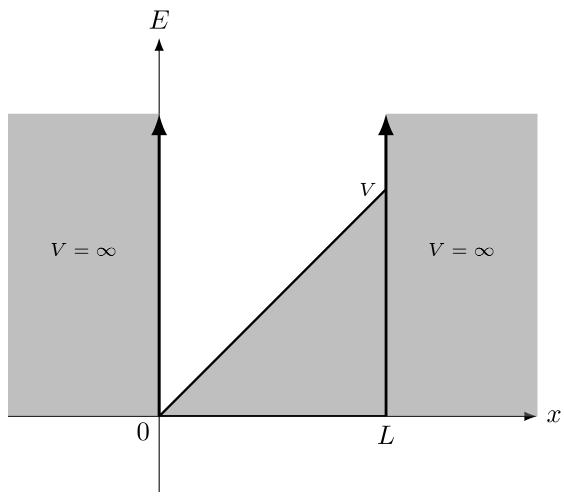
Problem 3 - Potential Well (Sakurai 5.2)
Consider a 1D potential well with infinite walls at $x = 0$, L. The bottom is *not* flat, but increases linearly from 0 at $x = 0$ to V at $x = L$. Find the first-order shift in the energy levels as a function of principal quantum number n.

Solution. The 1D potential well with infinite walls looks like



For the unperturbed potential of the infinite potential well, the wave functions $\left|\psi_n^{(0)}\right\rangle$ and the energy eigenvalues $E_n^{(0)}$ are given by

$$\left|\psi_n^{(0)}\right\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$
$$E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2mL^2}.$$

The Hamiltonian given by the perturbed potential is

$$\hat{\mathcal{H}}_p = \frac{V}{L}x.$$

The total Hamiltonian of the system is then given by

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_p = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{V}{L}x.$$

We know how to exactly solve the first term of the Hamiltonian, but our perturbation theory kicks in with the second term, which is the potential term.

The expected value of the energy of the perturbed potential is

$$\begin{aligned}
\left\langle \hat{\mathcal{H}}_p \right\rangle &= \left\langle \psi_n^{(0)} \middle| \hat{\mathcal{H}}_p \middle| \psi_n^{(0)} \right\rangle \\
&= \int_0^L \left(\psi_n^{(0)}\right)^* \hat{\mathcal{H}}_p \psi_n^{(0)} \,\mathrm{d}x \\
&= \int_0^L \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)\right)^* \left(\frac{V}{L}x\right) \left(\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L x \sin^2\left(\frac{n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L x \left(\frac{1 - \cos\left(\frac{2n\pi x}{L}\right)}{2}\right) \mathrm{d}x \\
&= \frac{2V}{L^2} \int_0^L \left[\frac{x}{2} - \frac{x}{2} \cos\left(\frac{2n\pi x}{L}\right)\right] \mathrm{d}x \\
&= \frac{2V}{L^2} \left[\frac{x^2}{4} - \frac{x}{2} \frac{L}{2n\pi} \sin\left(\frac{2n\pi x}{L}\right) + \frac{1}{2} \frac{L^2}{4n^2\pi^2} \cos\left(\frac{2n\pi x}{L}\right)\right]_0^L \\
&= \frac{2V}{L^2} \left[\frac{x^2}{4} - \frac{xL}{4n\pi} \sin\left(\frac{2n\pi x}{L}\right) + \frac{L^2}{8n^2\pi^2} \cos\left(\frac{2n\pi x}{L}\right)\right]_0^L \\
&= \frac{2V}{L^2} \left[\frac{L^2}{4} - \frac{L^2}{4n\pi} \sin(2n\pi) + \frac{L^2}{8n^2\pi^2} \cos(2n\pi) - \frac{L^2}{8n^2\pi^2}\right] \\
&= \frac{2V}{L^2} \left[\frac{L^2}{8n^2\pi^2} \left(2n^2\pi^2 - 2n\pi \sin(2n\pi) + \cos(2n\pi) - 1\right)\right] \\
&= \frac{2V}{L^2} \left[\frac{L^2}{8n^2\pi^2} \left(2n^2\pi^2\right)\right] \\
&= \frac{V}{2}.
\end{aligned}$$

Thus, the first-order energy shift is $\frac{V}{2}$. Notice that it does not depend on the principal quantum number n. ■

Problem 4 - 2D Harmonic Oscillator (Sakurai 5.7)
Consider an isotropic harmonic oscillator in *two* dimensions. The Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2} m\omega^2 \left(x^2 + y^2\right).$$

(a) Calculate the energies of the three lowest-lying states? Is there any degeneracy?

(b) We now apply a perturbation

$$V = \delta m\omega^2 xy,$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenstate and the corresponding energy to first order [that is, the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.

(c) Solve the $H + V$ problem *exactly*. Compare with the perturbation results obtained in (b).

Solution. (a) The energy for the state n of a harmonic oscillator with d degrees of freedom is given by

$$E = \left(\sum_{i=1}^{d} n_i + \frac{d}{2}\right) \hbar\omega.$$

In this case, we have two degrees of freedom. Hence, the energy for the state n of our isotropic harmonic oscillator will be

$$E = (n_x + n_y + 1)\hbar\omega.$$

We will now find the energy of the three lowest energy states.

