

## 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,

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

(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  $\Gamma$  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  $E_n \gg V_0$ .

Equation 9.17 gives the quantization condition which can be solved to determine the approximate allowed energies,

$$\int_0^a p(x) dx = n\pi\hbar, \quad n \in \mathbb{N},$$

where  $p(x)$  is given by Equation 9.2 to be

$$p(x) = \sqrt{2m(E - V(x))}.$$

Substituting our potential energy function yields

$$\int_0^{a/2} \sqrt{2mE} dx + \int_{a/2}^a \sqrt{2m(E - V_0)} dx = n\pi\hbar.$$

Both integrands are constants so are evaluated simply as

$$\frac{a}{2} \sqrt{2mE} + \frac{a}{2} \sqrt{2m(E - V_0)} = n\pi\hbar.$$

Then,

$$\sqrt{E} + \sqrt{E - V_0} = \sqrt{\frac{2}{m} \frac{n\pi\hbar}{a}}.$$

Equation 2.30 gives the energy levels of the infinite square well to be

$$E_n^0 = \frac{n^2 \pi^2 \hbar^2}{2ma^2}.$$

Then,

$$\sqrt{E} + \sqrt{E - V_0} = 2\sqrt{E_n^0}.$$

To solve for the allowed energies,  $E$ , both sides must be squared twice and arranged.

Indexed by the quantum number  $n$ , the allowed energies  $E_n$  are given by

$$E_n = E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0}.$$

3. 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.