PH 422: Quantum Mechanics II
Tutorial Sheet 3

This tutorial sheet contains problems related to the use of variational principle in quantum mechanics.

1. Obtain the energy of the ground state of a one-dimensional (1D) simple-harmonic oscillator (SHO) using the trial wave function $\psi(x) = Ce^{-\alpha x^2}$, where C is the normalization constant, and α is the variational parameter.

2. In the variational principle as applied to quantum mechanics, one minimizes the integral $I = \langle\psi|H|\psi\rangle = \int\{-\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + V\psi^*\psi\}d^3\mathbf{r}$, subject to the normalization condition $\int \psi^*\psi d^3\mathbf{r} = 1$. Show using integration by parts, that one can also use the expression $I = \int\{\frac{\hbar^2}{2m}\nabla\psi^* \cdot \nabla\psi + V\psi^*\psi\}d^3\mathbf{r}$.

3. Estimate the ground state energy of a 1D-SHO using the trial wave function of the form $\psi(x) = Ce^{-\alpha|x|}$, treating α as a variational parameter. (Helpful integral: $\int_0^\infty e^{-\alpha x}x^n dx = \frac{n!}{\alpha^{n+1}}$.)

4. Show that for a 1D-SHO, if one uses a trial wave function $\psi(x) = Cxe^{-\alpha x^2}$,where C is the normalization constant and α is the variational parameter, one obtains exact energy $E = \frac{3}{2}\hbar\omega$ of the first excited state.

5. Here we derive the "linear-combination of basis functions approach", quite commonly used in quantum mechanics, using a variational principle. Suppose that the Hamiltonian of a system is given by H, and we assume that the state ket $|\psi\rangle$ corresponding to its ground state can be approximated as

$$|\psi\rangle = \sum_{j=1}^{N} C_j|j\rangle,$$

where $|j\rangle$ denote the known basis kets, while C_j are the unknown expansion coefficients which are also the variational parameters in this approach, and, in general, are complex. In the $\mathbf{r}$ representation, the following notation is adopted $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle$, and $\phi_j(\mathbf{r}) = \langle\mathbf{r}|j\rangle$. Using the variational principle, show that the ground state energy E, and the state ket $|\psi\rangle$ can be obtained by solving the generalized eigenvalue problem

$$\tilde{H}\tilde{C} = E\tilde{S}\tilde{C},$$

where $\tilde{H}$ and $\tilde{S}$ denote the $N \times N$ matrices, representing the Hamiltonian and the overlap, with elements defined as $H_{ij} = \langle i|H|j\rangle$, $S_{ij} = \langle i|j\rangle$, respectively, while C_i form the N elements of the column vector $\tilde{C}$, denoting the ground state eigenfunction. Note that form an orthonormal basis set, $\langle i|j\rangle = \delta_{ij}$ so that $\tilde{S} = I$, and the previous generalized eigenvalue problem reduces to a normal eigenvalue problem.

6. This problem is a simple application of the linear-combination of basis functions approach. Suppose the wave function of a given quantum mechanical system can be expanded in terms of three basis functions $\{|i\rangle, i = 1, 2, 3\}$, which form an orthonormal set $\langle i|j\rangle = \delta_{ij}$. Defining the Hamiltonian matrix elements with respect to these basis functions as $H_{ij} = \langle i|H|j\rangle$, it is given that the only non-zero Hamiltonian matrix elements are $H_{12} = H_{21} = H_{23} = H_{32} = H_{13} = H_{31} = t$, where t is a real positive number. Obtain the eigenvalues and eigenvectors of this Hamiltonian. How do the results change when we set $H_{13} = H_{31} = 0$?

7. Estimate the ground state energy of a particle of mass m in a box with $V = 0$, for $0 \leq x \leq a$, and $V = \infty$, otherwise, using variational principle. For the purpose, take a wave function consisting of two linear components $\psi_1(x)$ and $\psi_2(x)$ defined by: (i) $\psi_1(0) = 0$, $\psi_1(x = \alpha) = C$ for $0 \leq x \leq \alpha$, and (ii) $\psi_2(x = \alpha) = C$, $\psi_2(x = a) = 0$, for $\alpha \leq x \leq a$, where C is the normalization constant, and α is the variational parameter.

8. Consider the Hamiltonian of a particle moving in a 1D Gaussian potential well $H = \frac{p^2}{2m} - V_0 e^{-ax^2}$, with V_0 and $a > 0$. Estimate its ground-state energy employing variational principle, with a trial wave function of the form $\psi(x) = Ce^{-\alpha x^2}$, with α as the variational parameter.

9. Using the trial wave function $\psi(\mathbf{r}) = Ce^{-\alpha r}$, where C is the normalization constant, and α is the variational parameter, estimate the ground state energy of the hydrogen atom.