Domača naloga pri predmetu Kvantna Mehanika I

EHRENFESTOV TEOREM

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1 Naloga

Za elektron v neskončni potencialni jami velja naslednja valovna funkcija:

$$\psi(x,t) = \frac{2}{\sqrt{5}}\,\psi_1(x)\exp\Big(-\frac{iE_1}{\hbar}t\Big) + \frac{1}{\sqrt{5}}\,\psi_2(x)\exp\Big(-\frac{iE_2}{\hbar}t\Big) =$$

$$= \frac{2}{\sqrt{5a}}\,\cos\Big(\frac{\pi}{2}\frac{x}{a}\Big)\exp\Big(-\frac{i\hbar\pi^2}{8ma^2}t\Big) + \frac{1}{\sqrt{5a}}\,\sin\Big(\pi\frac{x}{a}\Big)\exp\Big(-\frac{i\hbar\pi^2}{2ma^2}t\Big).$$

Poznamo še časovno odvisnost poprečnega položaja in gibalne količine:

$$\langle x\rangle = \frac{128a}{45\pi^2}\,\cos\Big(\frac{E_2-E_1}{\hbar}\,t\Big), \tag{1}$$

$$\langle p\rangle = -\frac{16\hbar}{15a}\,\sin\Big(\frac{E_2-E_1}{\hbar}\,t\Big). \tag{2}$$

Tu sta:

$$E_1 = \frac{\pi^2\hbar^2}{8ma^2} \qquad , \qquad E_2 = \frac{\pi^2\hbar^2}{2ma^2}$$

Preveriti moramo, da velja za izraza (1) in (2) Ehrenfestov teorem. Izračunali bomo silo, ki deluje na elektron v jami in spet preverili veljavnost teorema.

2 Reševanje

2.1 Izpeljava teorema

Zanima nas odvod po času pričakovane vrednosti operatorja A.

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\int \psi^*\,A\,\psi\,dx = \int \frac{d}{dt}(\psi^*\,A\,\psi)\,dx = \int \Big(\frac{d\psi^*}{dt}\,A\,\psi + \psi^*\,\frac{dA}{dt}\,\psi + \psi^*\,A\,\frac{d\psi}{dt}\Big)\,dx =$$

$$= \int \Big(\frac{d\psi^*}{dt}\,A\,\psi + \psi^*\,A\,\frac{d\psi}{dt}\Big)\,dx + \int \psi^*\,\frac{dA}{dt}\,\psi\,dx$$

Iz Schrödingerjeve enačbe pa poznamo časovni odvod valovne funkcije:

$$\frac{d\psi}{dt} = -\frac{i}{\hbar} H\psi \qquad , \qquad \frac{d\psi^*}{dt} = \frac{i}{\hbar} H^* \psi^*.$$

$$\frac{d}{dt}\langle A\rangle = \int \Big(\frac{i}{\hbar}\, H^*\psi^*\, A\,\psi + \psi^*\, A\Big(-\frac{i}{\hbar}\Big)H\psi\Big)\,dx + \int \psi^*\,\frac{dA}{dt}\,\psi\,dx =$$

$$= \int \Big(\frac{i}{\hbar}\,\psi^*\, H\, A\,\psi - \frac{i}{\hbar}\psi^*\, A\, H\psi\Big)\,dx + \int \psi^*\,\frac{dA}{dt}\,\psi\,dx = \frac{i}{\hbar}\int \psi^*\,(H\,A - A\,H)\psi\,dx + \int \psi^*\,\frac{dA}{dt}\,\psi\,dx$$

Vpeljemo *komutator* $[A, B] = AB - BA$. To je operacija med dvema operatorjema, ki vrne nov operator. Gornji izraz je torej enak:

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\,\langle\, [H, A]\,\rangle + \Big\langle \frac{dA}{dt}\Big\rangle.$$

2.2 Naša naloga

Poglejmo kaj je odvod povprečne vrednosti lege.

