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Prvi kolokvij 18. 4. 2023.

ZADATAK 1 Razmotrite sustav čija je valna funkcija u $t = 0$ jednaka

$$\Psi(x,0) = \frac{3}{\sqrt{50}}\psi_1(x) + \frac{4}{\sqrt{50}}\psi_2(x) + \frac{1}{\sqrt{6}}\psi_3(x)$$

gdje su $\psi_n(x)$ rješenja stacionarne Schrödingerove jednadžbe za beskonačnu potencijalnu jamu širine a.
(a) Nađite prosječnu energiju ovog sustava u $t = 0$.
(b) Nađite valnu funkciju $\Psi(x, t)$. Kolika je prosječna vrijednost energije za $t \neq 0$? Usporedite s (a).

ZADATAK 2 Razmotrite česticu mase m koja se giba pod utjecajem gravitacije. Hamiltonijan za ovaj problem glasi

$$H = \frac{p_z^2}{2m} + mgz$$

gdje je z visina u odnosu na površinu Zemlje.
(a) Izračunajte:

$$\frac{d\langle z\rangle}{dt}, \quad \frac{d\langle p_z\rangle}{dt}, \quad \frac{d\langle H\rangle}{dt}$$

(b) Napišite diferencijalnu jednadžbu za $\langle z\rangle$ i riješite je. Pretpostavite da je $\langle z\rangle$ u trenutku $t = 0$ jednaka z_0 i da je $\langle p_z\rangle$ u $t = 0$ jednak p_0 . Je li dobiveni rezultat sličan onome iz klasične fizike?

ZADATAK 3 Čestica mase m raspršena je na potencijalu

$$V(x) = V_0\delta(x-a) + V_0\delta(x+a)$$

gdje je $V_0 > 0$.
(a) Nađite koeficijent transmisije za česticu energije $E > 0$.
(b) Kad je V_0 vrlo velik ($V_0 \to \infty$), nađite rezonantne energije, odnosno, energije za slučaj $T \to 1$. Usporedite ih s energijama beskonačne potencijalne jame širine $2a$.

$\boxed{1.}$

$$\psi(x,0) = \frac{3}{\sqrt{50}}\psi_1(x) + \frac{4}{\sqrt{50}}\psi_2(x) + \frac{1}{\sqrt{6}}\psi_3(x)$$

(a) $\langle H \rangle = \int \psi^*(x,0) H \psi(x,0)\, dx$; $\boxed{E_n = \frac{\hbar^2\pi^2}{2m} n^2}$

$$H\psi(x,0) = \frac{3}{\sqrt{50}} H\psi_1 + \frac{4}{\sqrt{50}} H\psi_2 + \frac{1}{\sqrt{6}} H\psi_3$$

$$= \frac{3}{\sqrt{50}} E_1\psi_1 + \frac{4}{\sqrt{50}} E_2\psi_2 + \frac{1}{\sqrt{6}} E_3\psi_3$$

Uvrstimo u integral i koristimo uvjet ortonormiranosti za $\{\psi_n\}$

$$\int \psi_m^* \psi_n\, dx = \delta_{mn}$$

Ostaje,

$$\langle H \rangle = \left(\frac{3}{\sqrt{50}}\right)^2 E_1 + \left(\frac{4}{\sqrt{50}}\right)^2 E_2 + \left(\frac{1}{\sqrt{6}}\right)^2 E_3$$

$$= \frac{9}{50} E_1 + \frac{16}{50} E_2 + \frac{1}{6} E_3$$

$$= \frac{9}{50} \cdot \frac{\hbar^2\pi^2}{2ma^2} + \frac{16}{50} \cdot \frac{\hbar^2\pi^2}{2ma^2} \cdot 4 + \frac{1}{6} \cdot \frac{\hbar^2\pi^2}{2ma^2} \cdot 9$$

$$= \frac{\hbar^2\pi^2}{2ma^2} \underbrace{\left(\frac{9}{50} + \frac{64}{50} + \frac{9}{6}\right)}_{} = \frac{74}{25} \cdot \underbrace{\frac{\hbar^2\pi^2}{2ma^2}}_{E_1} = \frac{74}{25} E_1$$

