KVANTNI DELCI

1) De Broglieva zveza [delci]

$p = \frac{E}{c}$ $E = h\nu$ $p = \frac{h\nu}{c}$ $c = \lambda\nu$

$p = \frac{h}{\lambda}$ velja za svetlobo

$\boxed{\lambda = \frac{h}{p}}$ $\psi(\vec{r})$ $k = \frac{2\pi}{\lambda}$ $\frac{2\pi}{k} = \frac{h}{p}$ $p = \frac{h}{2\pi} k$

$$\left.\begin{aligned} &\boxed{p = \hbar k} \\ &E = \hbar\omega \end{aligned}\right\}$$

$(E, p) \longleftrightarrow (\omega, k)$

Dualnost delec-valovanje

Davisson, Germer (1927)

e^-

$|e_0 U| = \frac{1}{2} m_e v^2$ $p = m_e v$

$v = \sqrt{\frac{2e_0 U}{m_e}}$ $p = \sqrt{2m_e e_0 U}$

$\lambda = \frac{h}{\sqrt{2m_e e_0 U}} = \frac{1{,}23\,\mathrm{nm}}{\sqrt{U[V]}}$

$U = 50\,V$ $\lambda = 0{,}17\,\mathrm{nm}$

TEM : transmisijski el. mikroskop 1MV $\longrightarrow$ atomska ločljivost

GV $\longleftrightarrow$ GeV

TV $\longleftrightarrow$ TeV

Prah $r \sim 1\,\mu m$ $v \sim 1\,mm/s$ $m \sim 10^{-15}\,kg$

$\lambda = 0{,}7 \cdot 10^{-7}\,nm = 0{,}7 \cdot 10^{-10}\,\mu m$

Geometrijska optika (trajektorije, žarki)

Valovna optika (valovanje)

Ekviparticijski izrek $\frac{1}{2} m \langle v^2 \rangle = \frac{3}{2} k_B T$

$T = 20^\circ C \longrightarrow \underline{v \approx mm/s} \Rightarrow$ Brownovo gibanje

$v \longleftrightarrow \lambda = r \longrightarrow v = 1\mu m/s \longrightarrow T = 10^{-7} K$

2) VALOVNA FUNKCIJA $\psi(\vec{r}, t)$

$t = konst \qquad \psi(\vec{r})$

$\int_V |\psi(\vec{r})|^2 \, dV \longrightarrow$ verjetnost, da se delec nahaja v tem območju

$\int_{\text{cel prostor}} |\psi(\vec{r})|^2 \, dV = 1 \longrightarrow$ normalizacija valovne funkcije

$\hat{A}\psi(\vec{r}) = \varphi(\vec{r}) \qquad x, y, z, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \qquad \psi(x) \to \psi(x - 2cm)$ (krši lokalnost)

$(\varphi, \psi) = \int_{\text{celoten prostor}} \varphi(\vec{r})^* \psi(\vec{r}) \, dV = \langle \varphi | \psi \rangle$

$$\langle \varphi | \hat{A} | \psi \rangle = \int \varphi^*(\vec{r}) \underbrace{\hat{A}[\psi(\vec{r})]} \, dV = \int \varphi^*(\vec{r}) \eta(\vec{r}) \, dV \qquad \hat{A}[\psi(\vec{r})] = \eta(\vec{r})$$

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2 \psi(\vec{r}, t)}{\partial x^2} + \frac{\partial^2 \psi(\vec{r}, t)}{\partial y^2} + \frac{\partial^2 \psi(\vec{r}, t)}{\partial z^2}\right) + V(\vec{r})\psi(\vec{r}, t)$$

Schrödingerjeva enačba

$$\hat{H} = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \underbrace{V(\vec{r})}$$

$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \qquad \hat{H}$ operator celotne energije

3) PROSTI DELEC

$V = 0 \qquad \psi(x)$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_e}\frac{\partial^2 \psi}{\partial x^2} \qquad \longleftrightarrow \qquad \frac{1}{c^2}\frac{\partial^2 \psi}{\partial^2 t} = \frac{\partial^2 \psi}{\partial x^2}$$