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\,\langle\, [H, x]\,\rangle + \Big\langle \underbrace{\frac{dx}{dt}}_{0} \Big\rangle = \frac{i}{\hbar}\,\langle\, [H, x]\,\rangle \qquad (x \text{ in } t \text{ sta dve neodvisni koordinati}).$$

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) = \frac{p^2}{2m} + V(x)$$

Upoštevali bomo še naslednje zveze:

$$[x, p] = i\hbar \quad , \quad [x, x] = 0 \quad , \quad [f(x), x] = 0 \quad , \quad [AB, C] = A[B, C] + [A, C]B.$$

$$[H, x] = \Big[\frac{p^2}{2m} + V, x\Big] = \Big[\frac{p^2}{2m}, x\Big] + \underbrace{[V(x), x]}_{0} = \frac{p}{2m}[p, x] + [p, x]\frac{p}{2m} = \frac{p}{2m}(-i\hbar) + (-i\hbar)\frac{p}{2m} = -i\hbar\frac{p}{m}$$

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\,\langle\, [H, x]\,\rangle = \frac{i}{\hbar}\Big\langle -i\hbar\frac{p}{m}\Big\rangle = \frac{\langle p\rangle}{m}$$

Torej lahko $\langle p\rangle$ izračunamo po zgornji formuli z uporabo izraza (1).

$$\langle p\rangle = \frac{d\langle x\rangle}{dt}m = -\frac{128am}{45\pi^2}\frac{E_2 - E_1}{\hbar}\,\sin\Big(\frac{E_2 - E_1}{\hbar}\,t\Big) =$$

$$= -\frac{128am}{45\pi^2}\frac{3\pi^2\hbar^2}{8ma^2\hbar}\,\sin\Big(\frac{E_2 - E_1}{\hbar}\,t\Big) = -\frac{16\hbar}{15a}\,\sin\Big(\frac{E_2 - E_1}{\hbar}\,t\Big) \qquad \checkmark$$

To pa je enako izrazu (2).

Sedaj pa izračunamo silo z uporabo Ehrenfestovega teorema.

$$\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\,\langle\,[H,p]\,\rangle + \Big\langle\,\underbrace{\frac{dp}{dt}}_{0}\,\Big\rangle = \frac{i}{\hbar}\,\langle\,[\frac{p^2}{2m}+V,p]\,\rangle \qquad (p \text{ ni eksplicitno odvisno od časa}).$$

$$\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\Big(\Big\langle\underbrace{\Big[\frac{p^2}{2m},p\Big]}_{0}\Big\rangle + \langle\,[V,p]\,\rangle\Big) = \frac{i}{\hbar}\langle\,[V,p]\,\rangle$$

$$[V,p]\psi = -Vi\hbar\frac{\partial}{\partial x}\psi + i\hbar\frac{\partial}{\partial x}(V\psi) = -Vi\hbar\frac{\partial\psi}{\partial x} + i\hbar\frac{\partial V}{\partial x}\psi + i\hbar\frac{\partial\psi}{\partial x}V = i\hbar\frac{\partial V}{\partial x}\psi \quad\Rightarrow\quad [V,p] = i\hbar\frac{\partial V}{\partial x}$$

$$\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\langle\,[V,p]\,\rangle = \frac{i}{\hbar}\,i\hbar\Big\langle\frac{\partial V}{\partial x}\Big\rangle = \Big\langle -\frac{\partial V}{\partial x}\Big\rangle = \langle F\rangle \qquad \text{pričakovana vrednost sile}$$

Izračunamo silo za naš primer:

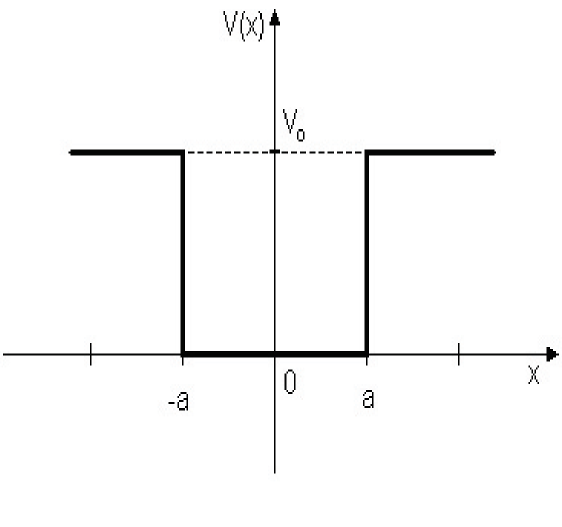
$$\langle F\rangle = \frac{d}{dt}\langle p\rangle = \langle p\rangle = -\frac{16\hbar}{15a}\frac{E_2-E_1}{\hbar}\cos\Big(\frac{E_2-E_1}{\hbar}\,t\Big) = -\frac{16\hbar}{15a}\frac{3\pi^2\hbar^2}{8ma^2\hbar}\cos\Big(\frac{E_2-E_1}{\hbar}\,t\Big).$$

$$\langle F\rangle = -\frac{2\pi^2\hbar^2}{5ma^3}\cos\Big(\frac{E_2-E_1}{\hbar}\,t\Big) \tag{3}$$

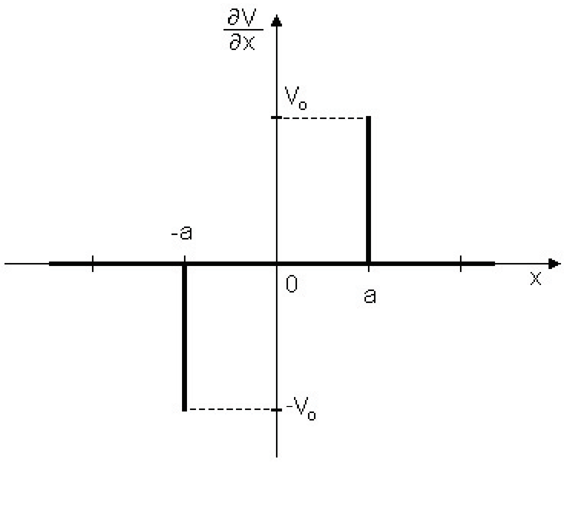
Izpeljali bomo silo za neskočno potencialno jamo še z uporabo integrala in preverili veljavnost izraza (3).

$$\langle F\rangle = \Big\langle -\frac{\partial V}{\partial x}\Big\rangle = \int \psi^*\Big(-\frac{\partial V}{\partial x}\Big)\psi dx$$

Tu pa ne znamo računati naprej ker ima potencial obliko neskončne škatle... Računamo za končno in nato limitiramo višino skoka v neskončnost.



Slika 1: Končna potencialna jama
$V(x) = V_0[\Theta(-a-x) + \Theta(x-a)]$



Slika 2: Odvod potenciala
$\partial V(x)/\partial x = V_0[-\delta(x+a) + \delta(x-a)]$

$$\langle F\rangle = \lim_{V_0\to\infty}\int \psi^* V_0[\delta(x+a)-\delta(x-a)]\psi dx = \lim_{V_0\to\infty} V_0\Big(\int \psi^*\delta(x+a)\psi dx - \int \psi^*\delta(x-a)\psi dx\Big) =$$

$$= \lim_{V_0\to\infty} \underbrace{V_0}_{\to\infty}(\psi^*(-a)\underbrace{\psi(-a)}_{\to 0} - \psi^*(a)\underbrace{\psi(a)}_{\to 0}) \qquad \text{Težave !}$$

Treba bo izračunati še popravek za valovno funkcijo delca v končni potencialni jami. Popravek bomo iskali le do prvega reda.