$$\frac{27 + 192 + 225}{150} = \frac{444}{150} = \frac{74}{25}$$

(b)

$$\psi(x,t) = \frac{3}{\sqrt{50}}\,\psi_1(x)\,e^{-iE_1 t/\hbar} + \frac{4}{\sqrt{50}}\,\psi_2(x)\,e^{-iE_2 t/\hbar} + \frac{1}{\sqrt{6}}\,\psi_3(x)\,e^{-iE_3 t/\hbar}$$

$$\langle H \rangle = \int \psi^*(x,t)\, H\, \psi(x,t)\, dx$$

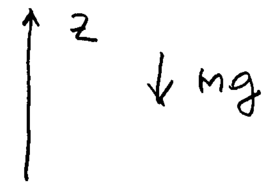
Zbog uvjeta ortonormalnosti te zbog toga što se faktori $e^{-iE_i t/\hbar}$ pokrate u integralima rezultat je identičan onome pod (a). To smo pokazali na vježbama gdje smo dokazali da je

$$\langle H \rangle = \sum_n |c_n|^2 E_n$$

ako potencijalna energija ne ovisi o vremenu.

$\boxed{2.}$ Čestica u gravitacijskom polju

$$H = \frac{p_z^2}{2m} + mgz$$



(a)

$$\frac{d}{dt}\langle z\rangle = \frac{i}{\hbar}\langle [H,z]\rangle$$

$$[H,z] = \left[\frac{p_z^2}{2m} + mgz, z\right] = \frac{1}{2m}[p_z^2, z]$$

$$= \frac{1}{2m}\Big(\underbrace{[p_z,z]}_{-i\hbar}p_z + p_z[p_z,z]\Big) = -\frac{2i\hbar}{2m}p_z$$

$$= -\frac{i\hbar}{m}p_z$$

$$\frac{d}{dt}\langle z\rangle = \frac{i}{\hbar}\cdot\left(-i\frac{\hbar}{m}\right)\langle p_z\rangle = \frac{\langle p_z\rangle}{m}$$

$$\frac{d}{dt}\langle p_z\rangle = \frac{i}{\hbar}\langle [H,p_z]\rangle$$

$$[H,p_z] = \left[\frac{p_z^2}{2m} + mgz, p_z\right] = mg\underbrace{[z,p_z]}_{i\hbar}$$

$$= i\hbar mg$$

$$\frac{d}{dt}\langle p_z\rangle = \frac{i}{\hbar}\cdot(i\hbar)mg\hbar = -mg$$

$$\frac{d}{dt}\langle H\rangle = \frac{i}{\hbar}\langle [H,H]\rangle = 0$$

$\langle H\rangle$ je konstanta gibanja; energija je očuvana

(b)

$$\frac{d}{dt}\langle z\rangle = \frac{1}{m}\langle p_z\rangle$$

$$\frac{d^2}{dt^2}\langle z\rangle = \frac{1}{m}\underbrace{\frac{d}{dt}\langle p_z\rangle}_{-mg} = \frac{1}{m}\cdot(-mg) = -g$$

$$\frac{d^2}{dt^2}\langle z\rangle = -g \Rightarrow \langle z\rangle = -g\frac{t^2}{2} + At + B$$

$\langle z\rangle$ u $t=0$ je z_0 $\Rightarrow$ $\boxed{B = z_0}$

$$\langle p_z\rangle = -mgt + C$$

$\langle p_z\rangle$ u $t=0$ je p_0 $\Rightarrow$ $\boxed{C = p_0}$

Imamo

$$\frac{d}{dt}\langle z\rangle = \frac{1}{m}\langle p_z\rangle = \frac{1}{m}\cdot(-mgt + p_0) = -gt + \frac{p_0}{m}$$

$$\langle z\rangle = -g\frac{t^2}{2} + \frac{p_0}{m}t + B$$

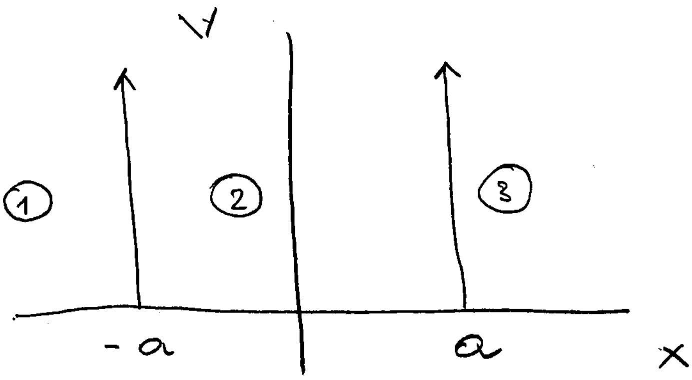
Vidimo da je $\boxed{A = \frac{p_0}{m}}$