$\psi = \psi \qquad \cancel{\frac{\partial^2 \psi}{\partial x^2} = 0} \qquad \cancel{\psi = ax + b}$

ψ nujno kompleksna funkcija

$$\boxed{\psi = e^{i(kx - \omega t)}}$$ ravni val (nastavek)

$p = \hbar k$

$$i\hbar(-i\omega)\cancel{\psi} = -\frac{\hbar^2}{2m_e}(+ik)^2\cancel{\psi}$$

$$+\hbar\omega = \frac{\hbar^2 k^2}{2m_e} = \frac{p^2}{2m_e} = \frac{1}{2}m_e v^2$$

$E \qquad E = p^2/2m_e$

$$\omega = \frac{E}{\hbar} = \frac{p^2/2m_e}{\hbar} \qquad k = p/\hbar$$

Prosti parameter: $p \leftrightarrow k$

$$\boxed{-i\hbar\frac{\partial}{\partial x}}\psi = \underbrace{\hbar k}_{p}\psi \qquad \boxed{\hat{p}_x = -i\hbar\frac{\partial}{\partial x}}$$

$$\left(\frac{\partial}{\partial x}\right)^2 = \frac{\partial}{\partial x}\frac{\partial}{\partial x} = \frac{\partial^2}{\partial x^2}$$

$$\frac{1}{2}p^2/m_e = \frac{1}{2m_e}(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) = -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = \hat{H}_{kin}$$

$\psi = A e^{i(kx - \omega t)}$

Gostota toka elektronov: $j = \frac{-i\hbar}{2m_e}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi\frac{\partial \psi^*}{\partial x}\right)$

$$\boxed{j = \frac{1}{2m_e}(\psi^* \hat{p}\psi - \psi\hat{p}\psi^*)}$$

$|\psi|^2 = |A|^2$

$j = \frac{p}{m}|A|^2 = v\,|A|^2$

hitrost, gostota

$A = \frac{1}{\sqrt{V}} \quad \rightarrow \quad j = 1$ delec/enota časa/enoto ploščice

$$\psi = A e^{i(kx - \omega t)} + B e^{i(-kx - \omega t)} \qquad p = \frac{\partial}{\partial x}$$

$k > 0$

$$j = \frac{1}{2m_e}\left(A^* e^{-i(kx-\omega t)} + B^* e^{-i(-kx-\omega t)}\right)\left(A\hbar k\, e^{i(kx-\omega t)} - B\hbar k\, e^{i(-kx-\omega t)}\right) \qquad \psi^* = A^* e^{-i(kx-\omega t)} + B^* e^{-i(-kx-\omega t)}$$

$$-\frac{1}{2m_e}\left(A e^{i(kx-\omega t)} + B e^{i(-kx-\omega t)}\right)\left(-A^*\hbar k\, e^{-i(kx-\omega t)} + B^*\hbar k\, e^{-i(-kx-\omega t)}\right)$$

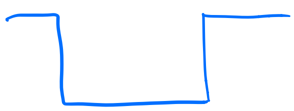
$$= \frac{1}{2m_e}\left(|A|^2\hbar k - |B|^2\hbar k + \cancel{A^* B\,\hbar k\, e^{-2ikx}} + \cancel{B^* A\,\hbar k\, e^{2ikx}}\right)$$

$$-\frac{1}{2m_e}\left(-|A|^2\hbar k + |B|^2\hbar k + \cancel{A^* B\,\hbar k\, e^{-2ikx}} + \cancel{B^* A\,\hbar k\, e^{2ikx}}\right)$$

$$j = \frac{1}{m_e}\left(|A|^2\hbar k - |B|^2\hbar k\right) = v\left(|A|^2 - |B|^2\right)$$

