9.1. Varyasyon ilkesini kullanarak bir boyutlu harmonik salınıcının taban durum enerjisini hesaplayınız.

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Deneme dalga fonksiyonu: $\psi(x) = A e^{-bx^2}$
(Gaussiyen)

b: sabit

• $\psi(x)$'i normalleyelim;

$$1 = \langle\psi|\psi\rangle = \int_{-\infty}^{+\infty} \psi^* \psi \, dx = |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2} dx$$

$$1 = |A|^2 \, 2 \int_0^{\infty} e^{-2bx^2} dx \qquad a^2 = \frac{1}{2b} \qquad a = \frac{1}{\sqrt{2b}} \qquad n=0$$

$$\int_0^{\infty} x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi}\,\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}$$

$$1 = |A|^2 \, 2\sqrt{\pi}\,\frac{(2.0)!}{0!}\left(\frac{1}{2\sqrt{2b}}\right)^{2.0+1} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$$

•

$$E_{td} \leq \langle\psi|H|\psi\rangle = \langle H\rangle \quad \text{olmalı (Varyasyon ilkesi)}$$

$$\langle H\rangle = \langle T\rangle + \langle V\rangle, \qquad \langle T\rangle = -\frac{\hbar^2}{2m}\langle\psi|\frac{d^2}{dx^2}|\psi\rangle$$

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle\psi|x^2|\psi\rangle$$

• $$\langle T\rangle = -\frac{\hbar^2}{2m}\langle\psi|\frac{d^2}{dx^2}|\psi\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}\frac{d^2}{dx^2}\left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2} dx$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{+\infty} e^{-bx^2}\frac{d^2}{dx^2}e^{-bx^2}dx = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{+\infty} e^{-bx^2}\frac{d}{dx}\left(-2xb\,e^{-bx^2}\right)dx$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{+\infty} e^{-bx^2}\left[-2b\left(e^{-bx^2} - 2bx^2 e^{-bx^2}\right)\right]dx$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left[-2b\underbrace{\int_{-\infty}^{+\infty} e^{-2bx^2}dx}_{\substack{n=0,\ a=\frac{1}{\sqrt{2b}} \\ 2\sqrt{\pi}\,\frac{(2\cdot 0)!}{0!}\left(\frac{1}{2\sqrt{2b}}\right)^{2\cdot 0+1}}} + 4b^2\underbrace{\int_{-\infty}^{+\infty} x^2 e^{-2bx^2}dx}_{\substack{n=1,\ a=\frac{1}{\sqrt{2b}} \\ 2\sqrt{\pi}\,\frac{(2\cdot 1)!}{1!}\left(\frac{1}{2\sqrt{2b}}\right)^{2\cdot 1+1}}}\right]$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\left[-2b\sqrt{\pi}\,2\left(\frac{1}{2\sqrt{2b}}\right) + \cancel{4}b^2\sqrt{\pi}\,2\,\frac{\cancel{2}}{1}\,\frac{1}{\cancel{2^3}}\,\frac{1}{(2b)^{3/2}}\right]$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\left[-2b+b\right] = \frac{\hbar^2 b}{2m} \Rightarrow \langle T\rangle = \frac{\hbar^2 b}{2m} \ //$$

- $$\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle = \frac{1}{2}m\omega^2\int_{-\infty}^{+\infty}\left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}x^2\left(\frac{2b}{\pi}\right)^{1/4}e^{-bx^2}dx$$

$$\langle V\rangle = \frac{1}{2}m\omega^2\sqrt{\frac{2b}{\pi}}\underbrace{\int_{-\infty}^{+\infty} x^2 e^{-bx^2}dx}_{I} \qquad \left.\begin{matrix} a=\frac{1}{\sqrt{2b}} \\ n=1\end{matrix}\right\} \ I = 2\sqrt{\pi}\,\frac{(2\cdot 1)!}{1!}\left(\frac{1}{2\sqrt{2b}}\right)^{2\cdot 1+1}$$

$$I = \frac{\sqrt{\pi}}{2}\,\frac{1}{(2b)^{3/2}}$$

$$\langle V\rangle = \frac{1}{2}m\omega^2\sqrt{\frac{2b}{\pi}}\left(\frac{\sqrt{\pi}}{2}\,\frac{1}{(2b)^{3/2}}\right) = \frac{m\omega^2}{8b} \Rightarrow \langle V\rangle = \frac{m\omega^2}{8b} \ //$$