Prema tome,

$$\langle z\rangle = -\frac{g}{2}t^2 + \frac{p_0}{m}t + z_0$$

identično klasičnoj mehanici!

3.



$$V(x) = V_0\,\delta(x-a) + V_0\,\delta(x+a)$$

$V_0 > 0$; potencijalna energija je parna funkcija

Rješavat ćemo Schrödingerovu jednadžbu u 3 područja

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \left[V_0\,\delta(x-a) + V_0\,\delta(x+a)\right]\psi = E\psi\,, \quad E > 0$$

Područje ①: $x < -a$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Rješenje: $\psi_1(x) = \underbrace{A\,e^{ikx}}_{\text{upadni val}} + \underbrace{B\,e^{-ikx}}_{\text{reflektirani val}}$

Područje ②: $-a < x < a$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Rješenje: $\psi_2(x) = C\,e^{ikx} + D\,e^{-ikx}$

moguće da nastane stojni val!

Područje ③: $x > a$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\psi_3 = \underbrace{F e}^{ikx}$$

transmitirani val

Koeficijente B, C, D i F treba izraziti pomoću A (upadni intenzitet je poznat!) koristeći rubne uvjete.

Neprekinutost valne funkcije:

$$1. \quad \psi_1 = \psi_2 \Big/_{x=-a}$$

$$2. \quad \psi_2 = \psi_3 \Big/_{x=a}$$

Uvrstimo valne funkcije

$$1. \quad A e^{-ika} + B e^{ika} = C e^{-ika} + D e^{ika}$$

$$2. \quad C e^{ika} + D e^{-ika} = e^{ika} F$$

Derivacije imaju prekid u točkama $x=-a$ i $x=a$.

Integrirat ćemo Schrödingerovu jednadžbu oko tih točaka.

Koristimo rezultate s vježbi! Oko točke $x=-a$ vrijedi:

$$\left(\frac{d\psi_2}{dx} - \frac{d\psi_1}{dx}\right)\Big/_{x=-a} = \frac{2m}{\hbar^2} V_0 \psi_1(-a)$$

↳ ili $\psi_2(-a)$

$$ikC e^{-ika} - ikD e^{ika} - ikA e^{-ika} + ikB e^{ika}$$

$$= \frac{2mV_0}{\hbar^2} \cdot \left(A e^{-ika} + B e^{+ika}\right)$$

Sredimo,

$$3. \quad B e^{ika}\left(1 + i\frac{2mV_0}{k\hbar^2}\right) + C e^{-ika} - D e^{ika}$$

$$= A e^{-ika}\left(1 - i\frac{2mV_0}{k\hbar^2}\right)$$

Oko točke $x=a$ imamo:

$$\left(\frac{d\psi_3}{dx} - \frac{d\psi_2}{dx} \right)_{x=a} = \frac{2mV_0}{\hbar^2} \psi_3(a)$$

↳ ili $\psi_2(a)$

$$ikE e^{ika} - ikC e^{ika} + ikD e^{-ika} = \frac{2mV_0}{\hbar^2} F e^{ika}$$

Sredimo,

$$4. \quad E e^{ika} \left(1 + i \frac{2mV_0}{k \cdot \hbar^2}\right) - C e^{ika} + D e^{-ika} = 0$$

Dobili smo sustav jednadžbi:

$$(1.) \quad B e^{ika} - C e^{-ika} - D e^{ika} = A e^{-ika}$$

$$(2.) \quad C e^{ika} + D e^{-ika} - F e^{ika} = 0$$

$$(3.) \quad B e^{ika} \left(1 + i \frac{2mV_0}{k\hbar^2}\right) + C e^{-ika} - D e^{ika} = A e^{-ika} \left(1 - i \frac{2mV_0}{k\hbar^2}\right)$$

$$(4.) \quad C e^{ika} - D e^{-ika} - F e^{ika} \left(1 + i \frac{2mV_0}{k\hbar^2}\right) = 0$$

