PHYS 661 - Quantum Mechanics II

Modern Quantum Mechanics by *J. J. Sakurai*

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Homework 3

Problem 1 - Variational Principle

In this problem you will learn the variational principle (see Sakurai Sec. 5.4 for more details) and apply it to the case of a double-well potential. The basic idea is that a guess $|\psi\rangle$ for the ground state of a Hamiltonian H satisfies $\langle\psi|H|\psi\rangle \geq E_0$, where E_0 is the exact ground state energy and $|\psi\rangle$ is assumed to be normalized. We can try to minimize $\langle\psi|H|\psi\rangle$ (and improve our bound on E_0) by taking derivative w.r.t. a parameter β in the guess state: $\partial_\beta \langle\psi(\beta)|H|\psi(\beta)\rangle = 0$.

1. Consider a 1D Harmonic oscillator Hamiltonian $H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega_0^2 x^2$. Find the energy $E(\beta) = \langle\psi|H|\psi\rangle$ and its minimum value $E(\beta_*)$ for the following variational wave functions. Interpret your results.

   (a) $\psi_a(x,\beta) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \exp\left(-\beta x^2\right)$

   (b) $\psi_b(x,\beta) = \begin{cases} \left(\frac{15}{16}\right)^{\frac{1}{4}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right), & |x| < \beta^{-\frac{1}{2}}, \\ 0, & |x| > \beta^{-\frac{1}{2}}. \end{cases}$

2. Let us consider the double well potential with Hamiltonian $H = \frac{p_x^2}{2m} + \frac{1}{2}m\frac{1}{4}\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)^2$

   (a) Using $\psi_1 = \left(\frac{2\beta}{\pi}\right)^{1/4} \exp\left(-\beta(x-a)^2\right)$, find $E_1(\beta) = \langle\psi_1| H |\psi_1\rangle$. Minimizing $E_1(\beta)$ is in general cumbersome, but show that for large a, the minimum is given by $\beta_* = \frac{m\omega_0}{2\hbar}$. Find $E_1(\beta_*)$ and comment on your result.

   (b) Use now instead $\psi_2 = A\left[\exp\left(-\beta(x-a)^2\right) + \exp\left(-\beta(x+a)^2\right)\right]$. Find the normalization constant A. Evaluate $E_2(\beta) = \langle\psi_2| H |\psi_2\rangle$. Minimizing E_2 in this case is hopeless to do analytically. However, by using the above value $\beta_* = \frac{m\omega_0}{2\hbar}$, find the difference $E_2(\beta_*) - E_1(\beta_*)$ in the limit of large a and comment on your result.

Solution. 1. (a) Notice that

$$|\psi_a\rangle = \langle\psi_a| = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2}.$$

Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle \psi_a | H | \psi_a \rangle \\
&= \int_{-\infty}^{\infty} \psi_a^* H \psi_a \, \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2} \left(\frac{p_x^2}{2m} + \frac{1}{2} m\omega_0^2 x^2\right) \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta x^2} \, \mathrm{d}x \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[\frac{1}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(p_x^2\right) \mathrm{e}^{-\beta x^2} \, \mathrm{d}x + m\omega_0^2 \int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(x^2\right) \mathrm{e}^{-\beta x^2} \, \mathrm{d}x\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \frac{\partial^2}{\partial x^2}\left(\mathrm{e}^{-\beta x^2}\right) \mathrm{d}x + m\omega_0^2 \int_{-\infty}^{\infty} x^2 \mathrm{e}^{-2\beta x^2} \, \mathrm{d}x\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{\hbar^2}{m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta x^2} \left(2\beta(2\beta x^2 - 1)\mathrm{e}^{-\beta x^2}\right) \mathrm{d}x + m\omega_0^2 \left(\frac{\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right)\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{2\beta\hbar^2}{m}\int_{-\infty}^{\infty} \left(2\beta x^2 - 1\right) \mathrm{e}^{-2\beta x^2} \, \mathrm{d}x + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[-\frac{2\beta\hbar^2}{m}\left(-\frac{\sqrt{\pi}}{2^{\frac{3}{2}}\sqrt{\beta}}\right) + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{1}{2}\left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}} \left[\frac{\hbar^2\sqrt{\beta\pi}}{\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{5}{2}}\beta^{\frac{3}{2}}}\right] \\
&= \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}.
\end{aligned}$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}\right) &= 0 \\
\frac{\hbar^2}{2m} - \frac{m\omega_0^2}{8\beta^2} &= 0 \\
\beta^2 &= \frac{m^2\omega_0^2}{4\hbar^2} \\
\beta &= \pm\sqrt{\frac{m^2\omega_0^2}{4\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \frac{m\omega_0}{2\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} \\
&= \frac{\hbar^2}{2m}\left(\frac{m\omega_0}{2\hbar}\right) + \frac{m\omega_0^2}{8}\left(\frac{2\hbar}{m\omega_0}\right) \\
&= \frac{\hbar\omega_0}{4} + \frac{\hbar\omega_0}{4} \\
&= \frac{\hbar\omega_0}{2}.
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}, \qquad E(\beta_*) = \frac{\hbar\omega_0}{2}.$$