Ker je potencial simetričen so lastne funkcije sode ali lihe. Videli smo, da osnovnemu stanju ustreza soda funkcija, prvemu vzbujenemu stanju pa liha lastna funkcija. Najprej izračunamo popravek za osnovno stanje.

$$\psi_1(x) = \begin{cases} A\cos kx & ; x\in[-a,a] \\ B\exp(-q(x-a)) & ; x>a \\ B\exp(q(x+a)) & ; x<-a \end{cases}$$

Tu sta:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \text{in} \qquad q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \quad .$$

Zaradi zveznosti funkcije in odvoda v točki a, mora veljati:

$$A\cos ka = B$$

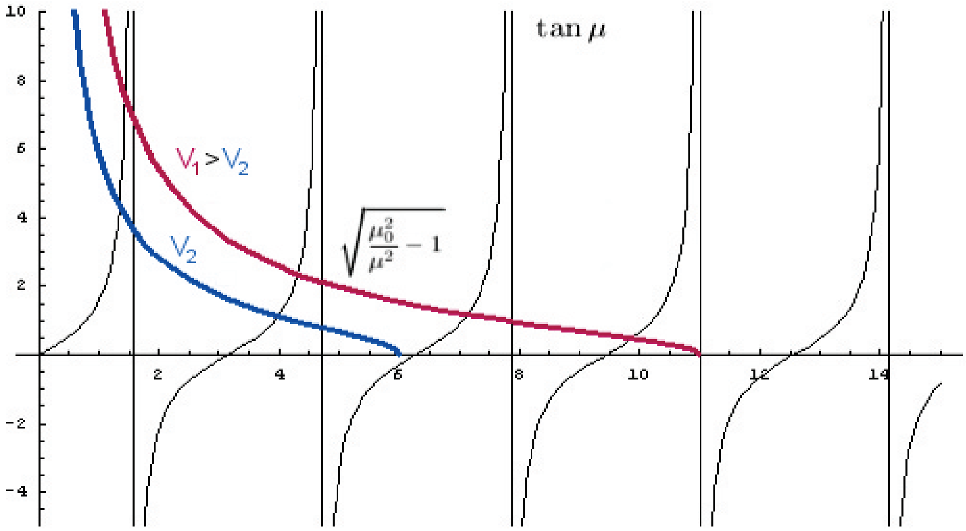
$$-Ak\sin ka = -Bq$$

Enačbi delimo ena z drugo in dobimo trascendentno enačbo:

$$k\tan ka = q \tag{4}$$

Kakor smo še prej storili, vpeljemo oznake μ in μ_0 ter dobimo:

$$\mu = ak = a\sqrt{\frac{2mE}{\hbar^2}} \quad , \quad \mu_0 = ak_0 = a\sqrt{\frac{2mV_0}{\hbar^2}} \qquad \Rightarrow \qquad \tan\mu = \sqrt{\frac{\mu_0^2}{\mu^2}-1}$$



Slika 3: Reševanje trascendentne enačbe $\tan\mu = \sqrt{\frac{\mu_0^2}{\mu^2}-1}$

Iz grafa je razvidno, da osnovnemu stanju ustreza vrednost $\mu \approx \pi/2$. Rekli bomo $\mu = ka = \pi/2 + \varepsilon$ in vstavili v enačbo (4).

$$\tan\mu = \tan ka = \frac{q}{k}$$

$$\tan\mu = \frac{\sin\mu}{\cos\mu} = \frac{\sin\left(\frac{\pi}{2}+\varepsilon\right)}{\cos\left(\frac{\pi}{2}+\varepsilon\right)} = \frac{\sin\left(\frac{\pi}{2}\right) + \varepsilon\cos\left(\frac{\pi}{2}\right) - \frac{\varepsilon^2}{2}\sin\left(\frac{\pi}{2}\right) + \dots}{\cos\left(\frac{\pi}{2}\right) - \varepsilon\sin\left(\frac{\pi}{2}\right) - \frac{\varepsilon^2}{2}\cos\left(\frac{\pi}{2}\right) + \dots} \approx \frac{1}{-\varepsilon}$$

Pri zadnjem koraku smo upoštevali, da je potencial zelo velik in zato je ε zelo blizu ničelni vrednosti.

$$-\varepsilon = \frac{ak}{aq} = \frac{\frac{\pi}{2}+\varepsilon}{aq} \approx \frac{\pi}{2aq}$$

