PROBLEM 6.4 (a) $\langle\psi_m^0|H'|\psi_n^0\rangle = \frac{2}{a}\alpha\int_0^a \sin\left(\frac{m\pi}{a}x\right)\delta\left(x-\frac{a}{2}\right)\sin\left(\frac{n\pi}{a}x\right)dx = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right)$,

which is zero unless both m and n are odd — in which case it is $\pm 2\alpha/a$. So [6.14] says

$$E_n^2 = \sum_{\substack{m\neq n\\(\text{odd})}}\left(\frac{2\alpha}{a}\right)^2\frac{1}{(E_n^0-E_m^0)}.\qquad \text{But [2.23] } E_n^0=\frac{\pi^2\hbar^2}{2ma^2}n^2, \text{ so}$$

$$\boxed{E_n^2=\begin{cases}0, & \text{if } n \text{ is even;}\\ 2m\left(\frac{2\alpha}{\pi\hbar}\right)^2\sum\limits_{\substack{m\neq n\\ \text{odd}}}\frac{1}{(n^2-m^2)}, & \text{if } n \text{ is odd.}\end{cases}}$$

To sum the series, note that $\frac{1}{(n^2-m^2)}=\frac{1}{2n}\left(\frac{1}{(m+n)}-\frac{1}{(m-n)}\right)$. Thus,

for n=1: $\sum = \frac{1}{2}\sum\limits_{3,5,7,\dots}\left(\frac{1}{m+1}-\frac{1}{m-1}\right)=\frac{1}{2}\left(\frac{1}{4}+\frac{1}{6}+\frac{1}{8}+\cdots-\frac{1}{2}-\frac{1}{4}-\frac{1}{6}-\frac{1}{8}\cdots\right)=\frac{1}{2}\left(-\frac{1}{2}\right)=-\frac{1}{4}$;

for n=3: $\sum = \frac{1}{6}\sum\limits_{1,5,7,\dots}\left(\frac{1}{m+3}-\frac{1}{m-3}\right)=\frac{1}{6}\left(\frac{1}{4}+\frac{1}{8}+\frac{1}{10}+\cdots+\frac{1}{2}-\frac{1}{2}-\frac{1}{4}-\frac{1}{6}-\frac{1}{8}-\frac{1}{10}\cdots\right)=\frac{1}{6}\left(-\frac{1}{6}\right)=\frac{-1}{36}$.

In general, there is perfect cancellation except for the "missing" term $\frac{1}{2n}$ in the first sum, so the total is $\frac{1}{2n}\left(-\frac{1}{2n}\right)=-\frac{1}{(2n)^2}$. Therefore:

$$\boxed{E_n^2=\begin{cases}0, & \text{if } n \text{ is even;}\\ -2m(\alpha/\pi\hbar n)^2, & \text{if } n \text{ is odd.}\end{cases}}$$

(b) $H'=\frac{1}{2}\epsilon kx^2$; $\langle\psi_m^0|H'|\psi_n^0\rangle=\frac{1}{2}k\epsilon\langle m|x^2|n\rangle$. Following Problem [2.37]:

$$\langle m|x^2|n\rangle = -\frac{1}{2m\omega^2}\langle m|(a_+^2-a_+a_--a_-a_++a_-^2)|n\rangle$$

$$=-\frac{1}{2m\omega^2}\left[\sqrt{(n+1)(n+2)}\,\hbar\omega\langle m|n+2\rangle-n\hbar\omega\langle m|n\rangle-(n+1)\hbar\omega\langle m|n\rangle+\sqrt{n(n-1)}\,\hbar\omega\langle m|n-2\rangle\right]$$

So, for $m\neq n$, $\langle\psi_m^0|H'|\psi_n^0\rangle=\left(\frac{1}{2}k\epsilon\right)\left(-\frac{\hbar}{2m\omega}\right)\left[\sqrt{(n+1)(n+2)}\,\delta_{m,n+2}+\sqrt{n(n-1)}\,\delta_{m,n-2}\right]$.

