PROBLEM SET 10 SOLUTIONS

Question 1:

a) For a Hamiltonian with matrix representation

$$E_0 \begin{pmatrix} 3 & 4 & 5 \\ 4 & 7 & 1 \\ 5 & 1 & 6 \end{pmatrix}$$

in some basis $|1\rangle, |2\rangle, |3\rangle$, we have by definition that the expectation value of H for the basis states gives

$$\langle 1|H|1\rangle = H_{11} = 3E_0$$
$$\langle 2|H|2\rangle = H_{22} = 7E_0$$
$$\langle 3|H|3\rangle = H_{33} = 6E_0$$

The lowest of these is $3E_0$, so this gives the best upper bound on the ground state energy.

EXTRA QUESTION: the true ground state energy is equal to the lowest eigenvalue of the matrix. So we are guaranteed that the lowest eigenvalue is less than or equal to the smallest diagonal element. By the same argument, this must be true for any Hermitian matrix.

b) In this case, we have from the class notes that

$$\psi(x) = \frac{A}{x^2+b^2} \text{ is normalized with } A=\sqrt{\frac{2b^3}{\pi}}$$

Also from the notes,

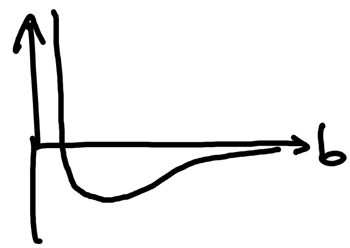
$$\langle\psi|\frac{p^2}{2m}|\psi\rangle = \frac{\hbar^2}{4b^2m}$$

Finally, $\langle\psi|V(x)|\psi\rangle = -\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 \cdot C\,\delta(x)$

$$= -C\,|\psi(0)|^2$$

$$= -C\cdot\frac{A^2}{b^4} = -C\cdot\frac{2}{\pi b}$$

So $\langle\psi|H|\psi\rangle = \frac{\hbar^2}{4b^2m} - \frac{2C}{\pi b}$



This has a minimum when

$$0 = \frac{d}{db}\left(\frac{\hbar^2}{4b^2m} - \frac{2C}{\pi b}\right) = -\frac{\hbar^2}{2b^3m} + \frac{2C}{\pi b^2} \Rightarrow b = \frac{\hbar^2\pi}{4Cm}$$

Plugging in to $\langle H\rangle(b)$, we get

$$E_{min} = \frac{4C^2m}{\hbar^2\pi^2} - \frac{8C^2m}{\hbar^2\pi^2} = -4\cdot\frac{C^2m}{\hbar^2\pi^2}$$

2 a) We have a Hamiltonian

$$H = \frac{p^2}{2m} + \alpha |x|^3$$

The ground state energy should be some function of the parameters m, α, and $\hbar$. To determine the possibilities, note that the dimensions of these are:

$$m \sim \text{Mass} \sim M$$

$$\alpha \sim \frac{\text{Energy}}{\text{Length}^3} \sim \frac{M}{L \cdot T^2}$$

$$\hbar \sim \text{Angular Momentum} \sim \frac{ML^2}{T}$$

The final answer should have dimensions of energy,

$$E_0 \sim \frac{ML^2}{T^2}$$

Thus, if $E_0 \sim m^{n_1} \alpha^{n_2} \hbar^{n_3}$ we must have:

mass units: $n_1 + n_2 + n_3 = 1$

length units: $-n_2 + 2n_3 = 2$

time units: $-2n_2 - n_3 = -2$

$$\Rightarrow \quad n_1 = -\frac{3}{5}, \quad n_2 = \frac{2}{5}, \quad n_3 = \frac{6}{5}$$

So $E_0 = c \cdot \left(\frac{\alpha^2 \hbar^6}{m^3}\right)^{\frac{1}{5}}$ for some number c.

b) The variational method says that the ground state energy is less than $\langle \psi | H | \psi \rangle$ for any choice of $|\psi\rangle$. Setting $\alpha = \hbar = m = 1$ by a choice of units, this means:

$$c \leq \int_{-\infty}^{\infty} dx\, \psi^*(x) \left(-\frac{1}{2} \psi''(x) + |x|^3 \psi(x) \right)$$

or (integrating by parts)

$$c \leq \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2} |\partial_x \psi|^2 + |x|^3 |\psi|^2 \right\}$$

for any function with $\int_{-\infty}^{\infty} dx \, |\psi(x)|^2 = 1$.

