CHAPTER 7

Problem 7.1 (a) $\langle V\rangle = 2\alpha A^2\int_0^\infty x e^{-2bx^2}dx = 2\alpha A^2\left(-\frac{1}{4b}e^{-2bx^2}\right)\Big|_0^\infty = \frac{\alpha A^2}{2b} = \frac{\alpha}{2b}\sqrt{\frac{2b}{\pi}} = \frac{\alpha}{\sqrt{2b\pi}}.$

$\therefore \langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2\pi b}}.\quad \frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha}{\sqrt{2\pi}}b^{-3/2} = 0 \Rightarrow b^{3/2} = \frac{\alpha}{\sqrt{2\pi}}\frac{m}{\hbar^2};\ b = \left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{2/3}.$

$$\langle H\rangle_{min} = \frac{\hbar^2}{2m}\left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{2/3} + \frac{\alpha}{\sqrt{2\pi}}\left(\frac{\sqrt{2\pi}\,\hbar^2}{m\alpha}\right)^{1/3} = \frac{\alpha^{2/3}\hbar^{2/3}}{m^{1/3}(2\pi)^{1/3}}\left(\frac{1}{2}+1\right) = \boxed{\frac{3}{2}\left(\frac{\alpha^2\hbar^2}{2\pi m}\right)^{1/3}}.$$

(b) $\langle V\rangle = 2\alpha A^2\int_0^\infty x^4 e^{-2bx^2}dx = 2\alpha A^2\frac{3}{8(2b)^2}\sqrt{\frac{\pi}{2b}} = \frac{3\alpha}{16b^2}\sqrt{\frac{\pi}{2b}}\sqrt{\frac{2b}{\pi}} = \frac{3\alpha}{16b^2}.$

$\therefore \langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}.\quad \frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0 \Rightarrow b^3 = \frac{3\alpha m}{4\hbar^2};\ b = \left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3}.$

$$\langle H\rangle_{min} = \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{2/3} = \frac{\alpha^{1/3}\hbar^{4/3}}{m^{2/3}}3^{1/3}4^{-1/3}\left(\frac{1}{2}+\frac{1}{4}\right) = \boxed{\frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{1/3}}.$$

Problem 7.2 Normalize: $1 = 2|A|^2\int_0^\infty \frac{1}{(x^2+b^2)^2}dx = 2|A|^2\frac{\pi}{4b^3} = \frac{\pi}{2b^3}|A|^2.\quad A = \sqrt{\frac{2b^3}{\pi}}.$

Kinetic energy: $\langle T\rangle = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{\infty}\frac{1}{(x^2+b^2)}\underbrace{\frac{d^2}{dx^2}\left(\frac{1}{(x^2+b^2)}\right)}dx$

$$\frac{d}{dx}\left(\frac{-2x}{(x^2+b^2)^2}\right) = \frac{-2}{(x^2+b^2)^2} + 2x\frac{4x}{(x^2+b^2)^3} = \frac{2(3x^2-b^2)}{(x^2+b^2)^3}$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\cdot\frac{2b^3}{\pi}\cdot 4\int_0^\infty\frac{(3x^2-b^2)}{(x^2+b^2)^4}dx = -\frac{4\hbar^2 b^3}{\pi m}\left\{3\int_0^\infty\frac{1}{(x^2+b^2)^3}dx - 4b^2\int_0^\infty\frac{1}{(x^2+b^2)^4}dx\right\}$$

$$= -\frac{4\hbar^2 b^3}{\pi m}\left\{3\cdot\frac{3\pi}{16b^5} - 4b^2\cdot\frac{5\pi}{32b^7}\right\} = \frac{\hbar^2}{4mb^2}.$$

Potential energy: $\langle V\rangle = \frac{1}{2}m\omega^2|A|^2\,2\int_0^\infty\frac{x^2}{(x^2+b^2)^2}dx = m\omega^2\frac{2b^3}{\pi}\cdot\frac{\pi}{4b} = \frac{1}{2}m\omega^2 b^2.$

