Quantum Physics III (8.06) Spring 2006
Solution Set 7

April 9, 2006

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

   The trial wave function is

   $$\psi(x) = Ae^{-bx^2} \tag{1}$$

   Normalizing the wavefunction we compute

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

   and therefore

   $$A = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}}. \tag{3}$$

   The expectation value of energy for this wave function is

   $$\begin{aligned} E(b) = \langle\psi|H|\psi\rangle &= A^2 \int_{-\infty}^{\infty} dx\, e^{-bx^2} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda x^4\right) e^{-bx^2} \\ &= \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} dx\, (\frac{\hbar^2}{2m}(2b - 4b^2x^2) + \lambda x^4) e^{-2bx^2} \\ &= \frac{\hbar^2 b}{2m} + \frac{3\lambda}{16b^2}. \end{aligned} \tag{4}$$

   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

   $$b_{\min} = \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}} \tag{5}$$

   with the energy at the minimum

   $$E_{\min} = \frac{3}{4}\frac{\hbar^2}{m}\left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}} \tag{6}$$

   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 $E_{\min}$.

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

   (a) **(6 points)** A generic wave function ψ can be expanded in terms of energy eigenfunctions

   $$|\psi\rangle = \sum_{n\geq 0} c_n|\psi_n\rangle. \tag{7}$$

   where $|\psi_0\rangle$ is the ground state and $|\psi_1\rangle$ is the first excited state with energy E_1. ψ_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

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

The expectation value of H is

$$
\begin{aligned}
\langle\psi|H|\psi\rangle &= \sum_{m,n\geq 1} c_m^* c_n \langle\psi_m|H|\psi_n\rangle \\
&= \sum_{m,n\geq 1} c_m^* c_n \delta_{m,n} E_n \\
&= \sum_{n\geq 1} |c_n|^2 E_n \\
&\geq \sum_{n\geq 1} |c_n|^2 E_1 \\
&= E_1 \sum_{n\geq 1} |c_n|^2 \\
&= E_1 .
\end{aligned}
\tag{8}
$$

Q.E.D.

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

$$
|\psi\rangle = Axe^{-bx^2} \tag{9}
$$

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

$$
\begin{aligned}
1 = \langle\psi|\psi\rangle &= A^2 \int_{-\infty}^{\infty} dx\, x^2 e^{-2bx^2} \\
&= A^2 \sqrt{\frac{\pi}{2^5 b^3}}
\end{aligned}
\tag{10}
$$

and thus

$$
A = \left(\frac{\pi}{2^5 b^3}\right)^{-\frac{1}{4}} \tag{11}
$$

The energy expectation value is

$$
\begin{aligned}
E(b) = \langle\psi|H|\psi\rangle &= A^2 \int_{-\infty}^{\infty} dx\, xe^{-bx^2} \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2}\right) xe^{-bx^2} \\
&= \sqrt{\frac{2^5 b^3}{\pi}} \int_{-\infty}^{\infty} dx \left(\frac{3\hbar^2 b}{m}x^2 + \left(\frac{m\omega^2}{2} - \frac{2\hbar^2 b^2}{m}\right) x^4\right) e^{-2bx^2} && (12) \\
&= \frac{3\hbar^2 b}{2m} + \frac{3m\omega^2}{8b} . && (13)
\end{aligned}
$$

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

$$
b_{\min} = \frac{m\omega}{2\hbar} \tag{14}
$$

with

$$E_{\min} = \frac{3\hbar\omega}{2}. \tag{15}$$

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 $\psi \sim xe^{-bx^2}$ 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 $1 = \int d^3x\, C^2\, e^{-2\lambda r} = 4\pi C^2 \int dr\, r^2 e^{-2\lambda r}$. Defining $x = 2\lambda r$, we find $1 = 4\pi C^2 (\frac{1}{2\lambda})^3 \int dx\, x^2 e^{-x}$. 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.Thefore 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 λ:

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

   This has the obvious solution $\lambda = 0$; the other solutions are found by solving the quartic equation $(\mu+\lambda)^4 - 3\alpha m\lambda\mu/\hbar^2 = 0$. By glancing at the quartic formula, it is easy to see that the quartic equation has no real roots unless $81\alpha m - 256\mu^2\hbar^2 > 0$, 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 α, minimum value of $E(\lambda)$ is 0, i.e. there are no bound states. [Note: You can solve the quartic equation $(\mu+\lambda)^4 = a\lambda$ using Mathematica, and you can see the occurrence of $\sqrt{27a^4 - 256a^3\mu^3}$ at several places. In order to have one or more real solutions, you need $27a - 256\mu^3$ to be positive. This is where you get the above condition.]

   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.

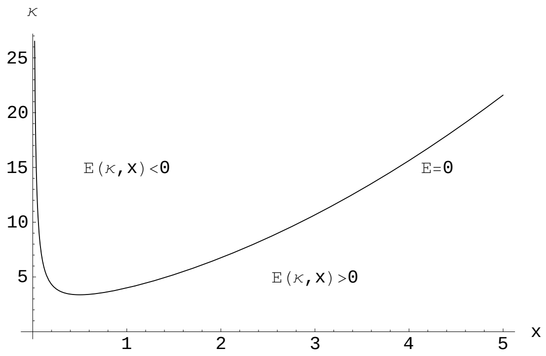

Figure 1: $\kappa = \frac{(1+x)^3}{2x}$

(Of course, this means that the probability of finding the particle at any specific point goes to zero as the volume of space goes to infinity.)

(d) **(4 points)** In terms of our dimensionless variables x and κ, we find

$$\begin{aligned} \mathcal{E} &= \frac{1}{2}\left(\frac{\lambda}{\mu}\right)^2 - \frac{m\alpha}{\hbar^2\mu^2}\left(\frac{\lambda/\mu}{1+\lambda/\mu}\right)^3 \\ &= \frac{1}{2}x^2 - \kappa\left(\frac{x}{1+x}\right)^3. \end{aligned}$$

We would like to know when it is possible to have $\mathcal{E} = 0$, 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 κ in figure 1. To have $\mathcal{E} = 0$, we must have $\kappa = \frac{(1+x)^3}{2x}$. The minimum value of κ satisfying that condition is obtained by setting $\frac{\partial \kappa}{\partial x} = 0$, yielding

$$\kappa_{min} = 3.375, \qquad\qquad x = \frac{1}{2}.$$

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