Vpoštevamo še, da velja $E \ll V_0$ in je zato:

$$q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \approx \sqrt{\frac{2mV_0}{\hbar^2}} = k_0 \qquad \Rightarrow \qquad \varepsilon = -\frac{\pi}{2ak_0}$$

Upoštevamo, da je $A = 1/\sqrt{a}$ kot za neskončno jamo. Popravek prvega reda za A bi namreč prispeval v vrednost funkcije popravek drugega reda. Vrednost funkcije v točki a je:

$$\psi_1(a) = \psi_1(-a) = A\cos ka = \frac{1}{\sqrt{a}}\cos\left(\frac{\pi}{2} - \frac{\pi}{2ak_0}\right) = \frac{1}{\sqrt{a}}\sin\left(\frac{\pi}{2ak_0}\right) \approx \frac{1}{\sqrt{a}}\frac{\pi}{2ak_0}$$

Sedaj pa izračunamo popravek za prvo vzbujeno stanje.

$$\psi_2(x) = \begin{cases} A'\sin kx & ; x \in [-a, a] \\ B'\exp(-q(x-a)) & ; x > a \\ -B'\exp(q(x+a)) & ; x < -a \end{cases}$$

Robni pogoji:

$$A' \sin ka = B'$$

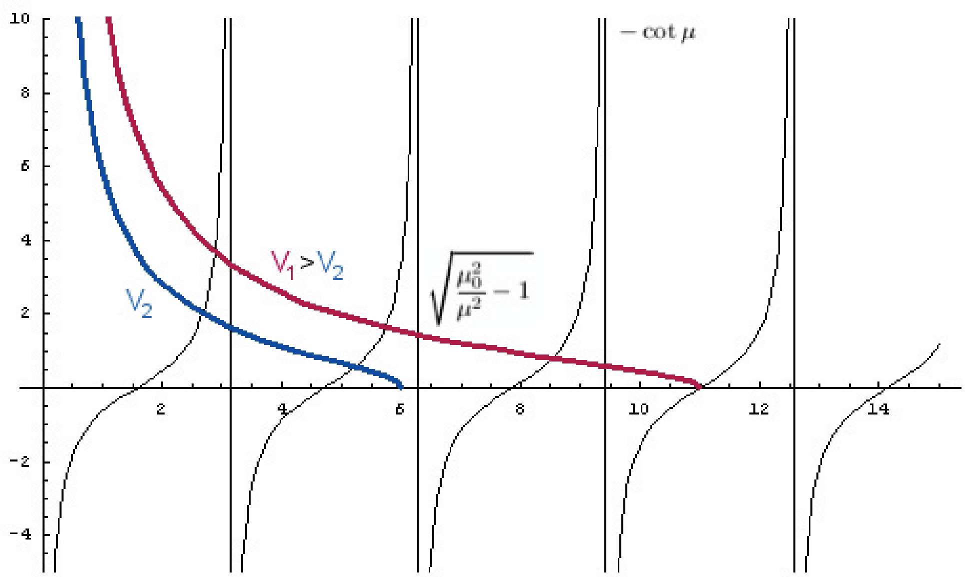
$$A' k \cos ka = -B' q$$

Enačbi delimo ena z drugo in dobimo trascendentno enačbo:

$$k \cot ka = -q \tag{5}$$

Vpeljemo μ in μ_0 kot prej in dobimo:

$$-\cot \mu = \sqrt{\frac{\mu_0^2}{\mu^2} - 1}$$



Slika 4: Reševanje trascendentne enačbe $-\cot \mu = \sqrt{\frac{\mu_0^2}{\mu^2} - 1}$

S pomočjo grafa nastavimo $\mu = ka = \pi + \varepsilon$.