$\therefore \langle H\rangle = \frac{\hbar^2}{4mb^2} + \frac{1}{2}m\omega^2 b^2.\quad \frac{\partial\langle H\rangle}{\partial b} = -\frac{\hbar^2}{2mb^3} + m\omega^2 b = 0 \Rightarrow b^4 = \frac{\hbar^2}{2m^2\omega^2} \Rightarrow b^2 = \frac{1}{\sqrt{2}}\frac{\hbar}{m\omega}.$

$$\therefore \langle H\rangle_{min} = \frac{\hbar^2}{4m}\frac{\sqrt{2}\,m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{1}{\sqrt{2}}\frac{\hbar}{m\omega} = \hbar\omega\left(\frac{\sqrt{2}}{4} + \frac{1}{2\sqrt{2}}\right) = \boxed{\frac{\sqrt{2}}{2}\hbar\omega} = 0.707\hbar\omega > \frac{1}{2}\hbar\omega.\ \checkmark$$

PROBLEM 7.4 (a) Follow the proof in §7.1 : $\psi = \sum_{n=1}^{\infty} c_n \psi_n$, where ψ_1 is the ground state. Since $\langle\psi_1|\psi\rangle = 0$, we have: $\sum_{n=1}^{\infty} c_n\langle\psi_1|\psi_n\rangle = c_1 = 0$ — the coefficient of the ground state is zero. So

$\langle H\rangle = \sum_{n=2}^{\infty} E_n|c_n|^2 \geq E_f \sum_{n\geq 2}^{\infty}|c_n|^2 = E_f$, since $E_n \geq E_f$ for all n except 1.

(b) $1 = |A|^2\int_{-\infty}^{\infty} x^2 e^{-2bx^2}dx = |A|^2\, 2\cdot\frac{1}{8b}\sqrt{\frac{\pi}{2b}} \Rightarrow |A|^2 = 4b\sqrt{\frac{2b}{\pi}}$.

$$\langle T\rangle = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{\infty} x e^{-bx^2}\underbrace{\frac{d^2}{dx^2}\left(xe^{-bx^2}\right)}dx$$

$$\frac{d}{dx}\left(e^{-bx^2} - 2bx^2e^{-bx^2}\right) = -2bxe^{-bx^2} - 4bxe^{-bx^2} + 4b^2x^3e^{-bx^2}$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}4b\sqrt{\frac{2b}{\pi}}\,2\int_0^{\infty}\left(-6bx^2 + 4b^2x^4\right)e^{-2bx^2}dx = -\frac{2\hbar^2 b}{m}\sqrt{\frac{2b}{\pi}}\,2\left\{-6b\frac{1}{8b}\sqrt{\frac{\pi}{2b}} + 4b^2\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}}\right\}$$

$$= -\frac{4\hbar^2 b}{m}\left(-\frac{3}{4} + \frac{3}{8}\right) = \frac{3\hbar^2 b}{2m} .$$

$$\langle V\rangle = \frac{1}{2}m\omega^2|A|^2\int_{-\infty}^{\infty} x^2e^{-2bx^2}x^2dx = \frac{1}{2}m\omega^2 4b\sqrt{\frac{2b}{\pi}}\,2\cdot\frac{3}{32b^2}\sqrt{\frac{\pi}{2b}} = \frac{3m\omega^2}{8b} .$$

$$\langle H\rangle = \frac{3\hbar^2 b}{2m} + \frac{3m\omega^2}{8b}\ ;\quad \frac{\partial\langle H\rangle}{\partial b} = \frac{3\hbar^2}{2m} - \frac{3m\omega^2}{8b^2} = 0 \Rightarrow b^2 = \frac{m^2\omega^2}{4\hbar^2} \Rightarrow b = \frac{m\omega}{2\hbar} .$$

$\therefore \langle H\rangle_{min} = \frac{3\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{3m\omega^2}{8}\frac{2\hbar}{m\omega} = \hbar\omega\left(\frac{3}{4}+\frac{3}{4}\right) = \boxed{\frac{3}{2}\hbar\omega}$. (Which is exact, since the trial wave function is in the form of the true first excited state.)

PROBLEM 7.5 (a) Use the unperturbed ground state (ψ_g^0) as the trial wave function. The variational principle says $\langle\psi_g^0|H|\psi_g^0\rangle \geq E_g$. But $H = H^0 + H'$, so $\langle\psi_g^0|H|\psi_g^0\rangle = \langle\psi_g^0|H^0|\psi_g^0\rangle + \langle\psi_g^0|H'|\psi_g^0\rangle$.
But $\langle\psi_g^0|H^0|\psi_g^0\rangle = E_g^0$ (the unperturbed ground state energy), and $\langle\psi_g^0|H'|\psi_g^0\rangle$ is precisely the first order correction to the ground state energy [6.9], so

$$E_g^0 + E_g^1 \geq E_g .\quad \text{QED.}$$

(b) The second-order correction (E_g^2) is $E_g^2 = \sum_{m\neq g}\frac{|\langle\psi_m^0|H'|\psi_g^0\rangle|^2}{E_g^0 - E_m^0}$. But the numerator is clearly positive, and the denominator is always negative (since $E_g^0 < E_m^0$ for all m), so E_g^2 is negative.

