PHY 407 QUANTUM MECHANICS Fall 05
Midterm Examination Nov 3 12:30 to 1:45 pm

1. Use a Gaussian variational ansatz to estimate the ground state energy of the hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda |x|^k, \quad \lambda > 0, k > 0. \tag{1}$$

Compare with the exact answer when $k = 2$.

Hint $\int_0^\infty e^{-t} t^{z-1} dt = \Gamma(z), \Gamma(z+1) = z\Gamma(z)$.

1 Solution

1.1 Dimensional Analysis

The hamiltonian can be written as

$$H = \frac{\hbar^2}{2m}\tilde{H}, \quad \tilde{H} = -\frac{\partial^2}{\partial x^2} + \tilde{\lambda}|x|^k, \quad \tilde{\lambda} = \frac{2m}{\hbar^2}\lambda. \tag{2}$$

$\tilde{H}$ has dimension of L^{-2}, so $[\tilde{\lambda}]L^k = L^{-2}$ so that $[\tilde{\lambda}] = L^{-2-k}$. Thus the ground state eigenvalue of $\tilde{H}$ should be proportional to $\tilde{\lambda}^{\frac{2}{2+k}}$ and that of H should be

$$\begin{aligned} E_0 &= \left[\frac{\hbar^2}{2m}\right]\left[\frac{\hbar^2}{2m}\right]^{-\frac{2}{2+k}} \lambda^{\frac{2}{2+k}} C \\ &= \left[\frac{\hbar^2}{2m}\right]^{\frac{k}{2+k}} \lambda^{\frac{2}{2+k}} C \end{aligned} \tag{1}$$

for some dimensionless constant C which will depend only on k. This will provide a check on our calculations.

1.2 Variational Ansatz

Let us choose a Gaussian variational ansatz:

$$\psi = e^{-\frac{1}{2}a^2x^2}. \tag{3}$$

We need to find

$$< H >= \frac{\frac{\hbar^2}{2m}\int\left[\frac{d\psi}{dx}\right]^2 dx + \lambda\int |x|^k|\psi(x)|^2 dx}{\int |\psi(x)|^2 dx} \tag{4}$$

Now,

$$\begin{aligned}\int |\psi(x)|^2 dx &= \int_{-\infty}^{\infty} e^{-a^2x^2}dx \\ &= a^{-1}\int_{-\infty}^{\infty} e^{-x^2}dx. \end{aligned} \tag{2}$$

$$\frac{d\psi}{dx} = -a^2x\psi, \tag{5}$$

$$\begin{aligned}\int\left[\frac{d\psi}{dx}\right]^2 dx &= \int a^4x^2e^{-a^2x^2}dx \\ &= a\int_{-\infty}^{\infty} x^2e^{-x^2}dx. \end{aligned} \tag{3}$$

$$\int |x|^k e^{-a^2x^2}dx = a^{-1-k}\int_{-\infty}^{\infty}|x|^k e^{-x^2}dx. \tag{4}$$

If we let

$$I(k) = \int_{-\infty}^{\infty}|x|^k e^{-x^2}dx, \tag{6}$$

we get

$$\begin{aligned}< H > &= \frac{\frac{\hbar^2}{2m}aI(2) + \lambda a^{-1-k}I(k)}{a^{-1}I(0)} \\ &= \frac{1}{I(0)}\left[\frac{\hbar^2}{2m}I(2)a^2 + \lambda I(k)a^{-k}\right] \end{aligned} \tag{5}$$

1.3 Minimization

Minimizing in a gives

$$2\frac{\hbar^2}{2m}I(2)a^2 - k\lambda I(k)a^{-k} = 0 \tag{7}$$

so at the minimum

$$< H >= \left\{1 + \frac{2}{k}\right\} \frac{1}{I(0)} \frac{\hbar^2}{2m} I(2)a^2 \tag{8}$$

where

$$a^{2+k} = \frac{2m\lambda}{\hbar^2} \frac{kI(k)}{2I(2)} \tag{9}$$

so that

$$< H >= \left\{\frac{k+2}{k}\right\} \frac{1}{I(0)} \frac{\hbar^2}{2m} I(2) \left[\frac{2m\lambda}{\hbar^2}\right]^{\frac{2}{2+k}} \left[\frac{kI(k)}{2I(2)}\right]^{\frac{2}{2+k}} \tag{10}$$

Simplifying this we get

$$E_0 \leq \left[\frac{\hbar^2}{2m}\right]^{\frac{k}{2+k}} \lambda^{\frac{2}{2+k}} \left\{\frac{k+2}{k}\right\} \frac{I(2)}{I(0)} \left[\frac{kI(k)}{2I(2)}\right]^{\frac{2}{2+k}} \tag{11}$$

This agrees with the form we got from dimensional analysis.