$$\therefore\ E_n^2=\left(\frac{\epsilon\hbar\omega}{4}\right)^2\sum_{m\neq n}\frac{\left[\sqrt{(n+1)(n+2)}\,\delta_{m,n+2}+\sqrt{n(n-1)}\,\delta_{m,n-2}\right]^2}{(n+\frac{1}{2})\hbar\omega-(m+\frac{1}{2})\hbar\omega}=\frac{\epsilon^2\hbar\omega}{16}\sum_{m\neq n}\frac{[(n+1)(n+2)\delta_{m,n+2}+n(n-1)\delta_{m,n-2}]}{(n-m)}$$

$$=\frac{\epsilon^2\hbar\omega}{16}\left[\frac{(n+1)(n+2)}{n-(n+2)}+\frac{n(n-1)}{n-(n-2)}\right]=\frac{\epsilon^2\hbar\omega}{16}\left[-\frac{1}{2}(n+1)(n+2)+\frac{1}{2}n(n-1)\right]$$

$$=\frac{\epsilon^2\hbar\omega}{32}(-n^2-3n-2+n^2-n)=\frac{\epsilon^2\hbar\omega}{32}(-4n-2)=\boxed{-\epsilon^2\frac{1}{8}\hbar\omega\left(n+\frac{1}{2}\right)}$$

(which agrees with the ϵ^2 term in the exact solution — Problem 15(a)).

PROBLEM 6.5 (a) $E_n^1=\langle\psi_n^0|H'|\psi_n^0\rangle=-qE\langle n|x|n\rangle=\boxed{0}$. (Problem 2.37.)

From [6.14] and Problem 3.50:

$$E_n^2=(qE)^2\sum_{m\neq n}\frac{|\langle m|x|n\rangle|^2}{(n-m)\hbar\omega}=\frac{(qE)^2}{\hbar\omega}\frac{\hbar}{2m\omega}\sum_{m\neq n}\frac{\left[\sqrt{n+1}\,\delta_{m,n+1}-\sqrt{n}\,\delta_{m,n-1}\right]^2}{(n-m)}$$

$$E_n^2 = \frac{(qE)^2}{2m\omega^2}\sum_{m\neq n}\frac{[(n+1)\delta_{m,n+1}+n\,\delta_{m,n-1}]}{(n-m)} = \frac{(qE)^2}{2m\omega^2}\left[\frac{(n+1)}{n-(n+1)}+\frac{n}{n-(n-1)}\right] = \frac{(qE)^2}{2m\omega^2}\left[-(n+1)+n\right]$$

$$= \boxed{\frac{-(qE)^2}{2m\omega^2}}.$$

(b) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \left(\frac{1}{2}m\omega^2x^2 - qEx\right)\psi = E\psi$. With the suggested change of variables,

$$\left(\tfrac{1}{2}m\omega^2x^2 - qEx\right) = \tfrac{1}{2}m\omega^2\left(x' + \left(\frac{qE}{m\omega^2}\right)\right)^2 - qE\left(x' + \left(\frac{qE}{m\omega^2}\right)\right) = \tfrac{1}{2}m\omega^2x'^2 + m\omega^2x'\frac{qE}{m\omega^2} + \tfrac{1}{2}m\omega^2\frac{(qE)^2}{m^2\omega^4}$$

$$-qEx' - (qE)^2/m\omega^2 = \tfrac{1}{2}m\omega^2x'^2 - \tfrac{1}{2}(qE)^2/m\omega^2.$$ So the Schrodinger equation says

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx'^2} + \tfrac{1}{2}m\omega^2x'^2\psi = \left(E + \tfrac{1}{2}(qE)^2/m\omega^2\right)\psi$$ — which is the Schrodinger equation for a simple harmonic oscillator, in the variable x'. The constant on the right must therefore be $(n+\frac{1}{2})\hbar\omega$, and we conclude that

$$\boxed{E_n = (n+\tfrac{1}{2})\hbar\omega - \tfrac{1}{2}(qE)^2/m\omega^2}.$$ The subtracted term is exactly what we got in part (a) using perturbation theory. Evidently all the higher corrections (like the first-order correction) are zero, in this case.