(b) Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_b|H|\psi_b\rangle \\
&= \int_{-\infty}^{\infty} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= \int_{-\beta^{-\frac{1}{2}}}^{\beta^{-\frac{1}{2}}} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= 2\int_{0}^{\beta^{-\frac{1}{2}}} \psi_b^* H \psi_b \,\mathrm{d}x \\
&= 2\int_{0}^{\beta^{-\frac{1}{2}}} \left(\frac{15}{16}\right)^{\frac{1}{2}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right) \left(\frac{p_x^2}{2m} + \frac{1}{2}m\omega_0^2 x^2\right) \left(\frac{15}{16}\right)^{\frac{1}{2}} \beta^{\frac{1}{4}} \left(1-\beta x^2\right) \mathrm{d}x \\
&= \frac{15\sqrt{\beta}}{8}\left[\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)\left(\frac{p_x^2}{2m}\right)\left(1-\beta x^2\right)\mathrm{d}x + \int_{0}^{\beta^{-\frac{1}{2}}} \left(\frac{1}{2}m\omega_0^2 x^2\right)\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)\frac{\partial^2}{\partial x^2}\left(1-\beta x^2\right)\mathrm{d}x + \frac{1}{2}m\omega_0^2\int_{0}^{\beta^{-\frac{1}{2}}} x^2\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\int_{0}^{\beta^{-\frac{1}{2}}} \left(1-\beta x^2\right)(-2\beta)\,\mathrm{d}x + \frac{1}{2}m\omega_0^2\int_{0}^{\beta^{-\frac{1}{2}}} x^2\left(1-\beta x^2\right)^2 \mathrm{d}x\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[-\frac{\hbar^2}{2m}\left(-\frac{4\sqrt{\beta}}{3}\right) + \frac{1}{2}m\omega_0^2\left(\frac{8}{105\beta^{\frac{3}{2}}}\right)\right] \\
&= \frac{15\sqrt{\beta}}{8}\left[\frac{2\sqrt{\beta}\hbar^2}{3m} + \frac{4m\omega_0^2}{105\beta^{\frac{3}{2}}}\right] \\
&= \frac{5\beta\hbar^2}{4m} + \frac{m\omega_0^2}{14\beta}.
\end{aligned}$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{5\beta\hbar^2}{4m} + \frac{1m\omega_0^2}{14\beta}\right) &= 0 \\
\frac{5\hbar^2}{4m} - \frac{m\omega_0^2}{14\beta^2} &= 0 \\
\beta^2 &= \frac{4m^2\omega_0^2}{70\hbar^2} \\
\beta &= \pm\sqrt{\frac{4m^2\omega_0^2}{70\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \sqrt{\frac{2}{35}}\frac{m\omega_0}{\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} \\
&= \frac{\hbar^2}{2m}\left(\sqrt{\frac{2}{35}}\frac{m\omega_0}{\hbar}\right) + \frac{m\omega_0^2}{8}\left(\sqrt{\frac{35}{2}}\frac{\hbar}{m\omega_0}\right) \\
&= \left(\sqrt{\frac{1}{70}} + \sqrt{\frac{35}{128}}\right)\hbar\omega_0
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{5\beta\hbar^2}{4m} + \frac{m\omega_0^2}{14\beta}, \qquad E(\beta_*) = \left(\sqrt{\frac{1}{70}} + \sqrt{\frac{35}{128}}\right)\hbar\omega_0.$$

2. Considering the Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{8}m\omega_0^2 a^2\left(\frac{x^2}{a^2} - 1\right)^2.$$

