

1. Using the test wavefunction

$$\psi(x) = A \exp[-bx^2],$$

obtain the lowest upper-bound you can on the ground-state energies associated with the following one-dimensional potential energies.

(a) $V(x) = \alpha|x|$.

(b) $V(x) = \alpha x^4$.

The normalization constant, A , is given by Griffiths Equation 8.3,

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

Then,

$$\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} \exp[-bx^2].$$

The expectation value of kinetic energy, $\langle T \rangle$, is independent of the potential energy function and can be found in general for a given test wavefunction. For the test wavefunction given, the expectation value of kinetic energy is given by Griffiths Equation 8.5,

$$\langle T \rangle = \frac{\hbar^2 b}{2m}.$$

The expectation value for total energy, $\langle H \rangle$, is given by Griffiths Equation 8.4,

$$\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 b}{2m} + \langle V \rangle,$$

where Griffiths Equation 8.5 was substituted.

(a) The expectation value of potential energy, $\langle V \rangle$, is given by

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^* V \psi \, dx = \sqrt{\frac{2b}{\pi}} \alpha \int_{-\infty}^{\infty} |x| e^{-2bx^2} \, dx.$$

The integrand is symmetric about $x = 0$; that is,

$$\langle V \rangle = 2\alpha \sqrt{\frac{2b}{\pi}} \int_0^{\infty} x e^{-2bx^2} \, dx.$$

$\langle V \rangle$ is of the form of Equation 8 on the class Integral Table,

$$\int_0^{\infty} x^m e^{-ax^2} \, dx = \frac{\Gamma\left(\frac{m+1}{2}\right)}{2a^{\frac{m+1}{2}}},$$

where $a = 2b$ and $m = 1$. Then,

$$\langle V \rangle = 2\alpha \sqrt{\frac{2b}{\pi}} \frac{1}{4b} = \frac{\alpha}{\sqrt{2b\pi}}.$$

The expectation value of total energy is then

$$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2b\pi}}.$$

To minimize with respect to b we first take the derivative with respect to b ,

$$\frac{d}{db} \langle H \rangle = \frac{\hbar^2}{2m} - \frac{1}{2} \frac{\alpha}{\sqrt{2\pi}} b^{-3/2}.$$

The minimum value is given by solutions to

$$\frac{d}{db} \langle H \rangle = 0.$$

This is satisfied for

$$b = \left(\frac{m\alpha}{\hbar^2 \sqrt{2\pi}} \right)^{2/3}.$$

The minimum expectation value of total energy is given by substituting the minimized value of b ,

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m} \left(\frac{m\alpha}{\hbar^2 \sqrt{2\pi}} \right)^{2/3} + \frac{\alpha}{\sqrt{2\pi}} \sqrt{\frac{1}{\left(\frac{m\alpha}{\hbar^2 \sqrt{2\pi}} \right)^{2/3}}} = \frac{3}{2} \left(\frac{\alpha^2 \hbar^2}{2\pi m} \right)^{1/3}.$$

Finally,

$$\frac{3}{2} \left(\frac{\alpha^2 \hbar^2}{2\pi m} \right) \geq E_{\text{gs}}.$$

(b) The expectation value of potential energy, $\langle V \rangle$, is given by

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^* V \psi \, dx = \alpha \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} x^4 e^{-2bx^2} \, dx.$$

Like in part (a), this integrand is symmetric about $x = 0$,

$$\langle V \rangle = 2\alpha \sqrt{\frac{2b}{\pi}} \int_0^{\infty} x^4 e^{-2bx^2} \, dx.$$

Also like in part (a), $\langle V \rangle$ is of the form of Equation 8 of the class Integral Table where $a = 2b$ and $m = 4$. Then, with Γ as the Gamma-function,

$$\langle V \rangle = 2\alpha \sqrt{\frac{2b}{\pi}} \frac{\Gamma\left(\frac{5}{2}\right)}{2(2b)^{5/2}} = 2\alpha \sqrt{\frac{2b}{\pi}} \frac{\frac{3\sqrt{\pi}}{4}}{2(2b)^{5/2}} = \frac{3\alpha}{16b^2}.$$

The expectation value of total energy is then

$$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}.$$

The minimum value of $\langle H \rangle$ is given by solutions to

$$\frac{d}{db} \langle H \rangle = 0,$$

where

$$\frac{d}{db} \langle H \rangle = \frac{\hbar^2}{2m} - \frac{3\alpha}{8} b^{-3}.$$

This is satisfied for

$$b = \left(\frac{3\alpha m}{4\hbar^2} \right)^{1/3}.$$

Then,

$$\langle H \rangle_{\min} = \frac{\hbar^2}{2m} \left(\frac{3\alpha m}{4\hbar^2} \right)^{1/3} + \frac{3\alpha}{16} \left(\frac{3\alpha m}{4\hbar^2} \right)^{-2/3} = \frac{3}{4} \left(\frac{3\alpha \hbar^4}{4m^2} \right)^{1/3}.$$

Finally,

$$\frac{3}{4} \left(\frac{3\alpha \hbar^4}{4m^2} \right)^{1/3} \geq E_{\text{gs}}.$$

2. Use the WKB approximation to determine the allowed energies, E_n , of an infinite-square well with a “shelf” of height V_0 extending half-way across,

$$V(x) = \begin{cases} V_0, & 0 < x < a/2, \\ 0, & a/2 < x < a, \\ \infty, & \text{else.} \end{cases}$$

Express the solution in terms of V_0 and E_n^0 , the energy for the n th state of the infinite-square well. Assume that $E_1^0 > V_0$, but do not assume $E_n \gg V_0$.

Response.

Use the WKB approximation result for transmission probability,

$$T \approx e^{-2\gamma},$$

where

$$\gamma \equiv \frac{1}{\hbar} \int_0^a |p(x)| \, dx,$$

to compute the approximate transmission probability for a particle with energy E that encounters a finite-square barrier with height $V_0 > E$ and width $2a$. Compare the solution to the exact result,

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left(\frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right),$$

which should reduce to the solution in the WKB regime where $T \ll 1$.

Response.