Problem 6.6 (a) $\langle\psi_+^0|\psi_-^0\rangle = \langle(\alpha_+\psi_a^0+\beta_+\psi_b^0)|(\alpha_-\psi_a^0+\beta_-\psi_b^0)\rangle$

$$= \alpha_+^*\alpha_-\langle\psi_a^0|\psi_a^0\rangle + \alpha_+^*\beta_-\langle\psi_a^0|\psi_b^0\rangle + \beta_+^*\alpha_-\langle\psi_b^0|\psi_a^0\rangle + \beta_+^*\beta_-\langle\psi_b^0|\psi_b^0\rangle$$

$$= \alpha_+^*\alpha_- + \beta_+^*\beta_-.$$ But $[6.21] \Rightarrow \beta_\pm = \alpha_\pm(E_\pm^1 - W_{aa})/W_{ab}$.

So $$\langle\psi_+^0|\psi_-^0\rangle = \alpha_+^*\alpha_-\left\{1 + \frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{W_{ab}^*W_{ab}}\right\} = \frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[|W_{ab}|^2 + (E_+^1-W_{aa})(E_-^1-W_{aa})\right].$$

The term in square brackets is:

$[\,] = E_+^1E_-^1 - W_{aa}(E_+^1+E_-^1) + |W_{ab}|^2 + W_{aa}^2$. But [6.26]: $E_\pm^1 = \frac{1}{2}\left[(W_{aa}+W_{bb}) \pm \sqrt{\;}\right]$, where $\sqrt{\;}$ is shorthand for the square root term. $E_+^1 + E_-^1 = W_{aa} + W_{bb}$, and

$$E_+^1E_-^1 = \frac{1}{4}\left[(W_{aa}+W_{bb})^2 - (\sqrt{\;})^2\right] = \frac{1}{4}\left[(W_{aa}+W_{bb})^2 - (W_{aa}-W_{bb})^2 - 4|W_{ab}|^2\right] = W_{aa}W_{bb} - |W_{ab}|^2.$$

So $[\,] = W_{aa}W_{bb} - |W_{ab}|^2 - W_{aa}(W_{aa}+W_{bb}) + |W_{ab}|^2 + W_{aa}^2 = 0$. $\therefore \langle\psi_+^0|\psi_-^0\rangle = 0$. QED.

(b) $$\langle\psi_+^0|H'|\psi_-^0\rangle = \alpha_+^*\alpha_-\langle\psi_a^0|H'|\psi_a^0\rangle + \alpha_+^*\beta_-\langle\psi_a^0|H'|\psi_b^0\rangle + \beta_+^*\alpha_-\langle\psi_b^0|H'|\psi_a^0\rangle + \beta_+^*\beta_-\langle\psi_b^0|H'|\psi_b^0\rangle$$

$$= \alpha_+^*\alpha_-W_{aa} + \alpha_+^*\beta_-W_{ab} + \beta_+^*\alpha_-W_{ba} + \beta_+^*\beta_-W_{bb} = \alpha_+^*\alpha_-\left\{W_{aa} + W_{ab}\frac{(E_-^1-W_{aa})}{W_{ab}} + W_{ba}\frac{(E_+^1-W_{aa})}{W_{ab}^*}\right.$$

$$+W_{bb}\frac{(E_+^1-W_{aa})}{W_{ab}^*}\frac{(E_-^1-W_{aa})}{W_{ab}}\Big\} = \alpha_+^*\alpha_-\Big\{W_{aa}+E_-^1-W_{aa}+E_+^1-W_{aa}+W_{bb}\frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{|W_{ab}|^2}\Big\}.$$