(a) Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_1|H|\psi_1\rangle \\
&= \int_{-\infty}^{\infty} \psi_1^* H \psi_1 \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta(x-a)^2}\left(\frac{p_x^2}{2m} + \frac{1}{8}m\omega_0^2 a^2\left(\frac{x^2}{a^2}-1\right)^2\right)\left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{1}{2m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta(x-a)^2}\left(p_x^2\right)\mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\int_{-\infty}^{\infty}\mathrm{e}^{-\beta(x-a)^2}\left(\frac{x^2}{a^2}-1\right)^2\mathrm{e}^{-\beta(x-a)^2}\,\mathrm{d}x\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \mathrm{e}^{-\beta(x-a)^2}\frac{\partial^2}{\partial x^2}\left(\mathrm{e}^{-\beta(x-a)^2}\right)\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\int_{-\infty}^{\infty}\left(\frac{x^2}{a^2}-1\right)^2\mathrm{e}^{-2\beta(x-a)^2}\,\mathrm{d}x\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(4\beta^2\left(x-a\right)^2 - 2\beta\right)\mathrm{e}^{-2\beta(x-a)^2}\,\mathrm{d}x + \frac{1}{8}m\omega_0^2a^2\left(\frac{\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{9}{2}}a^4\beta^{\frac{5}{2}}}\right)\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(2\beta x^2 - 1\right)\mathrm{e}^{-2\beta x^2}\,\mathrm{d}x + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[-\frac{\hbar^2}{2m}\left(-\frac{\sqrt{\pi\beta}}{\sqrt{2}}\right) + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{\hbar^2\sqrt{\beta\pi}}{2\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}\left(16a^2\beta+3\right)}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \left(\frac{2\beta}{\pi}\right)^{\frac{1}{2}}\left[\frac{\hbar^2\sqrt{\beta\pi}}{2\sqrt{2}m} + \frac{m\omega_0^2\sqrt{\pi}}{2^{\frac{7}{2}}\beta^{\frac{3}{2}}} + \frac{3m\omega_0^2\sqrt{\pi}}{2^{\frac{15}{2}}a^2\beta^{\frac{5}{2}}}\right] \\
&= \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta} + \frac{3m\omega_0^2}{2^7a^2\beta^2}.
\end{aligned}$$

For large a, the last term will tend to zero, and then

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}.$$

Now, we minimize the energy by setting its derivative with respect to β to 0. We have

$$\begin{aligned}
\frac{\partial E}{\partial \beta} &= 0 \\
\frac{\partial}{\partial \beta}\left(\frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta}\right) &= 0 \\
\frac{\hbar^2}{2m} - \frac{m\omega_0^2}{8\beta^2} &= 0 \\
\beta^2 &= \frac{m^2\omega_0^2}{4\hbar^2} \\
\beta &= \pm\sqrt{\frac{m^2\omega_0^2}{4\hbar^2}} \quad (-\text{rejected}) \\
\beta &= \frac{m\omega_0}{2\hbar} \equiv \beta_*.
\end{aligned}$$

Then, β_* is the variational parameter that minimizes the energy. The minimum value of the energy is then

$$\begin{aligned}
E(\beta_*) &= \frac{\hbar^2\beta_*}{2m} + \frac{m\omega_0^2}{8\beta_*} + \frac{3m\omega_0^2}{2^7a^2\beta_*^2} \\
&= \frac{\hbar^2}{2m}\frac{m\omega_0}{2\hbar} + \frac{m\omega_0^2}{8}\frac{2\hbar}{m\omega_0} + \frac{3m\omega_0^2}{2^7a^2}\left(\frac{2\hbar}{m\omega_0}\right)^2 \\
&= \frac{\hbar\omega_0}{4} + \frac{\hbar\omega_0}{4} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2} \\
&= \frac{\hbar\omega_0}{2} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2}.
\end{aligned}$$

Therefore, for $\psi_a(x,\beta)$, the energy E and its minimum value are

$$E(\beta) = \frac{\hbar^2\beta}{2m} + \frac{m\omega_0^2}{8\beta} + \frac{3m\omega_0^2}{2^7a^2\beta^2}, \qquad E(\beta_*) = \frac{\hbar\omega_0}{2} + \frac{3\hbar^2}{2^5m}\frac{1}{a^2}.$$

