Physics 741 – Graduate Quantum Mechanics 1

Solutions to Chapter 12

- 6. [20] A particle of mass *m* lies in one dimension with Hamiltonian near the origin of $H = P^2/2m + \frac{1}{2}m\omega^2X^2 + \gamma X^3$ where γ is very small.
 - (a) [8] Find the energy of all quantum states to second order in χ

If we treat γ as zero, then we have a harmonic oscillator, which has eigenstates $|n\rangle$ and energies $\hbar\omega(n+\frac{1}{2})$. Letting our perturbation act on an arbitrary state, we have

$$W|n\rangle = \gamma \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left(a+a^{\dagger}\right)^{3}|n\rangle = \gamma \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left(a+a^{\dagger}\right)^{2} \left(\sqrt{n+1}|n+1\rangle + \sqrt{n}|n-1\rangle\right)$$

$$= \gamma \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left(a+a^{\dagger}\right) \left(\sqrt{(n+1)(n+2)}|n+2\rangle + (2n+1)|n\rangle + \sqrt{n(n-1)}|n-2\rangle\right)$$

$$= \gamma \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left(\sqrt{(n+1)(n+2)(n+3)}|n+3\rangle + (3n+3)\sqrt{n+1}|n+1\rangle\right)$$

$$+3n\sqrt{n}|n-1\rangle + \sqrt{n(n-1)(n-2)}|n-3\rangle$$

The energies of our states, therefore, are

$$\begin{split} E_n &= \varepsilon_n + \left\langle n \middle| W \middle| n \right\rangle + \sum_{m \neq n} \frac{\left| \left\langle m \middle| W \middle| n \right\rangle \right|^2}{\varepsilon_n - \varepsilon_m} \\ &= \hbar \omega \left(n + \frac{1}{2} \right) + 0 + \frac{\left| \left\langle n - 3 \middle| W \middle| n \right\rangle \right|^2}{3\hbar \omega} + \frac{\left| \left\langle n - 1 \middle| W \middle| n \right\rangle \right|^2}{\hbar \omega} + \frac{\left| \left\langle n + 1 \middle| W \middle| n \right\rangle \right|^2}{-\hbar \omega} + \frac{\left| \left\langle n + 3 \middle| W \middle| n \right\rangle \right|^2}{-3\hbar \omega} \\ &= \hbar \omega \left(n + \frac{1}{2} \right) + \gamma^2 \left(\frac{\hbar}{2m\omega} \right)^3 \frac{1}{\hbar \omega} \begin{bmatrix} \frac{1}{3} n (n - 1) (n - 2) + (3n)^2 n - (3n + 3)^2 (n + 1) \\ -\frac{1}{3} (n + 1) (n + 2) (n + 3) \end{bmatrix} \\ &= \hbar \omega \left(n + \frac{1}{2} \right) + \frac{\gamma^2 \hbar^2}{8m^3 \omega^4} \left(\frac{1}{3} n^3 - n^2 + \frac{2}{3} n + 9n^3 - 9n^3 - 27n^2 - 27n - 9 - \frac{1}{3} n^3 - 2n^2 - \frac{11}{3} n - 2 \right) \\ &= \hbar \omega \left(n + \frac{1}{2} \right) - \frac{\gamma^2 \hbar^2}{8m^3 \omega^4} \left(30n^2 + 30n + 11 \right) \end{split}$$

(b) [5] Find the eigenstates of H to first order in χ

The states are given, to first order in γ , by

$$\begin{aligned} |\psi_{n}\rangle &= |n\rangle + \sum_{m\neq n} \frac{|m\rangle\langle n|W|p\rangle}{\varepsilon_{n} - \varepsilon_{m}} \\ &= |n\rangle + |n+3\rangle \frac{\langle n+3|W|n\rangle}{-3\hbar\omega} + |n+1\rangle \frac{\langle n+1|W|n\rangle}{-\hbar\omega} + |n-1\rangle \frac{\langle n-1|W|n\rangle}{\hbar\omega} + |n-3\rangle \frac{\langle n-3|W|n\rangle}{3\hbar\omega} \\ &= |n\rangle + \frac{\gamma}{3\hbar\omega} \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left(-\sqrt{(n+3)(n+2)(n+1)}|n+3\rangle - 9(n+1)^{3/2}|n+1\rangle + 9n^{3/2}|n-1\rangle \\ &+ \sqrt{n(n-1)(n-2)}|n-3\rangle \right) \end{aligned}$$