PROBLEM 10.10 (a) Check the answer given: $x_c = \omega \int_0^t f(t') \sin[\omega(t-t')]\,dt' \Rightarrow x_c(0)=0$ ✓

$$\dot{x}_c = \omega f(t) \sin[\omega(t-t)] + \omega^2 \int_0^t f(t') \cos[\omega(t-t')]dt' = \omega^2 \int_0^t f(t') \cos[\omega(t-t')]dt' \Rightarrow \dot{x}_c(0)=0 \checkmark$$

$$\ddot{x}_c = \omega^2 f(t)\cos[\omega(t-t)] - \omega^3\int_0^t f(t')\sin[\omega(t-t')]\,dt' = \omega^2 f(t) - \omega^2 x_c .$$

Now, the classical equation of motion is: $m\frac{d^2x}{dt^2} = -m\omega^2 x + m\omega^2 f$. For the proposed solution $m\frac{d^2x_c}{dt^2} = m\omega^2 f - m\omega^2 x_c$, so it does satisfy the equation of motion, with appropriate boundary conditions.

(b) Let $z \equiv x - x_c$ (so $\psi_n(x-x_c) = \psi_n(z)$, and z depends on t as well as x).

$$\frac{\partial\Psi}{\partial t} = \frac{d\psi_n}{dz}(-\dot{x}_c)e^{i\{\}} + \psi_n e^{i\{\}}\frac{i}{\hbar}\Big[-(n+\tfrac12)\hbar\omega + m\underset{\substack{\downarrow \\ \omega^2 f - \omega^2 x_c}}{\ddot{x}_c}\big(x-\tfrac{x_c}{2}\big) - \frac{m}{2}\dot{x}_c^2 + \frac{m\omega^2}{2}f x_c\Big]$$

$$[\;] = -(n+\tfrac12)\hbar\omega + \frac{m\omega^2}{2}\left(2x(f-x_c) + x_c^2 - \dot{x}_c^2/\omega^2\right).$$

$$\therefore \frac{\partial\Psi}{\partial t} = -\dot{x}_c\frac{d\psi_n}{dz}e^{i\{\}} + i\Psi\Big[-(n+\tfrac12)\omega + \frac{m\omega^2}{2\hbar}\Big(2x(f-x_c) + x_c^2 - \frac{1}{\omega^2}\dot{x}_c^2\Big)\Big].$$

$$\frac{\partial\Psi}{\partial x} = \frac{d\psi_n}{dz}e^{i\{\}} + \psi_n e^{i\{\}}\frac{i}{\hbar}[m\dot{x}_c]; \quad \frac{\partial^2\Psi}{\partial x^2} = \frac{d^2\psi_n}{dz^2}e^{i\{\}} + 2\frac{d\psi_n}{dz}e^{i\{\}}\frac{i}{\hbar}(m\dot{x}_c) - \Big(\frac{m\dot{x}_c}{\hbar}\Big)^2\psi_n e^{i\{\}}$$

$$\therefore H\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \tfrac12 m\omega^2x^2\Psi - m\omega^2 f x\Psi = -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dz^2}e^{i\{\}} - \frac{\hbar^2}{2m}2\frac{d\psi_n}{dz}e^{i\{\}}\frac{im\dot{x}_c}{\hbar} + \frac{\hbar^2}{2m}\Big(\frac{m\dot{x}_c}{\hbar}\Big)^2\Psi + \tfrac12 m\omega^2x^2\Psi$$

