SVEUČILIŠTE U RIJECI, FAKULTET ZA FIZIKU

Dipl. stud. Fizika i matematika Dipl. stud. Fizika i informatika Dipl. stud. Fizika i filozofija

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OSNOVE KVANTNE MEHANIKE

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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 Zadana su dva hermitska operatora A i B. Dokažite relaciju

$$\frac{d}{dt}\langle AB\rangle=\left\langle\frac{\partial A}{\partial t}B\right\rangle+\left\langle A\frac{\partial B}{\partial t}\right\rangle+\frac{1}{i\hbar}\langle[A,H]B\rangle+\frac{1}{i\hbar}\langle A[B,H]\rangle$$

gdje je H hamiltonijan.

$\boxed{1.}$

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

(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,

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

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

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

$$= \frac{\hbar^2\pi^2}{2ma^2}\underbrace{\left(\frac{9}{50} + \frac{64}{50} + \frac{9}{6}\right)}_{\frac{27+192+225}{150} = \frac{444}{150} = \frac{74}{25}} = \frac{74}{25}\cdot\underbrace{\frac{\hbar^2\pi^2}{2ma^2}}_{E_1} = \frac{74}{25}E_1$$

(b)

$$\psi(x,t) = \frac{3}{\sqrt{50}}\,\psi_1(x)\,e^{-iE_1t/\hbar} + \frac{4}{\sqrt{50}}\,\psi_2(x)\,e^{-iE_2t/\hbar} + \frac{1}{\sqrt{6}}\,\psi_3(x)\,e^{-iE_3t/\hbar}$$

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

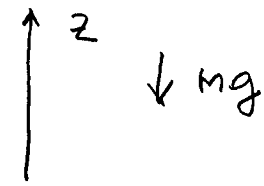
Zbog uvjeta ortonormalnosti te zbog toga što se faktori $e^{-iE_it/\hbar}$ pokrate u integralima rezultat je identičan onome pod (a). To smo pokazali na vježbama gdje smo dokazali da je

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

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.

$$\frac{d}{dt}\langle AB\rangle = \frac{d}{dt}\int \psi^* AB\psi\, d^3r = \int \frac{\partial \psi^*}{\partial t} AB\psi\, d^3r$$
$$+ \int \psi^* \frac{\partial}{\partial t}(AB)\psi\, d^3r + \int \psi^* AB \frac{\partial \psi}{\partial t} d^3r \qquad (*)$$

Schrödingerova jednadžba

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} H\psi$$
$$\frac{\partial \psi^*}{\partial t} = -\frac{1}{i\hbar}(H\psi)^*$$

Rodmamo prvi član u $(*)$; zamijenimo derivaciju po vremenu

$$-\frac{1}{i\hbar}\int (H\psi)^* AB\psi\, d^3r = -\frac{1}{i\hbar}\int \psi H(AB\psi)\, d^3r$$

jer je H hermitski operator. Treći član u $(*)$ je

$\frac{1}{i\hbar}\int \psi^* AB H\psi\, d^3r$. Imamo

$$\frac{d}{dt}\langle AB\rangle = \int \psi^* \frac{\partial}{\partial t}(AB)\psi\, d^3r$$
$$+ \frac{1}{i\hbar}\int \psi^* (\underbrace{ABH - HAB}_{[AB,H]})$$
$$= \frac{1}{i\hbar}\langle [A,H]B\rangle + \frac{1}{i\hbar}\langle A[B,H]\rangle$$
$$+ \langle \frac{\partial}{\partial t}(AB)\rangle$$

Zbog

$$\frac{\partial}{\partial t}(AB) = \frac{\partial A}{\partial t}B + A\frac{\partial B}{\partial t}$$

drugi član u (*) je

$$\int \psi^* \frac{\partial A}{\partial t} B \psi \, d^3r + \int \psi^* A \frac{\partial B}{\partial t} \psi \, d^3r = \langle \frac{\partial A}{\partial t} B \rangle + \langle A \frac{\partial B}{\partial t} \rangle$$

Ukupno

$$\frac{d}{dt}\langle AB \rangle = \langle \frac{\partial A}{\partial t} B \rangle + \langle A \frac{\partial B}{\partial t} \rangle + \frac{1}{i\hbar}\langle [A,H]B \rangle + \frac{1}{i\hbar}\langle A[B,H] \rangle$$

NAPOMENA: vidimo da smo mogli upotrijebiti uobičajenu formulu

$$\frac{d}{dt}\langle X \rangle = \frac{1}{i\hbar}\langle [X,H] \rangle + \langle \frac{\partial X}{\partial t} \rangle$$

i staviti

$$X = AB$$

Nije nužno da X bude hermitski operator! U našem slučaju, iako su A i B hermitski, AB nije hermitski!