Zbrojimo 2. i 4.

$$2 C e^{ika} = F e^{ika} \left(2 + i \frac{2mV_0}{k\hbar^2}\right)$$

$$C = F \left(1 + i \frac{mV_0}{k\hbar^2}\right)$$

Uvrstimo u 2.

$$E\left(1+i\frac{mV_0}{k\hbar^2}\right)e^{ikq}+De^{-ikq}-Fe^{ikq}=0$$

$$De^{-ikq}=-F\cdot i\frac{mV_0}{k\hbar^2}e^{ika}$$

$$D=-Fe^{2ikq}\cdot\frac{imV_0}{k\hbar^2}$$

Uvrstimo C i D koje smo izračunali u jednadžbe 1 i 3

① $$Be^{ikq}-Fe^{-ikq}\left(1+i\frac{mV_0}{k\hbar^2}\right)+Fe^{3ikq}\cdot\frac{imV_0}{k\hbar^2}=Ae^{-ikq}$$

$$Be^{ikq}+Fe^{ikq}\cdot\left[e^{2ikq}\cdot\frac{imV_0}{k\hbar^2}-e^{-2ikq}\cdot\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]=Ae^{-ika}$$

odnosno,

$$B+F\left[e^{2ikq}\cdot\frac{imV_0}{k\hbar^2}-e^{-2ikq}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]=Ae^{-2ikq} \qquad (*)$$

③ $$Be^{ikq}\left(1+i\frac{2mV_0}{k\hbar^2}\right)+F\left(1+i\frac{mV_0}{k\hbar^2}\right)e^{-ikq}+Fe^{3ikq}\cdot\frac{imV_0}{k\hbar^2}=Ae^{-ika}\left(1-i\frac{2mV_0}{k\hbar^2}\right)$$

$$B e^{ika}\left(1+i\frac{2mV_0}{k\hbar^2}\right)+Fe^{ika}\left[e^{2ika}\cdot\frac{imV_0}{k\hbar^2}+e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]=Ae^{-ika}\left(1-i\frac{2mV_0}{k\hbar^2}\right)$$

Prema tome,

$$B\left(1+i\frac{2mV_0}{k\hbar^2}\right)+F\left[e^{2ika}\frac{imV_0}{k\hbar^2}+e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]=Ae^{-2ika}\left(1-i\frac{2mV_0}{k\hbar^2}\right) \quad (**)$$

Imamo dvije jednadžbe za nepoznanice B i E. Treba nam E! Iz (*) je

$$B=Ae^{-2ika}-F\left[e^{2ika}\cdot\frac{imV_0}{k\hbar^2}-e^{-2ika}\cdot\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]$$

Uvstimo u (**)

$$\left(1+i\frac{2mV_0}{k\hbar^2}\right)Ae^{-2ika}-\left(1+i\frac{2mV_0}{k\hbar^2}\right)F\left[e^{2ika}\cdot\frac{imV_0}{k\hbar^2}-e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]$$

$$+F\left[e^{2ika}\frac{imV_0}{k\hbar^2}+e^{-2ikA}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]=Ae^{-2ika}\left(1-i\frac{2mV_0}{k\hbar^2}\right)$$

Sredimo; na desnoj strani ostaje koeficijent A

$$-iAe^{-2ika}\cdot\frac{4mV_0}{k\hbar^2}$$

Na drugoj strani je

$$F e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right) - i\frac{2mV_0}{k\hbar^2} F\left[e^{2ika} \cdot \frac{imV_0}{k\hbar^2} - e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right] + F e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right) =$$

$$2F\left\{e^{-2ika} + e^{-2ika} \cdot i\frac{mV_0}{k\hbar^2} - i\frac{mV_0}{k\hbar^2}\left[e^{2ika} \cdot \frac{imV_0}{k\hbar^2} - e^{-2ika}\left(1+i\frac{mV_0}{k\hbar^2}\right)\right]\right\}$$

$$= 2F\left\{e^{-2ika} + 2e^{-2ika} \cdot \frac{imV_0}{k\hbar^2} + e^{2ika} \cdot \left(\frac{mV_0}{k\hbar^2}\right)^2 - e^{-2ika}\left(\frac{mV_0}{k\hbar^2}\right)^2\right\}$$