Şimdi, $E_{Td} \leq \langle H\rangle$ denklemine göre, herhangi bir b değeri için enerji E_{Td}'yi geçer, en yakın sınırı bulmak için $\langle H\rangle$'yi b'ye göre türetilip b'nin değerini öyle bir bulalım ki $\langle H\rangle$ minimum olsun.

$$\frac{\partial}{\partial b}\langle H\rangle = 0 \Rightarrow \frac{\partial}{\partial b}\left(\frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}\right) = 0$$

$$0 = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} \Rightarrow b = \frac{m\omega}{2\hbar}$$

$$\Rightarrow \langle H\rangle_{min} = \frac{\hbar^2}{2m}\left(\frac{m\omega}{2\hbar}\right) + \frac{m\omega^2}{8}\left(\frac{\hbar 2}{m\omega}\right) \Rightarrow \langle H\rangle_{min} = \frac{\hbar\omega}{2} \ //$$

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9.2. Varyasyon ilkesini kullanarak delta fonksiyonu potansiyeli için taban durum enerjisini hesaplayınız.

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \left(-\alpha\,\delta(x)\right)$$

Deneme dalga fonksiyonu: $\psi(x) = A e^{-bx^2}$

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\,\delta(x)$$

• $\langle\psi|\psi\rangle = 1$ olmalı; $\quad 1 = \int_{-\infty}^{+\infty} |A|^2 e^{-2bx^2}\,dx \Rightarrow A = \left(\sqrt{\frac{2b}{\pi}}\right)^{1/2} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$

(Ayrıntılı çözüm 9.1.'de var)

• $E_{td} \leq \langle H\rangle \Rightarrow \langle H\rangle = \langle T\rangle + \langle V\rangle = -\frac{\hbar^2}{2m}\langle\psi|\frac{d^2}{dx^2}|\psi\rangle + \langle\psi|V|\psi\rangle$

• $\langle T\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}\frac{d^2}{dx^2}\left(\left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}\right)dx$

$\langle T\rangle = \frac{\hbar^2 b}{2m}$ // (Ayrıntılı çözüm 9.1'de var.)

• $\langle V\rangle = \langle\psi|\left(-\alpha\,\delta(x)\right)|\psi\rangle = -\sqrt{\frac{2b}{\pi}}\,\alpha\int e^{-bx^2}\delta(x)\,e^{-bx^2}\,dx$

$\langle V\rangle = -\alpha\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{+\infty}\delta(x)\,e^{-2bx^2}\,dx \qquad \int f(x)\,\delta(x)\,dx = f(0)$

$\langle V\rangle = -\alpha\sqrt{\frac{2b}{\pi}}\left(e^{-2b\cdot 0}\right) \Rightarrow \langle V\rangle = -\alpha\left(\frac{2b}{\pi}\right)^{1/2}$ //

$\Rightarrow \langle H\rangle = \frac{\hbar^2 b}{2m} - \alpha\left(\frac{2b}{\pi}\right)^{1/2}$

$\frac{d}{db}\langle H\rangle = 0 \Rightarrow \frac{\hbar^2}{2m} - \frac{\alpha}{\sqrt{2\pi b}} = 0 \qquad b = \frac{2m^2\alpha^2}{\pi\hbar^4}$ //

$\langle H\rangle_{min} = \frac{\hbar^2}{2m}\left(\frac{2m^2\alpha^2}{\pi\hbar^4}\right) - \alpha\left(\frac{4m^2\alpha^2}{\pi^2\hbar^4}\right)^{1/2} \Rightarrow \langle H\rangle_{min} = -\frac{m\alpha^2}{\pi\hbar^2}$ //

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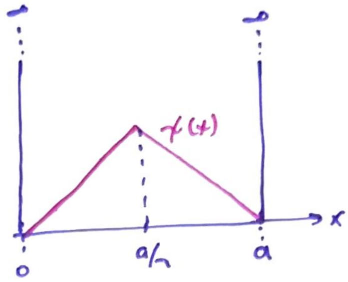
9.3. Aşağıda verilen "üçgen" deneme dalga fonksiyonunu kullanarak, bir boyutlu sonsuz kare kuyu potansiyelinin taban durum enerjisi için bir üst sınır bulunuz.