$-m\omega^2 f x\Psi$. But $-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dz^2} + \frac12 m\omega^2 z^2\psi_n = (n+\frac12)\hbar\omega\psi_n$, so

$$H\Psi = \cancel{(n+\tfrac12)\hbar\omega\Psi} - \tfrac12 m\omega^2 z^2\Psi - \cancel{i\hbar\dot{x}_c\frac{d\psi_n}{dz}e^{i\{\}}} + \frac{m}{2}\dot{x}_c^2\Psi + \tfrac12 m\omega^2x^2\Psi - m\omega^2 f x\Psi$$

$$\stackrel{?}{=} i\hbar\frac{\partial\Psi}{\partial t} = -\cancel{i\hbar\dot{x}_c\frac{d\psi_n}{dz}e^{i\{\}}} - \hbar\Psi\Big[-\cancel{(n+\tfrac12)}\omega + \frac{m\omega^2}{2\hbar}\Big(2xf - 2xx_c + x_c^2 - \frac{1}{\omega^2}\dot{x}_c^2\Big)\Big]$$

$$-\tfrac12 m\omega^2 z^2 + \cancel{\frac{m}{2}\dot{x}_c^2} + \tfrac12 m\omega^2 x^2 - \cancel{m\omega^2 f x} \stackrel{?}{=} -\frac{m\omega^2}{2}\Big(\cancel{2xf} - 2xx_c + x_c^2 - \cancel{\frac{1}{\omega^2}\dot{x}_c^2}\Big)$$

$$z^2 - x^2 \stackrel{?}{=} -2xx_c + x_c^2 \quad ; \quad z^2 \stackrel{?}{=} (x^2 - 2xx_c + x_c^2) = (x-x_c)^2 \;\checkmark$$

(c) [10.99] $\Rightarrow$ $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac12 m\omega^2(x^2 - 2xf + f^2) - \frac12 m\omega^2 f^2$. Shift origin: $u \equiv x - f$.

$$H = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial u^2} + \tfrac12 m\omega^2 u^2}_{\text{simple harmonic oscillator in variable } u} \underbrace{-\tfrac12 m\omega^2 f^2}_{\text{constant (with respect to position)}}.$$

So eigenfunctions are $\psi_n(u) = \psi_n(x-f)$, and eigenvalues are harmonic oscillator ones $(n+\frac12)\hbar\omega$, less the added constant: $E_n = (n+\frac12)\hbar\omega - \frac12 m\omega^2 f^2$.

(d) Note that $\sin[\omega(t-t')] = \frac{1}{\omega}\frac{d}{dt'}\cos[\omega(t-t')]$, so $x_c(t) = \int_0^t f(t')\frac{d}{dt'}\cos[\omega(t-t')]\,dt'$, or

$$x_c(t) = f(t')\cos[\omega(t-t')]\Big|_0^t - \int_0^t\Big(\frac{df}{dt'}\Big)\cos[\omega(t-t')]\,dt' = f(t) - \int_0^t\Big(\frac{df}{dt'}\Big)\cos[\omega(t-t')]\,dt' \quad (\text{since } f(0)=0).$$

Now, for <u>adiabatic</u> process we want df/dt very small – specifically, $\boxed{\frac{df}{dt'} \ll \omega f(t)}$ $(0 < t' \leq t)$.

Then the integral is negligible compared to $f(t)$, and we have $\boxed{x_c(t) \cong f(t)}$. (Physically, this says that if you pull on the spring very gently, no fancy oscillations will occur – the mass just moves along as though attached to a <u>string</u> of fixed length.)

(e) Put $x_c \cong f$ into [10.101], using [10.102]:

$$\Psi(x,t) = \psi_n(x,t)\, e^{\frac{i}{\hbar}\left[-(n+\frac{1}{2})\hbar\omega t + m\dot{f}(x - f/2) + \frac{m\omega^2}{2}\int_0^t f^2(t')dt'\right]}$$

The dynamic phase [10.41] is $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt' = -(n+\frac{1}{2})\hbar\omega t + \frac{m\omega^2}{2\hbar}\int_0^t f^2(t')dt'$, so

$$\Psi(x,t) = \psi_n(x,t)\, e^{i\theta_n(t)}\, e^{i\gamma_n(t)},$$ confirming [10.103], with the geometric phase given (ostensibly) by

$$\gamma_n(t) = \frac{m}{\hbar}\dot{f}(x - f/2).$$

But the eigen-functions here are <u>real</u>, and hence (see p. 338) the geometric phase should be <u>zero</u>.

The point is that (in the adiabatic approximation) $\dot{f}$ is extremely small (see above), and hence in this limit $\frac{m}{\hbar}\dot{f}(x - f/2) \cong 0$ (at least, in the only region of x where $\psi_n(x,t)$ is nonzero).