For example, we can try $\psi(x) = A e^{-ax^2/2}$. Normalizing,

$$\int_{-\infty}^{\infty} dx \, |\psi(x)|^2 = 1 \Rightarrow A = \left(\frac{a}{\pi}\right)^{1/4}$$

Then $c \leq \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2} (\psi'(x))^2 + |x|^3 |\psi(x)|^2 \right\}$

$$= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2} a^2 x^2 e^{-ax^2} + |x|^3 e^{-ax^2} \right\}$$

$$= \frac{a}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dy \, y^2 e^{-y^2} + \frac{1}{\sqrt{\pi} a^{3/2}} \int_{-\infty}^{\infty} dy \, |y|^3 e^{-y^2}$$

$$= \frac{a}{4} + \frac{1}{\sqrt{\pi} a^{3/2}}$$

Minimizing over a, we find a minimum where

$$\frac{1}{4} - \frac{3}{2} \cdot \frac{1}{\sqrt{\pi} a^{5/2}} = 0 \Rightarrow a = \left(\frac{6}{\sqrt{\pi}}\right)^{2/5}$$

This gives $c \leq \frac{5}{12} \cdot \left(\frac{36}{\pi}\right)^{1/5} \approx 0.67861$

We can do better by including more parameters. For example, with $\psi(x) = e^{-ax^2}(1 + bx^2)$, we get a bound of $c \leq 0.67492$

The exact answer is

$$E_0 \approx \left(\frac{\alpha^2 \hbar^6}{m^3}\right)^{1/5} \cdot 0.6748941\ldots$$

3 For $H = H_0 + H'(t)$, let the state be

$$|\psi(t)\rangle = \sum_n c_n(t)\, e^{-iE_n t/\hbar} |\psi_n\rangle$$

where $H_0|\psi_n\rangle = E_n|\psi_n\rangle$. The Schrödinger equation gives:

$$\boxed{i\hbar \frac{d}{dt}|\psi(t)\rangle = \left(H_0 + H'(t)\right)|\psi(t)\rangle}$$

$$\Rightarrow i\hbar \sum_n \left(\dot{c}_n(t)\, e^{-iE_n t/\hbar} - \frac{iE_n}{\hbar} c_n(t)\, e^{-iE_n t/\hbar}\right)|\psi_n\rangle$$

$$= \sum_n c_n(t)\, e^{-iE_n t/\hbar}\left(E_n + H'(t)\right)|\psi_n\rangle$$

$$\Rightarrow i\hbar \sum_n \dot{c}_n(t)\, e^{-iE_n t/\hbar}|\psi_n\rangle - \sum_n c_n(t)\, e^{-iE_n t/\hbar} H'(t)|\psi_n\rangle = 0$$

Taking the inner product with some state $|\psi_m\rangle$, we get:

$$i\hbar\, \dot{c}_m(t)\, e^{-iE_m t/\hbar} - \sum_n c_n(t)\, e^{-iE_n t/\hbar}\langle\psi_m|H'(t)|\psi_n\rangle = 0$$

$$\Rightarrow \boxed{\dot{c}_m(t) = -\frac{i}{\hbar}\sum_n e^{-i(E_n - E_m)t/\hbar} H'_{mn}(t)\, c_n(t)}$$

where $H'_{mn}(t) \equiv \langle\psi_m|H'(t)|\psi_n\rangle$

For $\frac{d}{dt}c(t) = f(t)c(t)$ we have:

$$\frac{1}{c(t)}\frac{d}{dt}c(t) = f(t)$$

$$\Rightarrow \frac{d}{dt}\ln(c(t)) = f(t)$$

$$\Rightarrow \boxed{c(t) = c(0)\, e^{\int_0^t f(t)\,dt}}$$

$$= c(0) + c(0)\int_0^t f(t)\,dt + \dots$$

$$= C(0) + C(0)\int_0 T(t)\,dt + \cdots$$

EXTRA:

1. For particles in a harmonic oscillator, the energy eigenstates are $|n\rangle$ with energies $\hbar\omega(n+\frac{1}{2})$.

With identical bosons, the state must be symmetric under interchange of the bosons. The states with lowest energy are:

$$|0\rangle\otimes|0\rangle \qquad \text{energy } \hbar\omega \quad - \text{ degeneracy } 1$$

$$\frac{1}{\sqrt{2}}\left(|0\rangle\otimes|1\rangle+|1\rangle\otimes|0\rangle\right) \qquad \text{energy } 2\hbar\omega \quad - \text{ degeneracy } 1$$

$$\left.\begin{array}{l}\frac{1}{\sqrt{2}}\left(|0\rangle\otimes|2\rangle+|2\rangle\otimes|0\rangle\right) \\ |1\rangle\otimes|1\rangle\end{array}\right\} \text{ energy } 3\hbar\omega \text{ - degeneracy } 2$$

With identical fermions, the state must be antisymmetric under interchange of the fermions. So the states with lowest energy are:

$$\frac{1}{\sqrt{2}}\left(|0\rangle\otimes|1\rangle-|1\rangle\otimes|0\rangle\right) \qquad \text{energy } 2\hbar\omega \quad \text{degeneracy } 1$$

$$\frac{1}{\sqrt{2}}\left(|0\rangle\otimes|2\rangle-|2\rangle\otimes|0\rangle\right) \qquad \text{energy } 3\hbar\omega \quad \text{degeneracy } 1$$

$$\left.\begin{array}{l}\frac{1}{\sqrt{2}}\left(|1\rangle\otimes|2\rangle-|2\rangle\otimes|1\rangle\right) \\ \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|3\rangle-|3\rangle\otimes|0\rangle\right)\end{array}\right\} \text{ degeneracy } 2 \quad \text{energy } 4\hbar\omega$$