1. Using the test wavefunction

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

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,

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

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

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

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

$$\langle V\rangle = 2\alpha\sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} x e^{-2bx^2}\,\mathrm{d}x.$$

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

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

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,

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

The minimum value is given by solutions to

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

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,

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

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

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

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

$$\langle V \rangle = 2\alpha \sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} x^4 e^{-2bx^2} \, \mathrm{d}x.$$

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

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

where

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

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,

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

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 nth 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,

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

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

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

Substituting our potential energy function yields

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

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

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

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 $T \ll 1$.

$p(x)$ is given by Griffiths Equation 9.3,

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

Substituting given values yields

$$p(x) = \sqrt{2m(E - V_0)} = i\sqrt{2m(V_0 - E)},$$

which is notably a constant in x and whose absolute value simply eliminates the i. Thus, γ is found as

$$\gamma = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}.$$

Then,

$$T \approx \exp\left[-\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right].$$

The exact result may be expressed as

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\gamma).$$

Then, $T \ll 1$ corresponds to the right hand side being much greater than one, in particular $\gamma \gg 1$. Then,

$$T^{-1} \approx \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\gamma).$$

The hyperbolic sine function may be expressed in terms of exponential functions,

$$\sinh(x) = \frac{e^x - e^{-x}}{2}.$$

Since $\gamma \gg 1$ we neglect the $e^{-\gamma}$ term and say

$$\sinh(\gamma) \approx \frac{1}{2}e^{\gamma}.$$

Then,

$$T^{-1} \approx \frac{V_0^2}{16E(V_0 - E)}e^{2\gamma}.$$

The leading coefficient is not significant compared to the exponential; therefore,

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

as expected.