# PHY521; Quantum Mechanics, Problem Set 8

Due Wed. 8 Nov.2006 at the beginning of class.

## 1. Variational calculation, 1D infinite square well.

In class we carried out a variational calculation for the 1D infinite square well, with $V(x)$ given by

$$V(x) = \begin{cases} 0, & |x| < d/2 \quad \text{(inside)} \\ \infty, & |x| > d/2 \quad \text{(outside).} \end{cases} \tag{1}$$

The trial wavefunction we assumed was an even power-law form,

$$\psi^T(x) = \begin{cases} \eta\Big((d/2)^p - |x|^p\Big), & |x| < d/2 \quad \text{(inside)} \\ 0, \quad |x| > d/2 & \text{(outside).} \end{cases} \tag{2}$$

The calculation proceeded by finding the expected energy

$$E^{estm}(p) = \langle \psi^T | H | \psi^T \rangle \tag{3}$$

where the Hamiltonian is as usual

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{4}$$

This was then minimized w.r.t. $p$ to find a variational upper bound on $E_0$. This was $5\hbar^2/md^2$, which compares rather well with the exact $E_0 = (\pi^2/2) \cdot \hbar^2/md^2$.

We can similarly apply the variational method to excited states, provided that the trial wavefunction is orthogonal to the exact lower energy eigenstates. In this problem this is possible for the first excited state by using an odd trial wavefunction.

Demonstrate this application by carrying deriving a variational upper bound for the energy of the first excited state (which has odd parity) of this problem, using the trial wavefunction

$$\psi^T(x) = \begin{cases} \eta x\Big((d/2)^p - |x|^p\Big), & |x| < d/2 \quad \text{(inside)} \\ 0, \quad |x| > d/2 & \text{(outside).} \end{cases} \tag{5}$$

Specifically,

a) (*2 pts*) Find the normalization constant $\eta$ for this odd wavefunction,

b) (*2 pts*) Find the expected energy

$$E^{estm}(p) = \langle \psi^T | H | \psi^T \rangle \tag{6}$$

c) (*2 pts*) Find the optimum variational parameter $p_{opt}$, and finally

d) (*2 pts*) Find the best variational upper bound on $E_1$,

$$E_1^{opt} = E_1^{estm}(p_{opt}) = \langle \psi^T(p_{opt}) | H | \psi^T(p_{opt}) \rangle \tag{7}$$

Express this in the form $E_1^{opt} = n \cdot \hbar^2/md^2$, where $n$ is a pure number (not necessarily an integer).

e) (*2 pts*) Compare this estimate to the exact $E_1$. By what fraction does your variational calculation overestimate $E_1$?

## 2. Variational calculation, 1D quartic potential.

In discussing perturbation theory we had some fun with the 1D SHO with a quartic perturbation, defined by the usual Hamiltonian (Prob.1, Eq.4) with the potential

$$V(x) = \frac{1}{2}kx^2 + gx^4. \tag{8}$$

We carried out perturbation theory to high order for this potential, and noted that the $E_0$ perturbation series is asymptotic (not convergent for any $g > 0$). So, what can one do with this potential in practice, especially when $g$ is large?

One method is to use a variational approach. If we assume a simple Gaussian as a trial wavefunction for the ground state of this potential

$$\psi^T(x) = (c/\pi)^{1/4}\, e^{-cx^2/2} \tag{9}$$

where $c$ is a variational parameter, derive the following expectation values:

a) (*2 pts*)

$$\langle \psi^T|T|\psi^T\rangle = \frac{1}{4}\frac{\hbar^2}{m}c \tag{10}$$

b) (*2 pts*)

$$\langle \psi^T|V|\psi^T\rangle = \frac{1}{4}kc^{-1} + g\frac{3}{4c^2}. \tag{11}$$

c) (*2 pts*)

Now minimize $E_0^{estm}(c)$ w.r.t. $c$ and show that the optimum value satisfies a cubic, which can be written as

$$c_{opt} = \frac{(mk)^{1/2}}{\hbar}\left(1 + \frac{6g}{k}c_{opt}^{-1}\right)^{1/2}. \tag{12}$$

d) (*2 pts*) This is easy to solve in the large-$g$ limit. Show that the solution is

$$\lim_{g\to\infty} c_{opt} = \left(\frac{6gm}{\hbar^2}\right)^{1/3}. \tag{13}$$

e) (*2 pts*) Find the resulting variational upper bound for the ground state energy of the pure $gx^4$ potential. This result should be expressed in the form $E_0^{estm}(c_{opt}) = n \cdot \left(\frac{\hbar^2}{m}\right)^{2/3} g^{1/3}$, where $n$ is a pure number. (This form is required by the units.)

## 3. Variational calculation, 3D SHO.

Variational methods can easily be extended to problems in higher dimensions. As an example, calculate the variational trial energy of the 3D SHO, defined by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2 \tag{14}$$

with the normalized Gaussian variational wavefunction

$$\psi^T(r) = (c/\pi)^{3/4}\, e^{-cr^2/2}, \tag{15}$$

where $c$ is a free variational paameter. Specifically, evaluate

a) (*3 pts*)

$$\langle \psi^T | T | \psi^T \rangle, \tag{16}$$

and

b) (*3 pts*)

$$\langle \psi^T | V | \psi^T \rangle. \tag{17}$$

c) (*4 pts*) Now sketch the expected energy $E_0^{estm}(c)$, and find the optimum variational parameter $c_{opt}$ and the corresponding upper bound on $E_0$. Show that these are exactly the 3D SHO results.