(b) We have

$$\psi_2 = A\left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right).$$

Normalizing, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} \left|\psi_2^2\right| \mathrm{d}x &= 1 \\
|A|^2\int_{-\infty}^{\infty}\left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right)^2 \mathrm{d}x &= 1 \\
|A|^2\int_{-\infty}^{\infty}\left(\mathrm{e}^{-2\beta(x-a)^2} + 2\mathrm{e}^{-2\beta(x^2+a^2)} + \mathrm{e}^{-2\beta(x+a)^2}\right) \mathrm{d}x &= 1 \\
|A|^2\left(\frac{\sqrt{2\pi}\,\mathrm{e}^{-2a^2\beta}\left(\mathrm{e}^{2a^2\beta}+1\right)}{\sqrt{\beta}}\right) &= 1 \\
|A|^2 &= \sqrt{\frac{\beta}{2\pi}}\frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
A &= \left(\frac{\beta}{2\pi}\right)^{\frac{1}{4}}\frac{1}{\left(1+\mathrm{e}^{-2a^2\beta}\right)^{\frac{1}{2}}}.
\end{aligned}$$

Replacing, we have

$$\psi_2 = \left(\frac{\beta}{2\pi}\right)^{\frac{1}{4}} \frac{1}{\left(1+\mathrm{e}^{-2a^2\beta}\right)^{\frac{1}{2}}} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right).$$

Computing the energy, we have

$$\begin{aligned}
E(\beta) &= \langle\psi_2|H|\psi_2\rangle \\
&= \int_{-\infty}^{\infty} \psi_2^* H \psi_2 \,\mathrm{d}x \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{p_x^2}{2m} + \frac{1}{8} m\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)\right)^2 \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{p_x^2}{2m}\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x \right.\\
&\quad \left. + \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{1}{8} m\omega_0^2 a^2 \left(\frac{x^2}{a^2} - 1\right)\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \frac{\partial^2}{\partial x^2} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x \right.\\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \left(\frac{x^2}{a^2} - 1\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
&\quad \left[-\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) 2\beta \mathrm{e}^{-2\beta\left(x^2+a^2\right)} \left(2\beta\left(x-a\right)^2 - 1\right) \mathrm{e}^{\beta(x+a)^2} \,\mathrm{d}x \right.\\
&\quad -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right) 2\beta \mathrm{e}^{-2\beta\left(x^2+a^2\right)} \left(2\beta\left(x+a\right)^2 - 1\right) \mathrm{e}^{\beta(x-a)^2} \,\mathrm{d}x \\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \int_{-\infty}^{\infty} \left(\frac{x^2}{a^2} - 1\right) \left(\mathrm{e}^{-\beta(x-a)^2} + \mathrm{e}^{-\beta(x+a)^2}\right)^2 \mathrm{d}x\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \\
&\quad \left[-\frac{\hbar^2}{2m} \left(-\frac{\sqrt{\pi}\sqrt{\beta}}{\sqrt{2}} + \frac{\sqrt{\pi}\sqrt{\beta}\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta}}{\sqrt{2}}\right)\right.\\
&\quad -\frac{\hbar^2}{2m} \left(\frac{\sqrt{\pi}\sqrt{\beta}\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta}}{\sqrt{2}} - \frac{\sqrt{\pi}\sqrt{\beta}}{\sqrt{2}}\right) \\
&\quad \left. + \frac{1}{8} m\omega_0^2 a^2 \left[\frac{\sqrt{\pi}}{2^{\frac{5}{2}} a^2 \beta^{\frac{3}{2}}} + - \frac{\sqrt{\pi}\left(8a^2\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{4a^2\beta^{\frac{3}{2}}} + \frac{\sqrt{\pi}}{2^{\frac{5}{2}} a^2 \beta^{\frac{3}{2}}}\right]\right] \\
&= \sqrt{\frac{\beta}{2\pi}} \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\left[-\frac{\hbar^2}{m}\sqrt{\frac{\pi\beta}{2}} \mathrm{e}^{-2a^2\beta} \left(\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta} - 1\right)\right]\right.\\
&\quad \left. + m\omega_0^2 \left[\frac{\sqrt{\pi}}{2^{\frac{11}{2}}\beta^{\frac{3}{2}}} + - \frac{\sqrt{\pi}\left(8\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{32\beta^{\frac{3}{2}}} + \frac{\sqrt{\pi}}{2^{\frac{11}{2}}\beta^{\frac{3}{2}}}\right]\right] \\
&= \frac{1}{1+\mathrm{e}^{-2a^2\beta}} \left[\left[-\frac{\hbar^2\beta}{m} \mathrm{e}^{-2a^2\beta} \left(\left(4a^2\beta - 1\right)\mathrm{e}^{-2a^2\beta} - 1\right)\right] + \frac{m\omega_0^2}{32\beta} \left[1 + - \frac{\left(8\beta - 1\right)\mathrm{e}^{-4a^2\beta}}{\sqrt{2}}\right]\right] \\
&= \frac{\hbar^2\beta}{m}\left(1 - 2a^2\beta\right) + \frac{m\omega_0^2}{8}\left(a^2 + \frac{1}{2\beta}\right),
\end{aligned}$$