- **Ground state**: We have $n_x = n_y = 0$, and the energy is

$$E = \hbar\omega.$$

- **First excited state**:
  - We have $n_x = 1$ and $n_y = 0$, and the energy is

$$E = 2\hbar\omega.$$

  - We have $n_x = 0$ and $n_y = 1$, and the energy is

$$E = 2\hbar\omega.$$

Thus, the two configurations of the first excited state both yield the same energy level and are therefore doubly degenerate.

(b) Given the perturbation

$$V = \delta m\omega^2 xy,$$

our total Hamiltonian becomes

$$\hat{\mathcal{H}} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + y^2\right) + \delta m\omega^2 xy$$

As we know, in time-independent perturbation theory, if we perturb an energy eigenvalue for the zeroth-order correction, then there will be no perturbation change in energy compared to the initial energy for the zeroth-order perturbation.

Finding the first-order energy correction, we have

$$\begin{aligned} E^{(1)}_{n_x,n_y} &= \langle n_x, n_y|V|n_x, n_y\rangle \\ &= \left\langle n_x, n_y\middle|\delta m\omega^2 xy\middle|n_x, n_y\right\rangle \\ &= \delta m\omega^2 \langle n_x, n_y|xy|n_x, n_y\rangle \\ &= \delta m\omega^2 \langle n_x|x|n_x\rangle \langle n_y|y|n_y\rangle, \end{aligned}$$

where the last step follows from the fact that x and y are independent.

The first-order energy shift is as follows

- For the ground state:

$$E^{(1)}_{0,0} = \langle 0,0|V|0,0\rangle = \delta m\omega^2 \langle 0|x|0\rangle \langle 0|y|0\rangle = 0.$$

- For the first excited state, this requires us to diagonalize the perturbation for the first order energy shift, but
  - For $(n_x, n_y) = (1, 0)$:

$$E^{(1)}_{1,0} = \langle 1,0|V|1,0\rangle = \delta m\omega^2 \langle 1|x|1\rangle \langle 0|y|0\rangle = 0.$$

  - For $(n_x, n_y) = (0, 1)$:

$$E^{(1)}_{1,0} = \langle 0,1|V|0,1\rangle = \delta m\omega^2 \langle 0|x|0\rangle \langle 1|y|1\rangle = 0.$$

The off-diagonal elements are

$$\begin{aligned}\langle 1,0|V|0,1\rangle &= \delta m\omega^2 \left\langle 1,0 \middle| \sqrt{\frac{\hbar}{2m\omega}}\sqrt{1}\sqrt{\frac{\hbar}{2m\omega}}\sqrt{1} \middle| 0,1 \right\rangle \\ &= \frac{\delta\hbar\omega}{2} \\ &= \langle 0,1|V|1,0\rangle .\end{aligned}$$

The first-order energy shifts in the first excited state are the eigenvalues $\Delta_1^{(1)}$, where

$$\left(\Delta_1^{(1)}\right)^2 - \left(\frac{\delta\hbar\omega}{2}\right)^2 = 0 \implies \Delta_1^{(1)} = \pm\frac{\delta\hbar\omega}{2},$$

and

$$E = \left(2 \pm \frac{\delta}{2}\right)\hbar\omega$$

for the degenerate first excited state. The corresponding eigenstates are

$$\frac{|1,0\rangle + ket0,1}{\sqrt{2}}.$$

(c) To solve $H + V$ exactly, we can rewrite the potential energy as

$$\begin{aligned}V &= \frac{1}{2}m\omega^2(x^2 + y^2 + 2\delta xy) \\ &= \frac{1}{2}m\omega^2\left[(1+\delta)\frac{(x+y)^2}{2} + (1-\delta)\frac{(x-y)^2}{2}\right].\end{aligned}$$

We can then rotate the xy-axes by $\frac{\pi}{4}$, and then the anharmonic oscillator has the normal coordinate $x' \equiv \frac{x+y}{\sqrt{2}}$ with frequency $\omega\sqrt{1+\delta}$, and $y' \equiv \frac{x-y}{\sqrt{2}}$ with frequency $\omega\sqrt{1-\delta}$.
Therefore, we have

- For $|0,0\rangle$:
$$\frac{1}{2}\hbar\omega\sqrt{1+\delta} + \frac{1}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(1 + \frac{\delta}{2} + 1 - \frac{\delta}{2}\right) = \hbar\omega.$$
- For $|1,0\rangle$:
$$\frac{3}{2}\hbar\omega\sqrt{1+\delta} + \frac{1}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(3 + \frac{3\delta}{2} + 1 - \frac{\delta}{2}\right) = \left(2 + \frac{\delta}{2}\right)\hbar\omega.$$
- For $|0,1\rangle$:
$$\frac{1}{2}\hbar\omega\sqrt{1+\delta} + \frac{3}{2}\hbar\omega\sqrt{1-\delta} \approx \frac{1}{2}\hbar\omega\left(1 + \frac{\delta}{2} + 3 - \frac{3\delta}{2}\right) = \left(2 - \frac{\delta}{2}\right)\hbar\omega.$$

All three cases are in agreement with our lowest order results from perturbation theory in part (b). ■