$$\cot \mu = \frac{\cos \mu}{\sin \mu} = \frac{\cos(\pi + \varepsilon)}{\sin(\pi + \varepsilon)} = \frac{\cos \pi - \varepsilon \sin \pi - \frac{\varepsilon^2}{2} \cos \pi + \dots}{\sin \pi + \varepsilon \cos \pi - \frac{\varepsilon^2}{2} \sin \pi + \dots} \approx \frac{1}{\varepsilon}$$

$$\frac{1}{\varepsilon} = -\frac{aq}{ak} = -\frac{aq}{\pi + \varepsilon}$$

$$\varepsilon = -\frac{\pi + \varepsilon}{aq} \approx -\frac{\pi}{aq} \approx -\frac{\pi}{ak_0}$$

Spet upoštevamo $A' = 1/\sqrt{a}$ in dobimo za točko a:

$$\psi_2(a) = -\psi_2(-a) = A' \sin ka = \frac{1}{\sqrt{a}} \sin\left(\pi - \frac{\pi}{ak_0}\right) = \frac{1}{\sqrt{a}} \sin\left(\frac{\pi}{ak_0}\right) \approx \frac{1}{\sqrt{a}} \frac{\pi}{ak_0}$$

Sedaj pa upoštevamo še časovni razvoj.

$$\psi(\pm a,t) = \frac{2}{\sqrt{5}}\,\psi_1(\pm a)\exp\Big(-\frac{iE_1}{\hbar}t\Big) + \frac{1}{\sqrt{5}}\,\psi_2(\pm a)\exp\Big(-\frac{iE_2}{\hbar}t\Big) =$$

$$= \frac{2}{\sqrt{5}}\frac{1}{\sqrt{a}}\frac{\pi}{2ak_0}\exp\Big(-\frac{iE_1}{\hbar}t\Big) \pm \frac{1}{\sqrt{5}}\frac{1}{\sqrt{a}}\frac{\pi}{ak_0}\exp\Big(-\frac{iE_2}{\hbar}t\Big) =$$

$$= \frac{\pi}{\sqrt{5}a\sqrt{a}k_0}\Big(\exp\Big(-\frac{iE_1}{\hbar}t\Big) \pm \exp\Big(-\frac{iE_2}{\hbar}t\Big)\Big)$$

Končno dobimo za silo:

$$\langle F\rangle = \lim_{V_0\to\infty} V_0(\psi^*(-a)\psi(-a) - \psi^*(a)\psi(a)) =$$

$$= \lim_{V_0\to\infty} V_0\Big[\Big(\frac{\pi}{\sqrt{5}a\sqrt{a}k_0}\Big)^2\Big(\exp\Big(\frac{iE_1}{\hbar}t\Big) - \exp\Big(\frac{iE_2}{\hbar}t\Big)\Big)\Big(\exp\Big(-\frac{iE_1}{\hbar}t\Big) - \exp\Big(-\frac{iE_2}{\hbar}t\Big)\Big) -$$

$$-\Big(\frac{\pi}{\sqrt{5}a\sqrt{a}k_0}\Big)^2\Big(\exp\Big(\frac{iE_1}{\hbar}t\Big) + \exp\Big(\frac{iE_2}{\hbar}t\Big)\Big)\Big(\exp\Big(-\frac{iE_1}{\hbar}t\Big) + \exp\Big(-\frac{iE_2}{\hbar}t\Big)\Big)\Big] =$$

$$= \lim_{V_0\to\infty} -2V_0\frac{\pi^2}{5a^3k_0^2}\Big[\Big(\exp\Big(\frac{-i(E_2-E_1)}{\hbar}t\Big) + \exp\Big(\frac{i(E_2-E_1)}{\hbar}t\Big)\Big] =$$

$$= \lim_{V_0\to\infty} -2V_0\frac{\pi^2\hbar^2}{5a^3 2mV_0}2\cos\Big(\frac{E_2-E_1}{\hbar}t\Big) = -\frac{2\pi^2\hbar^2}{5a^3m}\cos\Big(\frac{E_2-E_1}{\hbar}t\Big) \qquad \checkmark$$

To je isti rezultat, ki smo ga dobili z uporabo Ehrenfestovega teorema v enačbi (3).