Prema tome, koeficijent F je

$$F = -\frac{i\frac{2mV_0}{k\hbar^2} e^{-2ika} A}{e^{-2ika} + 2e^{-2ika} \cdot \frac{imV_0}{k\hbar^2} + e^{2ika}\left(\frac{mV_0}{k\hbar^2}\right)^2 - e^{-2ika}\left(\frac{mV_0}{k\hbar^2}\right)^2}$$

Pomnožimo brojnik i nazivnik s $e^{2ika} \cdot k^2\hbar^4$.

Dobijemo

$$\boxed{F = -\frac{2iAkmV_0\hbar^2}{k^2\hbar^4 - m^2V_0^2 + 2ikmV_0\hbar^2 + m^2V_0^2 e^{i4ka}}}$$

$$T = \frac{|F|^2}{|A|^2}.$$

Pretpostavimo da je

$$4ka = 2n\pi \quad , \quad n = 1, 2, 3, \dots \quad (k > 0)$$

Tada je $e^{i4ka} = 1$ pa imamo

$$F = -\frac{2ikmV_0\hbar^2 A}{k^2\hbar^4 + 2ikmV_0\hbar^2} = -\frac{2imV_0}{k\hbar^2 + 2imV_0} A$$

$$T = \frac{4m^2V_0^2}{k^2\hbar^4 + 4m^2V_0^2} \xrightarrow[V_0 \to \infty]{} T \to 1$$

Uvrstimo u uvjet $4ka = 2n\pi$ energiju $E = \frac{\hbar^2 k^2}{2m}$

$$16k^2a^2 = n^2\pi^2 \cdot 4$$

$$\underset{4}{\cancel{16}} \cdot \frac{2mE}{\hbar^2} a^2 = n^2\pi^2 \cdot \cancel{4}$$

$$E = \frac{\hbar^2\pi^2}{2m(2a)^2} n^2$$

i to je energija beskonačne potencijalne jame širine $2a$.

In[39]:= Solve[{B * Exp[i * k * a] - C * Exp[-i * k * a] - D * Exp[i * k * a] == A * Exp[-i * k * a],
C * Exp[i * k * a] + D * Exp[-i * k * a] - F * Exp[i * k * a] == 0,

$$B * Exp[i * k * a] * \left(1 + i * \frac{2 * m * V0}{\hbar^2 * k}\right) + C * Exp[-i * k * a] - D * Exp[i * k * a] == A * Exp[-i * k * a] * \left(1 - i * \frac{2 * m * V0}{\hbar^2 * k}\right),$$

$$C * Exp[i * k * a] - D * Exp[-i * k * a] - F * Exp[i * k * a] * \left(1 + i * \frac{2 * m * V0}{\hbar^2 * k}\right) == 0\}, \{B, C, D, F\}]$$

Out[39]=

$$\left\{\left\{B \to -\frac{A\, e^{-2 i a k} \left(-m^2 V0^2 + e^{4 i a k} m^2 V0^2 - k^2 \hbar^4\right)}{-m^2 V0^2 + e^{4 i a k} m^2 V0^2 + 2 i k m V0 \hbar^2 + k^2 \hbar^4},\right.\right.$$

$$C \to \frac{2 A m V0 \left(m V0 - i k \hbar^2\right)}{-m^2 V0^2 + e^{4 i a k} m^2 V0^2 + 2 i k m V0 \hbar^2 + k^2 \hbar^4},$$

$$D \to -\frac{2 A e^{2 i a k} m^2 V0^2}{-m^2 V0^2 + e^{4 i a k} m^2 V0^2 + 2 i k m V0 \hbar^2 + k^2 \hbar^4},$$

$$\left.\left.F \to -\frac{2 i A k m V0 \hbar^2}{-m^2 V0^2 + e^{4 i a k} m^2 V0^2 + 2 i k m V0 \hbar^2 + k^2 \hbar^4}\right\}\right\}$$

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