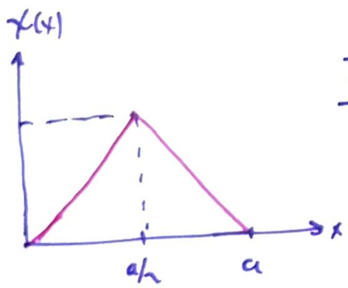
$$\psi(x) = \begin{cases} Ax, & 0 \leq x \leq a/2 \\ A(a-x), & a/2 \leq x < a \\ 0, & \text{diğer yerler} \end{cases}$$



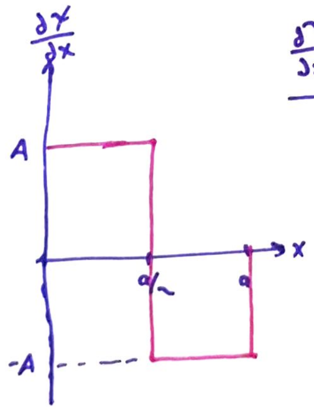
$$1 = \langle \psi | \psi \rangle = \int_0^{a/2} |A|^2 x^2 \, dx + \int_{a/2}^{a} |A|^2 (a-x)^2 \, dx = |A|^2 \left[\frac{x^3}{3} \Big|_0^{a/2} + \left(-\frac{x^3}{3} - \frac{2ax^2}{2} + a^2 x \right) \Big|_{a/2}^{a} \right]$$

$$A = \frac{2}{a}\sqrt{\frac{3}{a}}$$

- $\langle H \rangle = \langle T \rangle + \langle V \rangle = -\frac{\hbar^2}{2m} \langle \psi | \frac{d^2}{dx^2} | \psi \rangle + 0$



$\xrightarrow{\frac{d\psi}{dx}}$



$\xrightarrow{\frac{d^2\psi}{dx^2}}$ Basamak fonksiyonun türevi bir "delta" fonksiyonudur;

$$\frac{d^2\psi}{dx^2} = A\,\delta(x) - 2A\,\delta(x - a/2) + A\,\delta(x-a)$$

$$\langle H \rangle = -\frac{\hbar^2}{2m} A \Big[\underbrace{\int \psi(x)\,\delta(x)\,dx}_{\psi(0)} - 2\underbrace{\int \psi(x)\,\delta(x-a/2)\,dx}_{\psi(a/2)} + \underbrace{\int \psi(x)\,\delta(x-a)\,dx}_{\psi(a)} \Big]$$

$$\langle H \rangle = \frac{12\hbar^2}{2ma^2} < E_{TD}$$

9.4. Varyasyon ilkesini ve Gauss deneme fonksiyonunu kullanarak $V(x) = \alpha |x|$ potansiyeli için taban durumuna gelecek en düşük üst sınırı bulunuz.

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha |x| \quad , \qquad \psi = A e^{-bx^2} \, ,$$

- $$1 = \langle \psi | \psi \rangle = |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2} dx \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4} \rightarrow \psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}$$

- $$E_{tg} \leq \langle H \rangle \rightarrow \langle H \rangle = \langle T \rangle + \langle V \rangle = -\frac{\hbar^2}{2m} \langle \psi | \frac{d^2}{dx^2} | \psi \rangle + \alpha \langle \psi | |x| | \psi \rangle$$

- $\langle T \rangle = \dfrac{\hbar^2 b}{2m}$ (9.1'de ayrıntılı çözüm var.)

- $$\langle V \rangle = \int_{-\infty}^{+\infty} \psi^* \alpha |x| \psi \, dx = 2 \int_0^{\infty} \psi^* x \psi \, dx = 2\alpha \left(\frac{2b}{\pi}\right)^{1/2} \underbrace{\int_0^{\infty} x e^{-2bx^2} dx}_{I}$$

$$I = \int_0^{\infty} x e^{-2bx^2} dx \qquad \int_0^{\infty} x^{2n+1} e^{-x^2/a^2} dx = \frac{n!}{2} a^{2n+2}$$

$$n = 0, \quad a = \frac{1}{\sqrt{2b}}$$

$$I = \frac{0!}{2}\left(\frac{1}{\sqrt{2b}}\right)^{2 \cdot 1 + 2} = \frac{1}{2}\left(\frac{1}{\sqrt{2b}}\right)^4 = \frac{1}{8b^2}$$

$$\langle V \rangle = \frac{\alpha}{(2b\pi)^{1/2}} \; //$$

- $$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2b\pi}} \, , \qquad \frac{d\langle H \rangle}{db} = 0 \Rightarrow \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha \, b^{-3/2}}{\sqrt{2\pi}} = 0$$

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

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