1. Variational bound on the ground state in a power-like potential (10 points)

The trial wave function is

$$\psi(x) = Ae^{-bx^2}$$

(1)

Normalizing the wavefunction we compute

$$1 = \langle \psi | \psi \rangle = A^2 \int_{-\infty}^{\infty} dx e^{-2bx^2} = A^2 \frac{\sqrt{\pi}}{2b}$$

and therefore

$$A = \left( \frac{2b}{\pi} \right)^{\frac{1}{4}}.$$  

(2)

The expectation value of energy for this wave function is

$$E(b) = \langle \psi | H | \psi \rangle = A^2 \int_{-\infty}^{\infty} dx e^{-bx^2} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \lambda x^4 \right) e^{-bx^2}$$

$$= \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} dx \left( \frac{\hbar^2}{2m} (2b - 4b^2 x^2) + \lambda x^4 \right) e^{-2bx^2}$$

$$= \frac{\hbar^2 b}{2m} + \frac{3\lambda}{16b^2}.$$  

(3)

Requiring the derivative of $E(b)$ with respect to $b$ to be zero we find that the minimum of $\langle \psi | H | \psi \rangle$ is reached at

$$b_{\text{min}} = \left( \frac{3m\lambda}{4\hbar^2} \right)^{\frac{1}{2}}.$$  

(4)

with the energy at the minimum

$$E_{\text{min}} = \frac{3}{4} \frac{\hbar^2}{m} \left( \frac{3m\lambda}{4\hbar^2} \right)^{\frac{1}{2}}.$$  

(5)

The trial wave function $\psi(b)$ a linear combination of the ground and excited states. Therefore the energy in the ground state cannot be greater than $E_{\text{min}}$.

2. Variational bound on the excited states (15 points)

(a) (6 points) A generic wave function $\psi$ can be expanded in terms of energy eigenfunctions

$$|\psi\rangle = \sum_{n \geq 0} c_n |\psi_n\rangle.$$  

(6)

where $|\psi_0\rangle$ is the ground state and $|\psi_1\rangle$ is the first excited state with energy $E_1$. $\psi_n \ (n > 1)$ are higher excited states with $E_n \geq E_1$. The condition $\langle \psi | \psi_0 \rangle = 0$ implies that $c_0 = 0$ and thus $\langle \psi | \psi \rangle = 1$ leads to

$$\sum_{n \geq 1} |c_n|^2 = 1.$$  

(7)
The expectation value of $H$ is

$$
\langle \psi|H|\psi \rangle = \sum_{m,n \geq 1} c_m^* c_n \langle \psi_m|H|\psi_n \rangle
$$

$$
= \sum_{m,n \geq 1} c_m^* c_n \delta_{m,n} E_n
$$

$$
= \sum_{n \geq 1} |c_n|^2 E_n
$$

$$
\geq \sum_{n \geq 1} |c_n|^2 E_1
$$

$$
= E_1 \sum_{n \geq 1} |c_n|^2
$$

$$
= E_1.
$$

Q.E.D.

(b) (2 points) Since the potential $\lambda x^4$ is even, the ground state must also be even function of $x$. Then for example we may choose

$$
|\psi \rangle = A x e^{-bx^2}
$$

as a set of the trial functions. Since $|\psi \rangle$ is an odd function of $x$ it has zero overlap with $|\psi_0 \rangle$. The normalization constraint $\langle \psi|\psi \rangle = 1$ will determine $A$ in terms of $b$, thus giving a one-parametric set of trial functions.

(c) (7 points) The same set of trial functions as in (b) can be used to get an estimate for the harmonic oscillator. Normalizing (9) we write

$$
1 = \langle \psi|\psi \rangle = A^2 \int_{-\infty}^{\infty} dx x^2 e^{-2bx^2}
$$

$$
= A^2 \sqrt{\frac{\pi}{2^5 b^5}}
$$

and thus

$$
A = \left( \frac{\pi}{2^5 b^5} \right)^{-\frac{1}{4}}
$$

The energy expectation value is

$$
E(b) = \langle \psi|H|\psi \rangle = A^2 \int_{-\infty}^{\infty} dx x e^{-bx^2} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2} \right) x e^{-2bx^2}
$$

$$
= \sqrt{\frac{2^5 b^5}{\pi}} \int_{-\infty}^{\infty} dx \left( \frac{3\hbar^2 b}{m} x^4 + \left( \frac{m\omega^2}{2} - \frac{2\hbar^2 b^2}{m} \right) x^4 \right) e^{-2bx^2}
$$

$$
= \frac{3\hbar^2 b}{2m} + \frac{3m\omega^2}{8b}.
$$

Setting the derivative of $E(b)$ to zero we find that

$$
b_{\min} = \frac{m\omega}{2\hbar}
$$
with

\[ E_{\text{min}} = \frac{3\hbar \omega}{2}. \]  

(15)

Note that in this case the variational method gave us exact answer for the energy, which comes at no surprise since our set of trial wave functions \( \psi \sim x e^{-bx^2} \) includes that for the first excited state of the harmonic oscillator.

