PHYS 4301
Homework 4

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1. Find an approximate variational solution to the ground state of a particle of mass m exposed to the quartic potential (1). Use the trivial wave function (2) to find which value of the variational parameter α minimizes the expectation value of the total energy. How do the expectation values of the kinetic and potential energy compare in this variational solution?

$$V(x) = \lambda x^4,\ \lambda > 0 \tag{1}$$

$$\psi(x) \propto e^{-\frac{\alpha x^2}{2}} \tag{2}$$

$$\begin{aligned}
\psi(x) &= Ae^{-\frac{-\alpha x^2}{2}} \\
\int_{-\infty}^{\infty} |A|^2 e^{\frac{-\alpha x^2}{2}} dx &= 1 \\
|A|^2 \sqrt{\frac{\pi}{\alpha}} &= 1 \\
A &= \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} \\
\psi(x) &= \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{-\alpha x^2}{2}} \text{ (normalized)} \\
E(\alpha) &= \langle \psi | H | \psi \rangle \\
&= \langle \psi | T | \psi \rangle + \langle \psi | V | \psi \rangle \\
&= \langle T \rangle + \langle V \rangle = E(T) + E(V)
\end{aligned}$$

$$\begin{aligned}
\langle V \rangle &= \int_{-\infty}^{\infty} \psi^* V \psi dx \\
&= \lambda \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x^4 e^{-\alpha x^2} dx \\
&= 2\lambda \sqrt{\frac{\alpha}{\pi}} \int_{0}^{\infty} x^4 e^{-\alpha x^2} dx \\
&= 2\lambda \sqrt{\frac{\alpha}{\pi}} \frac{3}{8\alpha^2} \sqrt{\frac{\pi}{\alpha}} = \boxed{\frac{3\lambda}{4\alpha^2}}
\end{aligned}$$

$$
\begin{aligned}
\langle T \rangle &= \int_{-\infty}^{\infty} \psi^{*}(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} e^{-\frac{\alpha x^2}{2}} \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m} \frac{d}{dx} \left(-\frac{\alpha}{2} (2x)\, e^{-\frac{\alpha x^2}{2}} \right) \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m} \left(-\alpha \left(e^{-\frac{\alpha x^2}{2}} - \alpha x^2 e^{-\frac{\alpha x^2}{2}} \right) \right) \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m} \left(-\alpha e^{-\frac{\alpha x^2}{2}} + \alpha^2 x^2 e^{-\frac{\alpha x^2}{2}} \right) \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \left(-\frac{\hbar^2}{2m} \left(\alpha^2 x^2 - \alpha \right) e^{-\frac{\alpha x^2}{2}} \right) dx \\
&= \sqrt{\frac{\alpha}{\pi}} \left(\frac{\hbar^2 \alpha}{2m} \int_{-\infty}^{\infty} e^{-\alpha x^2 dx} - \frac{\hbar^2 \alpha^2}{2m} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx \right) \\
&= \sqrt{\frac{\alpha}{\pi}} \left(\frac{\hbar^2 \alpha}{2m} \sqrt{\frac{\pi}{\alpha}} - \frac{\hbar^2 \alpha^2}{2m} \int_{0}^{\infty} x^2 e^{-\alpha x^2} dx \right) = \sqrt{\frac{\alpha}{\pi}} \left(\frac{\hbar^2 \alpha}{2m} \sqrt{\frac{\pi}{\alpha}} - \frac{\hbar^2 \alpha^2}{2m} \left[\frac{1}{4\alpha} \right] \right) \\
&= \frac{\hbar^2 \alpha}{2m} - \sqrt{\frac{\alpha}{\pi}} \frac{\hbar^2 \alpha^2}{m} \sqrt{\frac{\pi}{\alpha}} \frac{1}{4\alpha} = \frac{\hbar^2 \alpha}{2m} - \frac{\hbar^2 \alpha^2}{4m\alpha} = \boxed{\frac{\hbar^2 \alpha}{4m}}
\end{aligned}
$$

$$
E(\alpha) = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 \alpha}{4m} + \frac{3\lambda}{4\alpha^2}
$$

To minimize,

$$
\begin{aligned}
\frac{\partial \langle E \rangle}{\partial \alpha} = \frac{\hbar^2}{4m} - 2\frac{3\lambda}{4x^3} &= 0 \\
\frac{\hbar^2}{4m} - \frac{3\lambda}{2x^3} &= 0 \\
\frac{\hbar^2}{4m} &= \frac{3\lambda}{2\alpha^3} \\
\alpha^3 &= \frac{6m\lambda}{\hbar^2} \\
\alpha &= \left(\frac{6m\lambda}{\hbar^2} \right)^{\frac{1}{3}} \text{ minimizes } E(\alpha)
\end{aligned}
$$

To compute the optimal value of the ground state of the particle:

$$
\begin{aligned}
E_0(\alpha) &= \frac{\hbar^2}{4m}\left(\frac{6m\lambda}{\hbar^2}\right)^{\frac{1}{3}} + \frac{3\lambda}{4}\left(\frac{\hbar^2}{6m\lambda}\right)^{\frac{2}{3}} \\
&= \frac{\hbar^{\frac{4}{3}}\lambda^{\frac{1}{3}}}{m^{\frac{2}{3}}}\left(\frac{6^{\frac{1}{3}}}{4} + \frac{3}{4\cdot 6^{\frac{2}{3}}}\right) \\
&\approx 0.681\left(\frac{\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}
\end{aligned}
$$

Expectation of kinetic energy is given by $\langle T\rangle = \frac{\hbar^2}{4m}\left(\frac{6m\lambda}{\hbar^2}\right)^{\frac{1}{3}} = \frac{6^{\frac{1}{3}}}{4}\left(\frac{\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}$.