(c) [7] Find the expectation value $\langle \psi_{\scriptscriptstyle n} | X | \psi_{\scriptscriptstyle n} \rangle$ for the eigenstates $|\psi_{\scriptscriptstyle n} \rangle$ to first order in \varkappa

We simply take

$$\begin{split} \left\langle \psi_{n} \left| X \right| \psi_{n} \right\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \left[\left\langle n \right| + \sum_{m \neq n} \frac{\left\langle n \right| W \left| m \right\rangle \left\langle m \right|}{\varepsilon_{n} - \varepsilon_{m}} \right] \left(a + a^{\dagger} \right) \left[\left| n \right\rangle + \sum_{m \neq n} \frac{\left| m \right\rangle \left\langle m \right| W \left| n \right\rangle}{\varepsilon_{n} - \varepsilon_{m}} \right] \\ &= \sqrt{\frac{\hbar}{2m\omega}} \sum_{m \neq n} \frac{1}{\varepsilon_{n} - \varepsilon_{m}} \left[\left\langle n \right| W \left| m \right\rangle \left\langle m \right| \left(a + a^{\dagger} \right) \left| n \right\rangle + \left\langle n \right| \left(a + a^{\dagger} \right) \left| m \right\rangle \left\langle m \right| W \left| n \right\rangle \right] \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left[\frac{\sqrt{n}}{\hbar \omega} \left(\left\langle n \right| W \left| n - 1 \right\rangle + \left\langle n - 1 \right| W \left| n \right\rangle \right) + \frac{\sqrt{n+1}}{-\hbar \omega} \left(\left\langle n \right| W \left| n + 1 \right\rangle + \left\langle n + 1 \right| W \left| n \right\rangle \right) \right] \\ &= \frac{2\gamma}{\hbar \omega} \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{\hbar}{2m\omega} \right)^{3/2} \left[\sqrt{n} 3n \sqrt{n} - \sqrt{n+1} \left(3n + 3 \right) \sqrt{n+1} \right] \\ &= \frac{6\gamma}{\hbar \omega} \left(\frac{\hbar}{2m\omega} \right)^{2} \left[n^{2} - \left(n + 1 \right)^{2} \right] = -\frac{3\gamma\hbar \left(2n + 1 \right)}{2m^{2}\omega^{3}} \end{split}$$

7. [15] A particle of mass m lies in a one-dimensional infinite slightly tilted square well

$$V(x) = \begin{cases} bx & \text{if } 0 < x < a \\ \infty & \text{otherwise} \end{cases}$$

where b is small.

(a) [2] What are the normalized eigenstates and energies if b = 0?

For b = 0, we just have an infinite square well, with wave functions and energies

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi nx}{a}\right)$$

$$\varepsilon_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}$$

(b) [6] Find the eigenstates and energies to first order in b.

The energies are given, to first order in b, by

$$E_{n} = \varepsilon_{n} + \left\langle \phi_{n} \middle| W \middle| \phi_{n} \right\rangle = \frac{\pi^{2} \hbar^{2} n^{2}}{2ma^{2}} + b \frac{2}{a} \int_{0}^{a} x \sin^{2} \left(\frac{\pi nx}{a} \right) dx = \frac{\pi^{2} \hbar^{2} n^{2}}{2ma^{2}} + b \frac{2}{a} \frac{a^{2}}{4} = \frac{\pi^{2} \hbar^{2} n^{2}}{2ma^{2}} + \frac{ba}{2} \frac{a^{2}}{2ma^{2}} + \frac{ba}{2ma^{2}} + \frac{ba}{2ma^{2}} \frac{a^{2}}{2ma^{2}} \frac{a^{2}}{2ma^{2}} + \frac{ba}{2ma^{2}} \frac{a^{2}}{2ma^{2}} \frac{a^{2}}{2ma^{2}} + \frac{ba}{2ma^{2}} \frac{a^{2}}{2ma^{2}} \frac{a$$

