Assignment 4 Solutions

4.1 The Variational Theorem tells us that we should first evaluate

$$<E> = \frac{\int_{-a}^{a} \phi(x)\hat{H}\phi(x)\ dx}{\int_{-a}^{a} \phi(x)\phi(x)\ dx} = \frac{\phi_0^2 \int_{-a}^{a} \cos\left(\frac{\pi x}{2a}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{kx^2}{2}\right]\cos\left(\frac{\pi x}{2a}\right) dx}{\phi_0^2 \int_{-a}^{a} \cos^2\left(\frac{\pi x}{2a}\right) dx}$$

where the definition of $\phi(x)$ allows us to limit the integration range to $-a \le x \le a$ since ϕ is zero elsewhere. Note that the normalization constant, ϕ_0, cancels from the problem. That's why normalization constants cannot be used as variational parameters! Let's start with the integral in the denominator:

$$\int_{-a}^{a} \cos^2\left(\frac{\pi x}{2a}\right) dx = \frac{2a}{\pi}\int_{-\pi/2}^{\pi/2} \cos^2 y\ dy = \frac{2a}{\pi}\left[\frac{\cos y \sin y + y}{2}\right]_{-\pi/2}^{\pi/2} = a\ .$$

The integral in the numerator can be written as a sum of two integrals, one for the kinetic energy operator and one for the potential energy operator. The first of these is

$$\int_{-a}^{a} \cos\left(\frac{\pi x}{2a}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2 \cos\left(\frac{\pi x}{2a}\right)}{dx^2}\right] dx = \frac{\hbar^2\pi^2}{8ma^2}\int_{-a}^{a} \cos^2\left(\frac{\pi x}{2a}\right) dx = \frac{\hbar^2\pi^2}{8ma}\ .$$

The second is

$$\int_{-a}^{a} \cos\left(\frac{\pi x}{2a}\right)\left[\frac{kx^2}{2}\right]\cos\left(\frac{\pi x}{2a}\right) dx = \frac{k}{2}\int_{-a}^{a} x^2 \cos^2\left(\frac{\pi x}{2a}\right) dx$$

$$= \frac{k}{2}\left(\frac{2a}{\pi}\right)^3 \int_{-\pi/2}^{\pi/2} y^2 \cos^2 y\ dy$$

$$= \frac{k}{2}\left(\frac{2a}{\pi}\right)^3 \frac{\pi}{24}\left(\pi^2 - 6\right) = a^3 k\left(\frac{1}{6} - \frac{1}{\pi^2}\right).$$

Putting everything together gives

$$<E> = \frac{\int_{-a}^{a} \phi(x)\hat{H}\phi(x)\ dx}{\int_{-a}^{a} \phi(x)\phi(x)\ dx} = \frac{\hbar^2\pi^2}{8ma^2} + a^2 k\left(\frac{1}{6} - \frac{1}{\pi^2}\right).$$

Now we have to find the value for a that makes this expression a minimum. We evaluate $d\langle E\rangle/da$, set the result equal to zero, and solve for a. A bit of algebra gives

$$a = \left(\frac{3}{4}\,\frac{\pi^4\hbar^2}{(\pi^2 - 6)\,km}\right)^{1/4}$$

and substituting this value for a into the expression for $\langle E\rangle$ gives, with a bit more algebra and the definition of ω,

$$\langle E\rangle = \frac{\hbar^2\pi^2}{8ma^2} + a^2k\left(\frac{1}{6} - \frac{1}{\pi^2}\right) = \frac{\sqrt{3}\,\sqrt{\pi^2 - 6}}{6}\,\hbar\omega = 0.568\ \hbar\omega.$$

Since the exact answer is $0.5\hbar\omega$, we see that this approximate wavefunction indeed predicts a ground state energy that is greater than the exact energy, as the Variational Theorem says it should.

4.2 We want to apply first-order perturbation theory to the perturbation

$$\hat{H}' = \begin{cases} 0 & 0 \le x < fL \quad \text{or} \quad (1-f)L < x \le L \\ V_0 & fL \le x \le (1-f)L \end{cases}$$

where f is anywhere in the range 0 to 1/2. Our unperturbed wavefunction is the particle-in-a-box ground-state wavefunction:

$$\psi_1^{(0)}(x) = \sqrt{\frac{2}{L}}\,\sin\frac{\pi x}{L}$$

We calculate the perturbation energy using the integral given in problem 13.11:

$$E_1^{(1)} = \int \psi_1^{(0)}\hat{H}'\psi_1^{(0)}\,dx = \frac{2V_0}{L}\int_{fL}^{(1-f)L} \sin^2\frac{\pi x}{L}\,dx = \frac{2V_0}{\pi}\int_{f\pi}^{(1-f)\pi} \sin^2 y^2\,dy$$

$$= \frac{2V_0}{\pi}\left\{\frac{(1-f)\pi - f\pi}{2} + \frac{1}{4}\left[\sin 2\pi f - \sin(2\pi - 2\pi f)\right]\right\}$$

$$= \frac{2V_0}{\pi}\left\{\frac{\pi - 2f\pi}{2} + \frac{1}{4}\left[2\sin 2\pi f\right]\right\} = V_0\left(1 - 2f + \frac{\sin 2\pi f}{\pi}\right)$$

and we check the answer for the follwing values of f: for $f = 0$ (the potential bump extends over the entire box), we find $E_1^{(1)} = V_0$, which makes great sense—the bump is no longer a bump, but just a change in the reference energy from zero at the bottom of the box to V_0 at the bottom; for $f = 1/2$ (the potential bump is gone), we find $E_1^{(1)} = 0$, again what we expect—no bump, no perturbation!— and finally for $f = 1/4$, the case considered in problem 13.11, we find $E_1^{(1)} = V_0\,(1/2 + 1/\pi)$, in agrement with the solution manual.

4.3 The Landé interval rule considers the energy difference (the "splitting") between two sequential spin-orbit states, i.e., states with quantum numbers j and $j + 1$. We keep l and s the same here and calculate, using Eq. (13.31),

$$\begin{aligned} E_{so}^{(1)}(j+1, l, s) - E_{so}^{(1)}(j, l, s) \\ &= \frac{\hbar^2 h_{so}}{2}\{[(j+1)(j+2) - l(l+1) - s(s+1)] - [j(j+1) - l(l+1) - s(s+1)]\} \\ &= \frac{\hbar^2 h_{so}}{2}\left(j^2 + 3j + 2 - j^2 - j\right) = \frac{\hbar^2 h_{so}}{2}(2j+2) = \hbar^2 h_{so}(j+1) \end{aligned}$$

which completes the proof: the energy splitting is directly proportional to the larger j value, i.e., to $j + 1$.