Expection of potential energy is given by $\langle V\rangle = \frac{3\lambda}{J}4\left(\frac{\hbar^2}{6m\lambda}\right)^{\frac{2}{3}} = \frac{3}{4\cdot 6^{\frac{2}{3}}}\left(\frac{\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}$

$\langle T\rangle/\langle V\rangle = \frac{6}{3} = 2 \longrightarrow \boxed{\langle T\rangle = 2\langle V\rangle}$

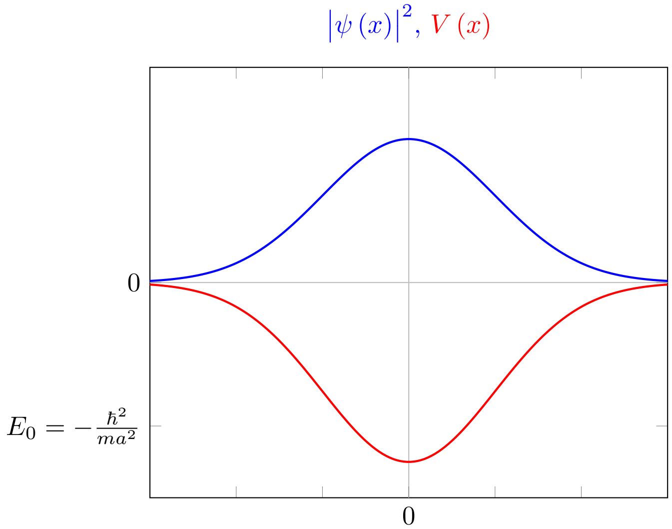
2. You are given the ground-state wave function $\psi_0(x)$ of a particle of mass m in an unknown potential $V(x)$

$$
\psi_0(x) \propto \frac{1}{cosh\left(\frac{x}{a}\right)} \tag{3}
$$

a) Given that the potential vanishes at infinity, find the potential $V(x)$ as well as the energy E_0 of the ground state, using the stationary Schrödinger equation directly

$$
\begin{aligned}
\psi_0(x) &= Asech\left(\frac{x}{a}\right),\ a>0 \\
\hat{H}_0\psi_0 &= E_0\psi_0 = -\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2} + V(x)\psi_0(x) \\
&= \left(-\frac{\hbar^2}{2m}\right)\frac{d\psi_0}{dx}\left(-Asech\left(\frac{x}{a}\right)tanh\left(\frac{x}{a}\right)\frac{1}{a}\right) + V(x)\psi_0(x) \\
&= \left(-\frac{\hbar^2}{2m}\right)\left(-\frac{A}{a}\right)\left(-sech\left(\frac{x}{a}\right)tanh^2\left(\frac{x}{a}\right)\frac{1}{a} + \frac{1}{a}sech\left(\frac{x}{a}\right)sech^2\left(\frac{x}{a}\right)\right) + V(x)\psi_0(x) \\
&= \left(-\frac{\hbar^2}{2m}\right)\left(\frac{A}{a^2}sech\left(\frac{x}{a}tanh^2\left(\frac{x}{a}\right) - \frac{A}{a^2}sech\left(\frac{x}{a}\right)sech^2\left(\frac{x}{a}\right)\right)\right) + V(x)\psi_0(x) \\
&= \left(-\frac{\hbar^2}{2m}\right)\left(tanh^2\left(\frac{x}{a} - sech^2\left(\frac{x}{a}\right)\right)\right)Asech\left(\frac{x}{a}\right) + V(x)\psi_0(x) \\
&= \left(-\frac{\hbar^2}{2m}\right)\left(tanh^2\left(\frac{x}{a} - sech^2\left(\frac{x}{a}\right)\right)\right)\psi_0(x) - \frac{\hbar^2}{ma^2}sech^2\left(\frac{x}{a}\right)\psi_0(x) \\
&= -\frac{\hbar^2}{2ma^2}\left(tanh^2\left(\frac{x}{a}\right) - sech^2\left(\frac{x}{a}\right) + 2sech^2\left(\frac{x}{a}\right)\right)\psi_0(x) \\
&= -\frac{\hbar^2}{2ma^2}\left(tanh^2\left(\frac{x}{a}\right) + sech^2\left(\frac{x}{a}\right)\right)\psi_0(x) = -\frac{\hbar^2}{2ma^2}\psi_0(x) \rightarrow \boxed{E_0 = -\frac{\hbar^2}{2ma^2}}
\end{aligned}
$$

b) The potential that you found has a minimum. The behavior of the potential "near" the minimum is approximated by a parabolic behavior. Perform this approximation for the found potential $V(x)$ and then find the resulting frequency ω of classical oscillations. You can now evaluate energy E of the ground state in this approximation. Sketch the behavior of the potential and its parabolic (harmonic) approximation and indicate positions of energies E_0 and E on the sketch



When close to the origin,

$$V(x) = -\frac{\hbar}{ma^2} sech^2\left(\frac{x}{a}\right)$$

$$\omega = \sqrt{\frac{k}{m}}$$

$$k = \frac{d^2V(x)}{dx^2} = \frac{\hbar^2}{ma^4} sech^4\left(\frac{x}{a}\right)$$

$$\omega = \boxed{\frac{\hbar}{a^2}}$$

$$E = \frac{1}{2}\hbar\omega = \boxed{\frac{1}{2}\frac{\hbar^2}{a^2} sech^2\left(\frac{x}{a}\right)}$$