But we know from (a) that $\frac{(E_+^1-W_{aa})(E_-^1-W_{aa})}{|W_{ab}|^2}=-1$, so

$$\langle\psi_+^0|H'|\psi_-^0\rangle = \alpha_+^*\alpha_-\left[E_-^1+E_+^1-W_{aa}-W_{bb}\right]=0.\quad \text{QED}.$$

(c) $\langle\psi_\pm^0|H'|\psi_\pm^0\rangle = \alpha_\pm^*\alpha_\pm\langle\psi_a^0|H'|\psi_a^0\rangle+\alpha_\pm^*\beta_\pm\langle\psi_a^0|H'|\psi_b^0\rangle+\beta_\pm^*\alpha_\pm\langle\psi_b^0|H'|\psi_a^0\rangle+\beta_\pm^*\beta_\pm\langle\psi_b^0|H'|\psi_b^0\rangle$

$$=|\alpha_\pm|^2\left\{W_{aa}+W_{ab}\frac{(E_\pm^1-W_{aa})}{W_{ab}}\right\}+|\beta_\pm|^2\left\{W_{ba}\frac{(E_\pm^1-W_{bb})}{W_{ba}}+W_{bb}\right\}$$ (this time I used [6.23] to express α in terms of β, in the third term).

$$\therefore\ \langle\psi_\pm^0|H'|\psi_\pm^0\rangle = |\alpha_\pm|^2(E_\pm^1)+|\beta_\pm|^2(E_\pm^1)=\left(|\alpha_\pm|^2+|\beta_\pm|^2\right)E_\pm^1=E_\pm^1\ .\ \text{QED}$$

PROBLEM 6.7 (a) (With slight change in notation this is precisely the solution obtained in Problem 2.43.)

(b) With $a\to n$, $b\to -n$, we have:

$$W_{aa}=W_{bb}=-\frac{V_0}{L}\int_{-L/2}^{L/2}e^{-x^2/a^2}dx\cong-\frac{V_0}{L}\int_{-\infty}^{\infty}e^{-x^2/a^2}dx=-\frac{V_0}{L}a\sqrt{\pi}.$$

$$W_{ab}=-\frac{V_0}{L}\int_{-L/2}^{L/2}e^{-x^2/a^2}e^{-4\pi nix/L}dx\cong-\frac{V_0}{L}\int_{-\infty}^{\infty}e^{-(x^2/a^2+4\pi nix/L)}dx$$

$$=-\frac{V_0}{L}a\sqrt{\pi}\,e^{-(2\pi n/L)^2a}.$$ (We did this integral in Problem 2.22.)

In this case $W_{aa}=W_{bb}$, and W_{ab} is real, so [6.26] $\Rightarrow$ $E_\pm^1=W_{aa}\pm|W_{ab}|$, or

$$E_\pm^1=\boxed{-\sqrt{\pi}\,\frac{V_0 a}{L}\left(1\mp e^{-(2\pi n/L)^2a}\right)}.$$

(c) [6.21] $\Rightarrow$ $\beta=\alpha\frac{(E^1-W_{aa})}{W_{ab}}=\alpha\left\{\frac{\pm\sqrt{\pi}\frac{V_0a}{L}e^{-(2\pi n/L)^2a}}{-\sqrt{\pi}\frac{V_0a}{L}e^{-(2\pi n/L)^2a}}\right\}=\mp\alpha$. Evidently the "good" linear combinations are: $\psi_+=\alpha\psi_n-\alpha\psi_{-n}=\frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}\left[e^{i2\pi nx/L}-e^{-i2\pi nx/L}\right]=\boxed{\sqrt{\frac{2}{L}}\,i\sin\left(\frac{2\pi nx}{L}\right)}$

