10.1. A normlama sabiti ve b ayarlanabilir bir parametre olmak üzere,

$$\chi(r) = A e^{-br^2}$$

Gauss deneme fonksiyonunu kullanarak, hidrojen atomunun taban durumu için elde edebileceğinizin en düşük sınırı bulunuz.

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{(-e^2)}{4\pi\varepsilon_0}\frac{1}{r}, \qquad \chi(r) = A e^{-br^2}$$

- $$1 = \langle \chi | \chi \rangle = |A|^2 \int e^{-2br^2}\, dV = |A|^2 \int_0^\infty e^{-2br^2} r^2 dr \underbrace{\int_0^\pi \sin\theta\, d\theta}_{2} \underbrace{\int_0^{2\pi} d\phi}_{2\pi}$$

$$1 = |A|^2 4\pi \int_0^\infty e^{-2br^2} r^2 dr \qquad I = \int_0^\infty x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi}\,\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}$$

$$a = \left(\frac{1}{2b}\right)^{1/2},\ n = 1 \qquad I = \sqrt{\pi}\,\frac{(2.1)!}{1!}\left(\frac{1}{2\sqrt{2b}}\right)^{2.1+1} = 2\sqrt{\pi}\,\frac{1}{8}\left(\frac{1}{2b}\right)^{3/2}$$

$$\Rightarrow 1 = |A|^2 \cancel{4}\pi\,\frac{\sqrt{\pi}}{\cancel{4}}\left(\frac{1}{2b}\right)^{3/2}$$

$$A = \left(\frac{2b}{\pi}\right)^{3/4} // \qquad \chi(r) = \left(\frac{2b}{\pi}\right)^{3/4} e^{-br^2}$$

- $$\langle T \rangle = -\frac{\hbar^2}{2m}\langle \chi | \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)|\chi\rangle$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}\left(\frac{2b}{\pi}\right)^{3/2}\int_0^\infty e^{-br^2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)e^{-br^2} r^2 dr \underbrace{\int_0^\pi \sin\theta\, d\theta}_{2}\underbrace{\int_0^{2\pi} d\phi}_{2\pi}$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}\left(\frac{2b}{\pi}\right)^{3/2} 4\pi \int_0^\infty e^{-br^2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)e^{-br^2} r^2 dr$$

$$\langle T \rangle = \frac{3\hbar^2 b}{2m} //$$

- $$\langle V \rangle = \frac{-e^2}{4\pi\varepsilon_0}\int_0^\infty e^{-br^2}\frac{1}{r}e^{-br^2} r^2 dr \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi = -\frac{e^2}{4\pi\varepsilon_0}\, 2\sqrt{\frac{2b}{\pi}} //$$

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$$\langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{3\hbar^2 b}{2m} - \frac{e^2}{4\pi\varepsilon_0}\, 2\sqrt{\frac{2b}{\pi}}$$

$$\frac{d\langle H\rangle}{db} = \frac{3\hbar^2}{2m} - \frac{e^2}{4\pi\varepsilon_0}\sqrt{\frac{2}{\pi}}\,\frac{1}{\sqrt{b}} = 0 \implies b = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{2}{\pi}\left(\frac{2m}{3\hbar^2}\right)^2 //$$

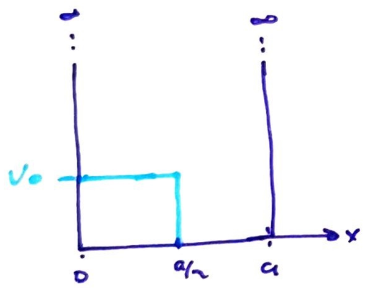
$$\langle H\rangle_{min} = \frac{3\hbar^2}{2m}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{2}{\pi}\left(\frac{2m}{3\hbar^2}\right)^2 - \frac{e^2}{4\pi\varepsilon_0}\, 2\sqrt{\frac{2}{\pi}}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\sqrt{\frac{2}{\pi}}\,\frac{2m}{3\hbar^2}$$

$$= \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m}{\hbar^2}\left(\frac{4}{3\pi} - \frac{8}{3\pi}\right)$$

$$= -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{8}{3\pi} = \frac{8}{3\pi} E_1 = -11,5\ eV$$

$$\langle H\rangle_{min} = -11,5\ eV //$$

10.2.



$$V(x) = \begin{cases} V_0, & 0 \le x \le a/2 \\ 0, & a/2 < x < a \\ \infty, & \text{diğer yerler} \end{cases}$$

Verilen $V(x)$ potansiyeli için izin verilen enerji değerlerini;

a) Pertürbasyon teorisini kullanarak,

b) WKB yaklaşıklığını kullanarak hesaplayınız.

a: Pertürbasyon teorisi ile;

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \qquad H = \underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{H^0} + \underbrace{V(x)}_{H'} \qquad \psi_n^0 = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

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

$$E_n^1 = \int_0^a \psi_n^{0*}\, V(x)\, \psi_n^0\, dx = \int_0^{a/2} \frac{2}{a} V_0 \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$E_n^1 = \frac{2V_0}{a}\int_0^{a/2}\left(\frac{1}{2} - \frac{\cos\left(\frac{2n\pi x}{a}\right)}{2}\right)dx = \frac{2V_0}{a}\left(\frac{a}{4}\right) = \frac{V_0}{2} \rightarrow E_n^1 = \frac{V_0}{2} //$$

$$E_n = E_n^0 + E_n^1 = \frac{\hbar^2\pi^2}{2ma^2}n^2 + \frac{V_0}{2} //$$

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b: WKB ile;

$$\int p(x)\,dx = n\pi\hbar$$

$n = 1, 2, 3 \ldots$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi$$

$$\left(\underbrace{\frac{p^2}{2m} + V(x) - E}_{0}\right)\psi = 0$$

$$\frac{p^2}{2m} = E - V(x) \longrightarrow p(x) = \frac{\left(2m(E-V(x))\right)^{1/2}}{1}$$

