Problem 9.1(L)

A trial wavefunction $\psi(x) = Ae^{-bx^2}$ is defined on the interval $x \in (-\infty, \infty)$. The real variational parameter $b > 0$.

a) Determine A in terms of b such that the trial wavefunction is normalized to 1.

b) Compute the expectation value of the operator x^2 in the state described by ψ.

c) Compute the expectation value of the operator $\frac{d^2}{dx^2}$ in the state described by ψ.

d) From the results in b) and c) write down the expectation value of the Hamiltonian of the 1d harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ in the state ψ, and minimize it with respect to b.

Problem 9.2(H)

A particle of mass m is located in a one-dimensional potential $V(x) = \alpha|x|$ where α is a real positive constant. Use the variational method to establish an upper bound on the ground state energy of this system. Choose the class of trial wavefunctions yourself.

Problem 9.3(H)

Consider a particle with mass m in a three-dimensional attractive Dirac delta-function potential

$$H_{3d} = \frac{\vec{p}^{\,2}}{2m} - \alpha\, \delta^3(\vec{r})$$

where $\delta^3(\vec{r}) = \delta(x)\delta(y)\delta(z)$ and $\alpha > 0$ is a constant that characterizes the strength of the potential.

Use the variational principle with Gaussian trial wavefunctions having a real variational parameter L

$$\psi_L(\vec{r}) = Ae^{-r^2/2L^2} = Ae^{-(x^2+y^2+z^2)/2L^2}$$

to demonstrate that the ground state energy of H_{3d} is not finite. H_{3d} is therefore unphysical. You might amuse yourself (not required) with repeating this for attractive delta-function potentials in two and one dimensions. It turns out that the two-dimensional delta-function potential is also unphysical. This is in contrast to the one-dimensional attractive delta-function potential which has a finite ground state energy.

Problem 9.4(H)

A problem of importance in astrophysics is whether or not a single proton can bind two electrons. This question can be addressed by the variational method using the trial wavefunctions

$$\psi(\vec{r}_1, \vec{r}_2) = A\left[\psi_1(r_1)\psi_2(r_2) + \psi_2(r_1)\psi_1(r_2)\right], \qquad \psi_i(r) = \sqrt{\frac{Z_i^3}{\pi a_0^3}} e^{-Z_i r/a_0}, \quad i \in 1, 2$$

where a_0 is the Bohr radius and Z_1 and Z_2 are the variational parameters. (The spin part is omitted.) Using this class of trial wavefunctions one can show that the trial energy in terms of $x = Z_1 + Z_2$ and $y = 2\sqrt{Z_1 Z_2}$ is

$$E_{tr} = \frac{E_1}{x^6 + y^6}\left(-x^8 + 2x^7 + \frac{1}{2}x^6y^2 - \frac{1}{2}x^5y^2 - \frac{1}{8}x^3y^4 + \frac{11}{8}xy^6 - \frac{1}{2}y^8\right)$$

where $E_1 = -13.6eV$. Minimize E_{tr} numerically with respect to Z_1 and Z_2 and determine if a proton and two electrons can form a bound state.

Problem 9.5(H)

Two distinguishable particle, but with the same mass m are moving in a one dimensional well of extension a and with infinitely high walls. The particles are imprenetrable, so that particle 1 is always to the left of particle 2. Write down the simplest polynomial trial wavefunction that describes these particles and their boundary conditions. Use this trial wavefunction to work out an upper bound for the ground state energy of this system.

Problem 9.6(X)

Two identical spinless bosons of mass m are located in a one dimensional harmonic oscillator potential of characteristic frequency ω. The bosons also have a repulsive interaction so that in real space there is a particle-particle interaction

$$H_{int} = g\delta(x_1 - x_2)$$

where g is a positive quantity with units energy times length, and $\delta(x_1 - x_2)$ is the Dirac delta-function.

a) Use the following normalized trial wavefunctions

$$\psi(x_1, x_2) = \left(\frac{2b}{\pi}\right)^{1/2} e^{-b(x_1^2 + x_2^2)}$$

to calculate the variational energy (trial energy) as a function of b ($b > 0$) for the two interacting particles in the harmonic oscillator well. You may use without proof the integral $\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} dx e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)e^{-bx^2} = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$. Do not try to minimize the obtained variational energy exactly. Instead, find approximately how the minimum variational energy behaves as a function of g for large g ($g \gg \hbar\omega\sqrt{\frac{\hbar}{m\omega}}$).

b) Which of the following variational wavefunctions is (are) most likely better variational wavefunction(s) (i.e. have a lower energy) for large positive values of g than the ones considered in a)?

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\begin{aligned}
a) \quad & \psi = \tfrac{2b}{\sqrt{\pi}}|x_1 + x_2|e^{-b(x_1^2+x_2^2)} \\
b) \quad & \psi = \tfrac{2b}{\sqrt{\pi}}|x_1 - x_2|e^{-b(x_1^2+x_2^2)} \\
c) \quad & \psi = \tfrac{2b}{\sqrt{\pi}}(x_1 + x_2)e^{-b(x_1^2+x_2^2)} \\
d) \quad & \psi = \tfrac{2b}{\sqrt{\pi}}(x_1 - x_2)e^{-b(x_1^2+x_2^2)}
\end{aligned}
$$

To get credit on this subproblem you should give reasons for your answer. NB! Do not attempt to perform the actual variational calculation. All you need to do is to discuss the different alternatives.