1.4 Evaluation of Integrals

$$\begin{aligned} I(k) &= \int_{-\infty}^{\infty} |x|^k e^{-x^2} dx = 2\int_0^{\infty} x^k e^{-x^2} dx \\ &= \int_0^{\infty} t^{\frac{k}{2}} e^{-t} t^{-\frac{1}{2}} dt = \int_0^{\infty} t^{(\frac{k}{2}+\frac{1}{2})-1} e^{-t} dt \\ &= \Gamma\left(\frac{k+1}{2}\right). \end{aligned} \tag{6}$$

Thus

$$\frac{I(2)}{I(0)} = \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{1}{2})} = \frac{1}{2}. \tag{12}$$

$$\frac{kI(k)}{2I(2)} = \frac{k\Gamma(\frac{k+1}{2})}{2\Gamma(\frac{3}{2})}. \tag{13}$$

$$E_0 \leq \left[\frac{\hbar^2}{2m}\right]^{\frac{k}{2+k}} \lambda^{\frac{2}{2+k}} \left\{\frac{k+2}{2k}\right\} \left[\frac{k\Gamma(\frac{k+1}{2})}{2\Gamma(\frac{3}{2})}\right]^{\frac{2}{2+k}} \tag{14}$$

1.5 The special case $k = 2$

This corresponds to the harmonic oscillator:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda x^2 \tag{15}$$

has ground state energy $\frac{1}{2}\hbar\omega$ where $\lambda = \frac{1}{2}m\omega^2$.

If we put $k = 2$ in the above variatioan estimate,

$$E_0 \leq \left[\frac{\hbar^2}{2m}\right]^{\frac{1}{2}} \lambda^{\frac{1}{2}} = \frac{1}{2}\hbar\omega. \tag{7}$$

Thus we get the exact answer in this case, which is because the Gaussian is the true ground state wave function of the harmonic oscillator.

2. A metal contains electrons trapped in a potential barrier of height $V_0 > 0$ ("Work Function"). An external electric field $F > 0$ is applied to strip electrons out of the metal. The potential seen by the electron can be taken to be

$$V(x) = -V_0, \quad \text{for } x < 0, \quad V(x) = -qFx \text{ for } x > 0. \tag{16}$$

where q is the magnitude of the charge of the electron. Using the WKB approximation, calculate the probability that an electron will be emitted, assuming it is in the ground state inside the metal.

2 Solution

2.1 Dimensional Analysis

The probability can depend only on dimensionless ratios of the parameters $\hbar, m, q, F, V_0$ of the problem. The wavelength of the electron in its ground state will be given by

$$\frac{\hbar^2}{2m}\lambda^{-2} = V_0, \Rightarrow \lambda = \left[\frac{\hbar^2}{2mV_0}\right]^{\frac{1}{2}} \tag{17}$$

the distance over which the electron will have to tunnel is another length parameter (potential energy divided by force)

$$\frac{V_0}{qF}. \tag{18}$$

The probability can only depend on the ratio of these two lengths:

$$\left[\frac{2mV_0^3}{\hbar^2}\right]^{\frac{1}{2}}\frac{1}{qF}. \tag{19}$$

2.2 Tunnelling amplitude

Let the electron have energy E; in the ground state $E = -V_0$. It has to tunnel through a potential barrier to escape to infinity when $E < 0$.

The tunneling amplitude is

$$e^{-\frac{1}{\hbar}\int_{x_1}^{x_2}\sqrt{2m[V(x)-E]}dx} \tag{20}$$

where x_1, x_2 are the points where $E = V(x)$. In our case $x_1 = 0$, and

$$-qFx_2 = E. \tag{21}$$

The integral is

$$\begin{aligned}
\int_{x_1}^{x_2}\sqrt{2m[V(x)-E]}dx &= \sqrt{2m}\int_0^{x_2}\sqrt{-E-qFx}dx \\
&= \sqrt{2m}|E|^{\frac{1}{2}}\int_0^{x_2}\left[1-\frac{qFx}{|E|}\right]^{\frac{1}{2}}dx \\
&= \sqrt{2m}|E|^{\frac{1}{2}}\left[\frac{qF}{|E|}\right]^{-1}\int_0^1[1-y]^{\frac{1}{2}}dy \\
&= \sqrt{2m}|E|^{\frac{3}{2}}\frac{1}{qF}\frac{2}{3}. \qquad (8)
\end{aligned}$$

The tunneling aomplitude is

$$\exp\left(-\frac{1}{\hbar}\sqrt{2m}|E|^{\frac{3}{2}}\frac{1}{qF}\frac{2}{3}\right) \tag{22}$$

and the tunneling probabiity is its square:

$$\exp\left(-\frac{4}{3qF}\sqrt{\frac{2m}{\hbar^2}}|E|^{\frac{3}{2}}\right) \tag{23}$$

In the ground state $E = -V_0$ so that we have

$$\exp\left(-\frac{4}{3qF}\sqrt{\frac{2m}{\hbar^2}}V_0^{\frac{3}{2}}\right) \tag{24}$$

This agrees with our dimensional analysis.