4) DELEC V POTENCIALU

$V = -q\Phi \qquad q = -e_0 \qquad V = e_0\Phi$



$$\psi(\vec r, t) = \phi(\vec r)\,\chi(t) \qquad \psi \sim e^{-i\omega t}$$

$$i\hbar\, \phi(x)\frac{\partial \chi(t)}{\partial t} = \chi(t)\left[-\frac{\hbar^2}{2m_e}\frac{\partial^2\phi(x)}{\partial x^2} + V(x)\phi(x)\right]$$

$$i\hbar\, \dot\chi(t)/\chi(t) = \left[-\frac{\hbar^2}{2m_e}\phi''(x) + V(x)\phi(x)\right]/\phi(x) = \text{konst} = E$$

$$i\hbar\dot\chi = E\chi \qquad \chi = e^{-i\omega t} \qquad E = \hbar\omega$$

$$\boxed{-\frac{\hbar^2}{2m_e}\phi''(x) + V(x)\,\phi(x) = E\,\phi(x)}$$

Stacionarna Schröd. enačba

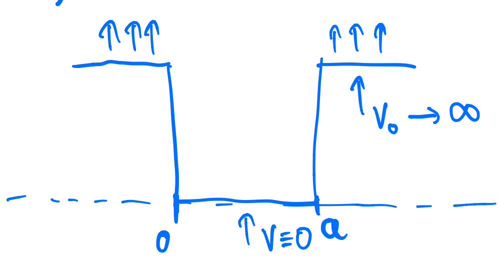
problem lastnih vrednosti

$$\psi = \phi(r)\, e^{-i\omega t} \qquad E = \hbar\omega$$

$$\hat H = -\frac{\hbar^2}{2m_e} + V \qquad \hat H|\phi\rangle = E|\phi\rangle$$

$$(\hat H - E\hat{1})\,|\phi\rangle = 0 \qquad \det(\hat H - E1) = 0$$

4a) KVADRATNA POTENCIALNA JAMA



$\psi(x) \equiv 0 \quad x < 0$ ali $x > a$

$\psi(0) = 0 \qquad \psi(a) = 0$

$-\frac{\hbar^2}{2m_e}\phi'' = E\phi \qquad \phi(0)=0 \qquad \phi(a)=0$ [0:a] rešujemo na tem intervalu

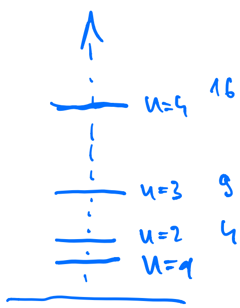
$\phi = A\sin(kx) \qquad ka = n\pi \qquad n = 1,2,3,\dots$

$k = \frac{n\pi}{a} \qquad \phi_n = A\sin\left(\frac{n\pi}{a}x\right)$

↑ kvantno število

Pojav kvantizacije

$E = +\frac{\hbar^2}{2m_e}\left(\frac{n\pi}{a}\right)^2 = \frac{(\hbar\pi n)^2}{2m_e a^2}$ dovoljene energija za elektron v pasti

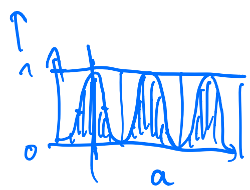


$E_{n=1} = \frac{\hbar^2\pi^2}{2m_e a^2} > 0$ → ničelna energija

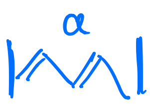
$$\int_0^a |\phi_n|^2\,dx = 1 = A^2\int_0^a \sin^2\frac{n\pi}{a}x = A^2\frac{a}{2} = 1$$

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

$\phi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$



$A = 1\cdot a$



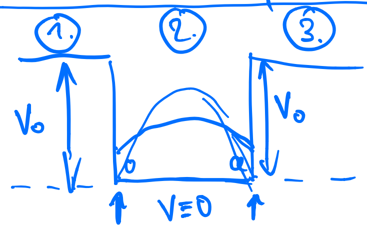
π-konjugirane vezi

$a = 0{,}416\,\text{nm}$

$E = 10{,}8\,\text{eV}$

↳ 114 nm UV

4b) KVADRATNA JAMA, KONČNO VISOK POTENCIAL



$-\frac{\hbar^2}{2m_e}\phi''(x) + V\phi(x) = E\phi(x)$

1) $-\frac{\hbar^2}{2m_e}\phi_1'' + V_0\phi_1 = E\phi_1 \qquad \phi_1(x\to-\infty) = 0$