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

$$\Rightarrow \int_0^a \left(2m(E-V(x))\right)^{1/2} dx = n\pi\hbar \Rightarrow \int_0^{a/2} \left[2m(E-V_0)\right]^{1/2} dx + \int_{a/2}^{a} \left[2m(E-\cancel{V_0})\right]^{1/2} dx = n\pi\hbar$$

$$\Rightarrow \left[2m(E-V_0)\right]^{1/2} \int_0^{a/2} dx + \left[2mE\right]^{1/2} \int_{a/2}^{a} dx = n\pi\hbar$$

$$\Rightarrow \left[2m(E-V_0)\right]^{1/2} \frac{a}{2} + \left[2mE\right]^{1/2} \frac{a}{2} = n\pi\hbar$$

$$\Rightarrow E + E - V_0 + 2\sqrt{E(E-V_0)} = \frac{4}{2m}\left(\frac{n\pi\hbar}{a}\right)^2 = 4E_n^0$$

$$\Rightarrow 2\sqrt{E(E-V_0)} = (4E_n^0 - 2E + V_0)$$

$$4E(E-V_0) = 4E^2 - 4EV_0 = 16E_n^{0\,2} + 4E^2 + V_0^2 - 16EE_n^0 + 8E_n^0 V_0 - 4EV_0$$

$$\Rightarrow 16EE_n^0 = 16E_n^{0\,2} + 8E_n^0 V_0 + V_0^2 \Rightarrow E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0} = E_n$$

$$\Rightarrow E_n = E_n^0 + \frac{V_0}{2} + \frac{V_0^2}{16E_n^0} \quad //$$

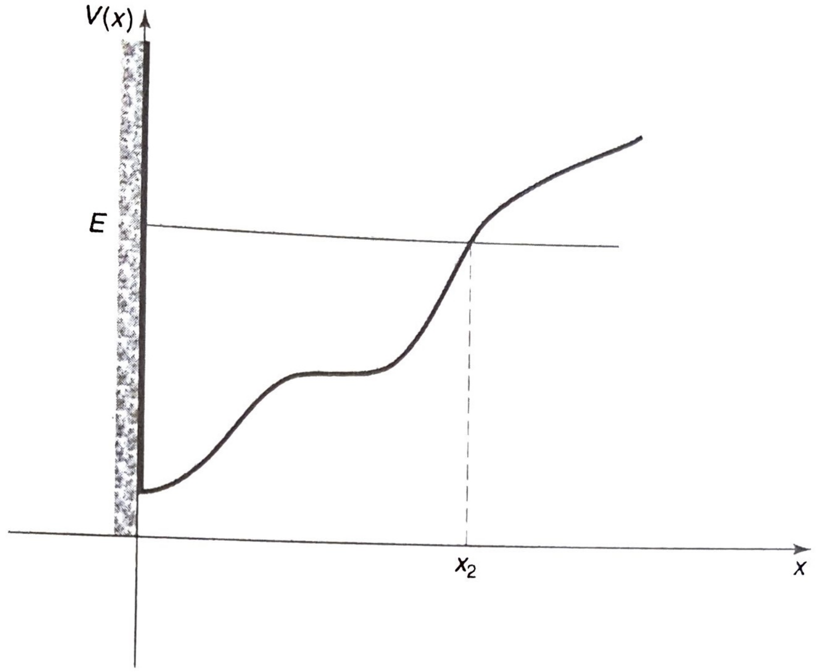
$n = 1, 2, 3$

Örnek 8.3 Tek dik duvarlı potansiyel kuyusu: 8.10 nolu şekil ile verilen potansiyel kuyusunu ele alın: $x = 0$'da dik bir duvar var ve diğer taraf eğimli. Bu durumda $\psi(0) = 0$ olur ve böylece 8.46 nolu denklem

$$\frac{1}{\hbar}\int_0^{x_2} p(x)\,dx + \frac{\pi}{4} = n\pi, \quad (n = 1, 2, 3, \ldots)$$

ya da

$$\boxed{\int_0^{x_2} p(x)\,dx = \left(n - \frac{1}{4}\right)\pi\hbar} \qquad [8.47]$$



ŞEKİL 8.10: Tek dik duvarlı potansiyel kuyusu.

"Yarım harmonik salınıcı" örneğini göz önüne alalım:

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & x > 0 \\ \infty & \text{diğer yerlerde.} \end{cases} \qquad \textbf{[8.48]}$$

Bu durumda

$$p(x) = \sqrt{2m[E - (1/2)m\omega^2 x^2]} = m\omega\sqrt{x_2^2 - x^2}$$

dir ve burada

$$x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

dönüm noktasıdır. Böylece

$$\int_0^{x_2} p(x)\,dx = m\omega\int_0^{x_2}\sqrt{x_2^2 - x^2}\,dx = \frac{\pi}{4}m\omega x_2^2 = \frac{\pi E}{2\omega}$$

olur ve 8.47 nolu denklem ile verilen kuantumlama koşulu

$$E_n = \left(2n - \frac{1}{2}\right)\hbar\omega = \left(\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots\right)\hbar\omega \qquad [8.49]$$

elde edilir. Bu özel durumda WKB yaklaşıklığı aslında izin verilen *kesin* enerji değerlerini verir ve bunlar *tam* olarak harmonik salınıcının *tek* enerji değerleridir. (2.42 nolu probleme bakın).