where, for large a, we take $\frac{1}{a}, \mathrm{e}^{-a^2} \to 0$.
By using the value for $\beta_* = \frac{m\omega_0}{2\hbar}$ from part 1, we minimize E_2

$$\begin{aligned} E_2(\beta_*) &= \frac{\hbar^2\beta_*}{m}\left(1 - 2a^2\beta_*\right) + \frac{m\omega_0^2}{8}\left(a^2 + \frac{1}{2\beta_*}\right) \\ &= \frac{\hbar^2}{m}\left(\frac{m\omega_0}{2\hbar}\right)\left(1 - 2a^2\frac{m\omega_0}{2\hbar}\right) + \frac{m\omega_0^2}{8}\left(a^2 + \frac{1}{2}\left(\frac{2\hbar}{m\omega_0}\right)\right) \\ &= \frac{\hbar\omega_0}{2} + \frac{m\omega_0^2 a^2}{2} + \frac{m\omega_0^2 a^2}{8} + \frac{\hbar\omega_0}{8} \\ &= \frac{5\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8}. \end{aligned}$$

In the limit of large a, the difference of the energies is then

$$\begin{aligned} E_2(\beta_*) - E_1(\beta_*) &= \frac{5\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8} - \frac{\hbar\omega_0}{2} \\ &= \frac{\hbar\omega_0}{8} + \frac{3m\omega_0^2 a^2}{8} \\ &= \frac{1}{8}\left(\hbar\omega_0 + \frac{3}{m}\omega_0^2 a^2\right). \end{aligned}$$

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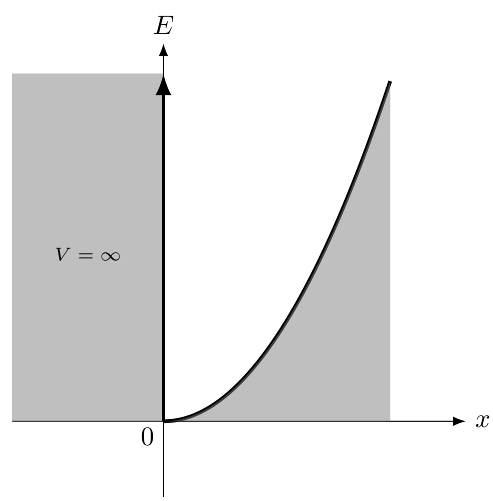
Problem 2 - WKB Approximation
Consider a 1D potential

$$V(x) = \begin{cases} \infty, & x < 0, \\ \frac{1}{2}m\omega_0^2 x^2, & x > 0, \end{cases}$$

i.e. a harmonic trap interrupted by a hard wall. By using the WKB approximation, find the bound state energies.

Solution. The 1D potential given is as follows



The momentum is given by $p(x) = \sqrt{2m(E - V(x))} = \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)}$.

We proceed by finding the turning points. In this case, we only need to find the right turning point. Additionally, the potential is equal to the energy at the turning point. Thus, we have

$$\begin{aligned} V(x) = \frac{1}{2}m\omega_0^2 x^2 = E \\ \implies x^2 = \frac{2E}{m\omega_0^2} \\ x = \pm\sqrt{\frac{2E}{m\omega_0^2}}. \end{aligned}$$

Since $x > 0$, then we reject the negative solution, and we have that $x_1 = 0$ and $x_2 = \sqrt{\frac{2E}{m\omega_0^2}}$. The momentum can then be written as

$$\begin{aligned} p(x) &= \sqrt{2m\left(E - \frac{1}{2}m\omega_0^2 x^2\right)} \\ &= \sqrt{2m\left(\frac{1}{2}m\omega_0^2 x_{2,1}^2 - \frac{1}{2}m\omega_0^2 x^2\right)} \\ &= m\omega\sqrt{(x_2^2 - x^2)}. \end{aligned}$$

Integrating the momentum over the turning points, we get

$$\begin{aligned} \int_a^b p(x')\,\mathrm{d}x' &= m\omega_0 \int_{x_1}^{x_2} \sqrt{x_2^2 - x'^2}\,\mathrm{d}x' \\ &= m\omega_0 \int_0^{x_2} \sqrt{1 - \frac{x'^2}{x_2^2}}\,\mathrm{d}x' \\ &= \frac{\pi m\omega_0 x_2}{4}. \end{aligned}$$