and $\psi_-=\alpha\psi_n+\alpha\psi_{-n}=\boxed{\sqrt{\frac{2}{L}}\cos\left(\frac{2\pi nx}{L}\right)}$. Using [6.9], we have:

$$\left.\begin{aligned}E_+^1&=\langle\psi_+|H'|\psi_+\rangle=\frac{2}{L}(-V_0)\int_{-L/2}^{L/2}e^{-x^2/a^2}\sin^2\left(\frac{2\pi nx}{L}\right)dx\\ E_-^1&=\langle\psi_-|H'|\psi_-\rangle=\frac{2}{L}(-V_0)\int_{-L/2}^{L/2}e^{-x^2/a^2}\cos^2\left(\frac{2\pi nx}{L}\right)dx\end{aligned}\right\}\ \text{Use}\ \left\{\begin{aligned}\sin^2\theta&=\tfrac12(1-\cos2\theta)\\ \cos^2\theta&=\tfrac12(1+\cos2\theta)\end{aligned}\right\}\ \text{to obtain:}$$

$$E_\pm^1\cong-\frac{V_0}{L}\int_{-\infty}^{\infty}e^{-x^2/a^2}\left(1\mp\cos\left(\frac{4\pi nx}{L}\right)\right)dx.$$

$$E_{\pm}^{1} = -\frac{V_0}{L}\left\{\int_{-\infty}^{\infty} e^{-x^2/a^2}dx \mp \int_{-\infty}^{\infty} e^{-x^2/a^2}\cos\left(\frac{4\pi n x}{L}\right)dx\right\}$$

$$= -\frac{V_0}{L}\left\{\sqrt{\pi}\,a \mp a\sqrt{\pi}\,e^{-(2\pi n/L)^2 a}\right\} = -\sqrt{\pi}\,\frac{V_0 a}{L}\left(1 \mp e^{-(2\pi n/L)^2 a}\right) \text{— same as (b).}$$

(d) $A f(x) = f(-x)$ (The parity operator). The eigenstates are <u>even</u> functions (with eigenvalue +1) and <u>odd</u> functions (with eigenvalue −1). The linear combinations we found in (c) are precisely the odd and even linear combinations of ψ_n and ψ_{-n}.

$$E^1_\pm = -\frac{V_0}{L}\left\{\int_{-\infty}^{\infty} e^{-x^2/a^2}dx \mp \int_{-\infty}^{\infty} e^{-x^2/a^2}\cos\left(\frac{4\pi n x}{L}\right)dx\right\}$$

$$= -\frac{V_0}{L}\left\{\sqrt{\pi}\,a \mp a\sqrt{\pi}\, e^{-(2\pi n/L)^2 a}\right\} = -\sqrt{\pi}\,\frac{V_0 a}{L}\left(1 \mp e^{-(2\pi n/L)^2 a}\right) \text{ — same as (b).}$$

(d) $\hat{A}f(x) = f(-x)$ (the parity operator). The eigenstates are <u>even</u> functions (with eigenvalue +1) and <u>odd</u> functions (with eigenvalue −1). The linear combinations we found in (c) are precisely the odd and even linear combinations of ψ_n and ψ_{-n}.

PROBLEM 6.27 (a) Let the unperturbed Hamiltonian be $H(\lambda_0)$, for some fixed value λ_0. Now tweak λ to $\lambda_0 + d\lambda$. The perturbing Hamiltonian is

$$H' = H(\lambda_0 + d\lambda) - H(\lambda_0) = \frac{\partial H}{\partial \lambda}\, d\lambda \quad \text{(derivative evaluated at } \lambda_0\text{)}.$$

The change in energy is given by [6.9]:

$$dE_n = E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle\, d\lambda \quad \text{(all evaluated at } \lambda_0\text{)}.$$

$$\therefore \quad \frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial H}{\partial \lambda} | \psi_n \rangle.$$ [Note: even though we used perturbation theory, the result is exact, since all we needed is the infinitesimal change in E_n.]

