Homework 10 Key

1. Find the ground state energy of the 1D harmonic oscillator using the variational method for each of the following test wavefunctions:

   (a) $\psi = e^{-ax^2}$

   Since it is not normalized, we need to use $\dfrac{\int \psi^* \hat{H} \psi d\tau}{\int \psi^* \psi d\tau} \geq E_1$

   Recall:

   $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$,

   $V = \frac{1}{2}kx^2,\ V = 2\pi^2\nu^2 m x^2$

   $\hat{H} = \hat{T} + \hat{V},\ \hat{T} = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2},\ \hat{V} = 2\pi^2\nu^2 m x^2$

$$\int \psi^* \hat{H} \psi d\tau = \int \psi^* \hat{T} \psi d\tau + \int \psi^* \hat{V} \psi d\tau$$
$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} e^{-ax^2}\frac{d^2 e^{-ax^2}}{dx^2}dx + 2\pi^2\nu^2 m \int_{-\infty}^{\infty} x^2 e^{-2ax^2}dx$$
$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} e^{-ax^2}\cdot(-2ae^{-ae^2} + 4a^2x^2e^{-ax^2})dx + 2\pi^2\nu^2 m \int_{-\infty}^{\infty} x^2 e^{-2ax^2}dx$$
$$= -\frac{2\hbar^2}{2m}\int_{0}^{\infty}(-ae^{-2ax^2} + 2a^2x^2e^{-2ax^2})dx + 4\pi^2\nu^2 m \int_{0}^{\infty} x^2 e^{-2ax^2}dx$$
$$= \frac{\hbar^2 a \pi^{\frac{1}{2}}}{m(2a)^{\frac{1}{2}}} - \frac{4a^2\hbar^2\pi^{\frac{1}{2}}}{4m(2a)^{\frac{3}{2}}} + \frac{4\pi^2\nu^2 m \pi^{\frac{1}{2}}}{4(2a)^{\frac{3}{2}}}$$
$$= \frac{\hbar^2 a^{\frac{1}{2}}\pi^{\frac{1}{2}}}{2^{\frac{1}{2}}m} - \frac{a^{\frac{1}{2}}\hbar^2\pi^{\frac{1}{2}}}{2^{\frac{3}{2}}m} + \frac{\pi^{\frac{5}{2}}\nu^2 m}{8^{\frac{1}{2}}a^{\frac{3}{2}}}$$
$$= \frac{\hbar^2 a^{\frac{1}{2}}\pi^{\frac{1}{2}}}{2^{\frac{3}{2}}m} + \frac{\pi^{\frac{5}{2}}\nu^2 m}{2^{\frac{3}{2}}a^{\frac{3}{2}}}$$

$$\int \psi^* \psi d\tau = \int_{-\infty}^{\infty} e^{-ax^2}dx = 2\int_{0}^{\infty} e^{-2ax^2} = \frac{\pi^{\frac{1}{2}}}{2^{\frac{1}{2}}a^{\frac{1}{2}}}$$

$$\frac{\int \psi^* \hat{H}\psi d\tau}{\int \psi^* \psi d\tau} = \frac{\hbar^2 a^{\frac{1}{2}}\pi^{\frac{1}{2}}}{2^{\frac{3}{2}}m} \cdot \frac{2^{\frac{1}{2}}a^{\frac{1}{2}}}{\pi^{\frac{1}{2}}} + \frac{\pi^{\frac{5}{2}}\nu^2 m}{2^{\frac{3}{2}}a^{\frac{3}{2}}} \cdot \frac{2^{\frac{1}{2}}a^{\frac{1}{2}}}{\pi^{\frac{1}{2}}}$$

$$\frac{\int \psi^* \hat{H}\psi d\tau}{\int \psi^* \psi d\tau} = \frac{a\hbar^2}{2m} + \frac{\pi^2\nu^2 m}{2a}$$

$$\frac{\hbar^2}{2m} - \frac{\pi^2\nu^2 m}{2a^2} = 0$$

$$a = \frac{m\pi\nu}{\hbar}$$

$$E = \hbar\pi\nu$$

(b) $\psi = \sin(\alpha x)$

$$\frac{\int \psi^* \hat{H}\psi d\tau}{\int \psi^* \psi d\tau} \geq E_1$$

$$\int \psi^* \hat{H}\psi d\tau = \int \psi^* \hat{T}\psi d\tau + \int \psi^* \hat{V}\psi d\tau$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \sin(\alpha x)\frac{d^2 \sin \alpha x}{dx^2}dx + 2\pi^2\nu^2 m \int_{-\infty}^{\infty} x^2 \sin \alpha x dx$$

$\psi = \sin \alpha x$ is an invalid wavefunction because it diverges from $-\infty$ to ∞, which are the bounds of the quantum harmonic oscillator.

2. Find the ground state energy of the 1D particle in a box using the variational method for each of the following test wavefunctions:

   (a) $\psi = e^{-ax^2}$

   Insolvable for the ground state energy of the 1d. Recall the bounds for particle in a box is between 0 to L. Because $e^{a(0)^2} = 1$. This wavefunction violates the boundary condition.

   (b) $\psi = x^a$

   Insolvable because it violates boundary conditions because it is not 0 at the bounds.

3. Given a Hamiltonian H with (non-degenerate) eigenvectors ψ_k and eigenvalues E_k: $E_0 < E_1 < ....$ Let $H' = H + K|\psi_0\rangle\langle\psi_0|$ be an auxiliary operator (K is a constant). Under which conditions you could use the variational principle and the auxiliary operator to study some of the excited states of H?

   K must be bigger than the gap between ground and 1st excited state because if $K > E_1 - E_0$, then the ground state of H' is the first excited state of H.

4. $H = \frac{p_x^2}{2m} + ax + \frac{bx^2}{2} + \frac{c}{6}x^3$. use perturbation theory to provide the best estimate (up to 1st order) of the energy of its 2nd excited state.

   The perturbation is $V = ax + \frac{c}{6}x^3$ because the other two terms can be separated into the $\hat{H}$ for harmonic oscillator.

   $\lambda = 1$ for first order correction.

   $E = E_0^2 + \int_{-\infty}^{\infty} \psi * (ax + \frac{c}{6}x^3)\psi$

   $E = \hbar\omega(n + \frac{1}{2}) + 0$ because odd functions in the integral part.

   $E = \hbar\omega(2 + \frac{1}{2}) = \frac{5}{2}\hbar\omega$ Energy from first order perturbation for the 2nd excited state is the same as 2nd excited state for the harmonic oscillator.

5. Let h be the Hamiltonian of a single fermion, with normalized eigenfunctions k. Show that the Slater determinant:

$$\begin{bmatrix} \psi_1(1) & \psi_1(2) & \dots & \psi_1(n) \\ \psi_2(1) & \psi_2(2) & \dots & \psi_2(n) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_n(1) & \psi_n(2) & \dots & \psi_n(n) \end{bmatrix}$$

$\hat{H} = h1 + h2 + ... + h_N$

To prove that there will it will normalize to $\frac{1}{N!}$, we know there are N! terms in the slater determinant of the $n \times n$ matrix. Different spin state will be orthogonal. So it will be $\frac{1}{\sqrt{N!}}$