2) $-\frac{\hbar^2}{2m_e}\phi_2'' = E\phi_2$

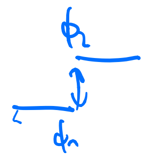
3) $-\frac{\hbar^2}{2m_e}\phi_3'' + V_0\phi_3'' = E\phi_3$

$$\begin{cases} \phi_1(0)=\phi_2(0) & \phi_1'(0)=\phi_2'(0) \\ \phi_2(a)=\phi_3(a) & \phi_2'(a)=\phi_3'(a) \end{cases}$$

$\phi_3(x\to+\infty)=0$

Zvezna: $\phi_1(x-0)=\phi_2(x+0)$

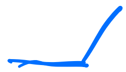
$p=-i\hbar\frac{\partial}{\partial x}$



$\frac{\partial}{\partial x}\phi = \lim_{\Delta x\to 0}\frac{\phi_2-\phi_1}{\Delta x} = \infty$

Zvezno odvedljivo: $\phi_1'(x-0)=\phi_2'(x+0)$

(razen za ∞ visoke potenciale)

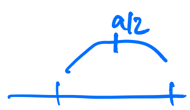


kappa

1) $\phi_1 = Ae^{\varkappa_1 x}$ $\qquad \varkappa_1>0$

$-\frac{\hbar^2}{2m_e}\varkappa_1^2 + V_0 = E \quad\to\quad \varkappa_1=\frac{\sqrt{2m_e(V_0-E)}}{\hbar}$

2) $\phi_2 = B\cos\left(k\left(x-a/2\right)\right)$



$+\frac{\hbar^2}{2m_e}k^2 = E \qquad k=\frac{\sqrt{2m_eE}}{\hbar}$

kappa $\varkappa$ $\qquad$ chi χ

3) $\phi_3 = A\, e^{-\varkappa_3(x-a)}$ $\qquad \varkappa_3=\varkappa_1$

$A,\ B,\ E \searrow k,\ \varkappa_1=\varkappa_3$

$\phi_1(0)=\phi_2(0)$

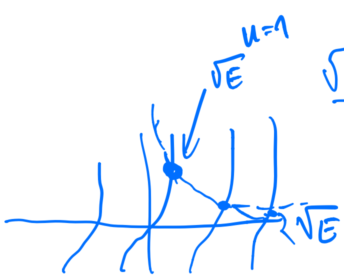
$\phi_1'(0)=\phi_2'(0)$

$A = B\cos(ka/2)$

$A\varkappa_1 = -kB\sin\left(k\left(\overset{0}{x}-a/2\right)\right) = -kB\sin(-ka/2)$

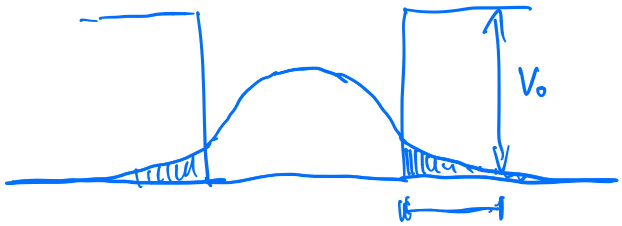
$A\varkappa_1 = kB\sin(ka/2)$

$\varkappa_1 = k\tan(ka/2)$



$\frac{\sqrt{2m_e(V_0-E)}}{\hbar} = \frac{\sqrt{2m_eE}}{\hbar}\tan\left(\frac{\sqrt{2m_eE}}{\hbar}\cdot\frac{a}{2}\right)$ $\qquad E=?$

$\sqrt{\frac{V_0-E}{E}} = \tan\left(\frac{\sqrt{2m_eE}}{\hbar}\frac{a}{2}\right)$ $\qquad \sqrt{E}$

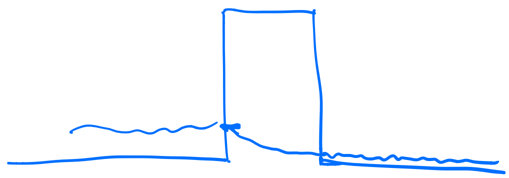


$E < V_0$

"vezana stanja"

klasično prepovedano območje

bariera



tuneliranje

kvantnomehansko prehajanje delcev skozi potencialno bariero

Evanescentni valovi