(b) $E_n = (n+\frac{1}{2})\hbar\omega$; $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$.

(i) $\frac{\partial E_n}{\partial \omega} = (n+\frac{1}{2})\hbar$; $\frac{\partial H}{\partial \omega} = m\omega x^2$; so theorem $\Rightarrow (n+\frac{1}{2})\hbar = \langle n | m\omega x^2 | n \rangle$. $V = \frac{1}{2}m\omega^2 x^2$,

So $\langle V \rangle = \langle n | \frac{1}{2}m\omega^2 x^2 | n \rangle = \frac{1}{2}\omega(n+\frac{1}{2})\hbar = \boxed{\frac{1}{2}(n+\frac{1}{2})\hbar\omega = \langle V \rangle}$.

(ii) $\frac{\partial E_n}{\partial \hbar} = (n+\frac{1}{2})\omega$; $\frac{\partial H}{\partial \hbar} = -\frac{\hbar}{m}\frac{d^2}{dx^2} = \frac{2}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) = \frac{2}{\hbar}T$; so theorem $\Rightarrow (n+\frac{1}{2})\omega = \frac{2}{\hbar}\langle n | T | n \rangle$,

or $\boxed{\langle T \rangle = \frac{1}{2}(n+\frac{1}{2})\hbar\omega}$.

(iii) $\frac{\partial E_n}{\partial m} = 0$; $\frac{\partial H}{\partial m} = \frac{\hbar^2}{2m^2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2 = -\frac{1}{m}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) + \frac{1}{m}\left(\frac{1}{2}m\omega^2 x^2\right) = -\frac{1}{m}T + \frac{1}{m}V$.

So theorem $\Rightarrow 0 = -\frac{1}{m}\langle T \rangle + \frac{1}{m}\langle V \rangle$, or $\boxed{\langle T \rangle = \langle V \rangle}$.

These results are consistent with what we found in Problems 2.37 and 3.53.

PROBLEM 6.28 (a) $\frac{\partial E_n}{\partial e} = \frac{-4me^3}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^2} = \frac{4}{e}E_n$; $\frac{\partial H}{\partial e} = -\frac{2e}{4\pi\epsilon_0}\frac{1}{r}$.

So the theorem says: $\frac{4}{e}E_n = -\frac{e}{2\pi\epsilon_0}\langle \frac{1}{r} \rangle$, or $\langle \frac{1}{r} \rangle = -\frac{8\pi\epsilon_0}{e^2}E_n = -\frac{8\pi\epsilon_0 E_1}{e^2 n^2}$

$\therefore \langle \frac{1}{r} \rangle = -\frac{8\pi\epsilon_0}{e^2}\left[-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{e^2 m}{4\pi\epsilon_0\hbar^2}\frac{1}{n^2}$. But $\frac{4\pi\epsilon_0\hbar^2}{me^2} = a$ [4.72], so $\boxed{\langle \frac{1}{r} \rangle = \frac{1}{n^2 a}}$

(Agrees with [6.54].)

(b) $\frac{\partial E_n}{\partial l} = \frac{2me^4}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^3} = -\frac{2E_n}{n}$; $\frac{\partial H}{\partial l} = \frac{\hbar^2}{2mr^2}(2l+1)$; theorem says

$-\frac{2E_n}{n} = \frac{\hbar^2(2l+1)}{2m}\langle \frac{1}{r^2} \rangle$, or $\langle \frac{1}{r^2} \rangle = -\frac{4mE_n}{n(2l+1)\hbar^2} = -\frac{4mE_1}{n^3(2l+1)\hbar^2}$. But $-\frac{4mE_1}{\hbar^2} = \frac{2}{a^2}$, so

$\boxed{\langle \frac{1}{r^2} \rangle = \frac{1}{n^3(l+\frac{1}{2})a^2}}$. (Agrees with [6.55].)