Additionally, we know that

$$\frac{1}{\hbar}\int_b^a p(x')\,\mathrm{d}x = \left(n + \frac{3}{4}\right)\pi \leq 0,$$

then

$$\begin{aligned} \frac{1}{\hbar}\frac{\pi m\omega_0 x_2}{4} &= \left(n + \frac{3}{4}\right)\pi \\ \frac{1}{\hbar}\frac{\pi m\omega_0}{4}\left(\frac{2E}{m\omega_0^2}\right) &= \left(n + \frac{3}{4}\right)\pi \\ m\omega_0\left(\frac{2E}{m\omega_0^2}\right) &= (4n+3)\,\hbar \\ E &= \left(2n + \frac{3}{2}\right)\hbar\omega_0. \end{aligned}$$

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Problem 3 - Wave Function Normalization in Perturbation Theory
In the lectures we chose the perturbed state $|n\rangle$ (with energy E_n) to be such that $\langle n^{(0)}|n\rangle = 1$. Let us define a normalized perturbed state $|n\rangle_N = Z_n^{\frac{1}{2}}|n\rangle$ (see lecture notes Sec. 2.1.1) which satisfies ${}_N\langle n|n\rangle_N = 1$. Show that

$$Z_n = \frac{\partial E_n}{\partial E_n^{(0)}}$$

where $E_n^{(0)}$ is the energy of the unperturbed state $\left|n^{(0)}\right\rangle$.

Solution. The Brillouin-Wigner expansion is given by

$$|n\rangle = \left|n^{(0)}\right\rangle + \sum_{p=0}^{\infty}\left(\frac{\phi_n}{E_n - H_0}\lambda V\right)^p \left|n^{(0)}\right\rangle,$$

where the energy E_n is

$$E_n = E_n^{(0)} + \lambda\sum_{p=0}^{\infty}\left\langle n^{(0)}\middle|V\left(\frac{\phi_n}{En - H_0}\lambda V\right)^p\middle|n^{(0)}\right\rangle.$$

Let $|n\rangle_N = \sqrt{Z_n}\,|n\rangle$ be the normalized perturbed state. By normalization, we have

$${}_N\langle n|n\rangle_N = Z_n\langle n|n\rangle = 1 \implies \langle n|n\rangle = \frac{1}{Z_n}.$$

Computing the inner product using Brillouin-Wigner up to the second-order, we have

$$\begin{aligned}
\langle n|n\rangle &= \left(\left\langle n^{(0)}\right| + \left\langle n^{(0)}\right|\frac{\phi_n}{E_n - H_0}\lambda V\right)\left(\left|n^{(0)}\right\rangle + \lambda V\frac{\phi_n}{E_n - H_0}\left|n^{(0)}\right\rangle\right) \\
&= \left\langle n^{(0)}\middle|n^{(0)}\right\rangle + \lambda\left\langle n^{(0)}\middle|\frac{\phi_n}{E_n - H_0}V\middle|n^{(0)}\right\rangle + \lambda\left\langle n^{(0)}\middle|V\frac{\phi_n}{E_n - H_0}\middle|n^{(0)}\right\rangle + \lambda^2\left\langle n^{(0)}\middle|V\frac{\phi_n^2}{E_n - H_0)^2}V\middle|n^{(0)}\right\rangle \\
&= 1 + \sum_{k\neq n}\frac{\lambda^2|V_{kn}|^2}{(E_n - E_n^{(0)})^2}.
\end{aligned}$$

Thus,

$$Z_n = \left(1 + \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2}\right)^{-1}$$

Using the sum of a geometric series formula, we can see that

$$Z_n = 1 - \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2}$$

Computing the energy up tot he second-order, we have

$$\begin{aligned}
E_n &= E_n^{(0)} + \lambda^2\left\langle n^{(0)}\middle|V\frac{\phi_n}{E_n - H - 0}V\middle|n^{(0)}\right\rangle \\
&= E_n^{(0)} + \lambda^2\sum_{k\neq n}\frac{|V_{nk}|^2}{E_n - E_n^{(0)}}.
\end{aligned}$$

Taking the derivative, we get

$$\frac{\partial E_n}{\partial E_n^{(0)}} = 1 - \lambda^2\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_n^{(0)})^2} = Z_n.$$

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