3. Variational bound on the ground state in an exponential potential (15 points)

(Full credit will be given to answers to this problem that set \( \hbar = 1. \))

(a) (2 points) The condition that the wave function be normalized yields

\[ 1 = \int d^3 x \, C^2 \, e^{-2\lambda r} = 4\pi C^2 \int dr \, r^2 e^{-2\lambda r}. \]

Defining \( x = 2\lambda r \), we find

\[ 1 = 4\pi C^2 \left( \frac{1}{2\lambda} \right)^3 \int dx \, x^2 e^{-x}. \]

Using the identity \( \int_0^\infty dx \, x^2 e^{-x} = 2 \), we find

\[ C^2 = \frac{\lambda^3}{\pi}. \]

(b) (3 points) Our trial wavefunction has only radial dependence, therefore angular parts in kinetic energy give 0 when they act on the wavefunction. It is sensible to choose an s-wave ansatz, as was given in the problem, since we expect an s-wave ground state for a particle in a spherically symmetric potential. Therefore expectation value of the energy in our trial wave function is given by the integral

\[ E = 4\pi C^2 \int dr \, r^2 \left[ \frac{\hbar^2}{2m} \lambda^2 e^{-2\lambda r} - \alpha e^{-2(\mu + \lambda)r} \right], \]

which we can rewrite as

\[ E = 4\pi C^2 \int dx \, x^2 e^{-x} \left( \frac{\hbar^2 \lambda^2}{2m} \left( \frac{1}{2\lambda} \right)^3 - \frac{\alpha}{8(\mu + \lambda)^3} \right), \]

or, using part (a),

\[ E = \frac{\hbar^2 \lambda^2}{2m} - \alpha \left( \frac{\lambda}{\mu + \lambda} \right)^3. \]

(c) (4 points) We minimize \( E \) with respect to \( \lambda \):

\[ \frac{\partial E}{\partial \lambda} = \frac{\hbar^2 \lambda}{m} - 3\alpha \left( \frac{\lambda}{\mu + \lambda} \right)^2 \left( \frac{\mu}{(\mu + \lambda)^2} \right) = 0. \]

This has the obvious solution \( \lambda = 0 \); the other solutions are found by solving the quartic equation \( (\mu + \lambda)^4 - 3\alpha m \lambda / \hbar^2 = 0 \). By glancing at the quartic formula, it is easy to see that the quartic equation has no real roots unless \( 81m - 256\mu^2 \hbar^2 > 0 \), or, in other words, only for \( \alpha > \frac{256\mu^2 \hbar^2}{81m} \) does \( E \) have extrema other than at \( \lambda = 0 \). Therefore for small \( \alpha \), minimum value of \( E(\lambda) \) is 0, i.e. there are no bound states. \cite{footnote}

When \( \lambda = 0 \), the energy also vanishes, and we are left with something that looks very much like a zero momentum plane wave. The wave function is distributed uniformly through space.
We would like to know when it is possible to have \( E = 0 \), as this is the dividing line between having a bound state and having no bound states. We plot this dividing line as a function of \( x \) and \( \kappa \) in figure 1. To have \( E = 0 \), we must have \( \kappa = \frac{(1+x)^3}{2x} \). The minimum value of \( \kappa \) satisfying that condition is obtained by setting \( \frac{\partial \kappa}{\partial x} = 0 \), yielding

\[
\kappa_{\text{min}} = 3.375, \quad x = \frac{1}{2}.
\]

(e) (2 points) Recall that the variational method gives only an upper bound on the ground state energy. If \( E < 0 \), we know that there exists a bound state, but if \( E > 0 \), we cannot conclude that there is no bound state. Therefore, the previous section gives us neither a minimum nor a maximum value of \( \alpha \) required for a bound state. All it tells us is that if \( \alpha \geq \frac{\hbar^2 \kappa_{\text{min}}}{m} \), then we know that a bound state exists, while if \( \alpha < \frac{\hbar^2 \kappa_{\text{min}}}{m} \), we do not know if a bound state exists.