To find the wave functions, we need to find

$$\langle \phi_p | W | \phi_n \rangle = b \frac{2}{a} \int_0^a x \sin\left(\frac{\pi nx}{a}\right) \sin\left(\frac{\pi px}{a}\right) dx = \frac{4banp\left[\left(-1\right)^{n+p} - 1\right]}{\pi^2 \left(n^2 - p^2\right)^2}$$

We are avoiding the letter m so as not to confuse it with the mass. The expression in []'s vanishes when n + p is even, and is -2 when n + p is odd. So we have

$$\begin{aligned} \left|\psi_{n}\right\rangle &=\left|\phi_{n}\right\rangle + \sum_{p\neq n}\left|\phi_{p}\right\rangle \frac{\left\langle\phi_{p}\left|W\right|\phi_{n}\right\rangle}{\varepsilon_{n} - \varepsilon_{p}} &=\left|\phi_{n}\right\rangle + \sum_{\substack{p+n\\ \text{odd}}} \frac{-8banp}{\pi^{2}\left(n^{2} - p^{2}\right)^{2}} \frac{2ma^{2}}{\pi^{2}\hbar^{2}\left(n^{2} - p^{2}\right)}\left|\phi_{p}\right\rangle \\ &=\left|\phi_{n}\right\rangle - \frac{16bma^{3}}{\pi^{4}\hbar^{2}} \sum_{\substack{p+n\\ \text{odd}}} \frac{np}{\left(n^{2} - p^{2}\right)^{3}}\left|\phi_{p}\right\rangle. \end{aligned}$$

(c) [7] Find the ground state energy to second order in b. If you can't do the sums exactly, do them numerically.

Using our formula, we have

$$\begin{split} E_{1} &= \varepsilon_{1} + \left\langle \phi_{1} \left| W \right| \phi_{1} \right\rangle + \sum_{p \neq 1} \frac{\left| \left\langle \phi_{p} \left| W \right| \phi_{1} \right\rangle \right|^{2}}{\varepsilon_{1} - \varepsilon_{p}} = \frac{\pi^{2} \hbar^{2}}{2ma^{2}} + \frac{ba}{2} + \sum_{p \text{ even}} \left[\frac{-8bap}{\pi^{2} \left(1 - p^{2} \right)^{2}} \right]^{2} \frac{2ma^{2}}{\pi^{2} \hbar^{2} \left(1 - p^{2} \right)} \\ &= \frac{\pi^{2} \hbar^{2}}{2ma^{2}} + \frac{ba}{2} - \frac{128mb^{2}a^{4}}{\pi^{6} \hbar^{2}} \sum_{p \text{ even}} \frac{p^{2}}{\left(p^{2} - 1 \right)^{5}} \end{split}$$

The final sum can be performed numerically very quickly, since the terms fall as p^{-8} , or we can do it analytically by hand or with the help of Maple.

> sum(4*n^2/(4*n^2-1)^5,n=1..infinity);

$$\begin{split} E_1 &= \frac{\pi^2 \hbar^2}{2ma^2} + \frac{ba}{2} - \frac{128mb^2 a^4}{\pi^6 \hbar^2} \left(\frac{5\pi^2}{1024} - \frac{\pi^4}{3072} \right) = \frac{\pi^2 \hbar^2}{2ma^2} + \frac{ba}{2} - \frac{\left(15 - \pi^2\right)mb^2 a^4}{24\pi^4 \hbar^2} \\ &= \frac{\pi^2 \hbar^2}{2ma^2} + \frac{ba}{2} - 0.002195 \frac{mb^2 a^4}{\hbar^2} \end{split}$$