- konečná jáma, konečná jáma v PBC – stavy, GS, variace
- rozptyl – sch.
- schod

- z cvičení 7.4. víme

$$\psi = e^{ikx} \quad E \quad k \quad E = \frac{\hbar^2 k^2}{2m} \to k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi = e^{\pm kx} \quad E \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

- Pro jistotu ověříme

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} e^{ikx} = -\frac{\hbar^2}{2m}(ik)^2 e^{ikx} = \frac{\hbar^2 k^2}{2m} e^{ikx} = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} e^{\pm kx} = -\frac{\hbar^2 k^2}{2m} e^{\pm kx} = E\psi$$

- Uvažujme rozptyl na bariéře (napři)

E, něco, $E + V$, $E - V$

$$\psi = e^{ikx} + Be^{-ikx} \qquad \psi = Ae^{ik'x}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad k' = \sqrt{\frac{2m(E-V)}{\hbar^2}}$$

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

j_{in} j_T j_{out}

Ukažte $R + T = 1$

$$R = \frac{j_{out}}{j_{in}} \qquad T = \frac{j_T}{j_{in}}$$

a pozn. zjevně $j_{in} = j_{out} + j_T$

trochu důkaz ☺

pro $+\infty$:
$$j_+ = \frac{\hbar}{2mi}\left[A^* e^{-ik'x}\, ik' A e^{ik'x} - A e^{ik'x}(-ik')A^* e^{-ik'x}\right]$$
$$= \frac{\hbar}{2mi}|A|^2(+2ik')$$
$$= \frac{\hbar k'|A|^2}{m}$$

pro $-\infty$
$$j_- = \frac{\hbar}{2mi}\Big[\left(e^{-ikx} + B^* e^{ikx}\right)\left(ik e^{ikx} - ikBe^{-ikx}\right) - \left(e^{ikx} + Be^{-ikx}\right)\left(-ike^{-ikx} + B^* ik e^{ikx}\right)\Big]$$
$$= \frac{\hbar}{2mi}\Big[ik - ikBe^{-2ikx} + ikB^* e^{2ikx} - ik|B|^2 + ik - B^* ik e^{2ikx} + Bike^{-2ikx} - |B|^2 ik\Big]$$
$$= \frac{\hbar}{2mi}\left[2ik - 2ik|B|^2\right]$$
$$= \frac{\hbar k}{m}\left[1 - |B|^2\right]$$

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$j_+ = \frac{\hbar k'}{m}|A|^2 \qquad j_- = \frac{\hbar k}{m}(1-|B|^2)$

• Nyní "stacionární stav" $\to \frac{d|\psi|^2}{dt} = 0 \Rightarrow \frac{dj}{dt} = 0$

$\Rightarrow j(-\infty) = j(\infty) \qquad \frac{dj}{dx} = 0$ & $j = const$ $\left(\underbrace{\frac{\partial\rho}{\partial t}}_{=0} + \underbrace{\nabla\cdot j}_{=0} = 0\right)$

$$\frac{\hbar k'}{m}|A|^2 = \frac{\hbar k}{m}(1-|B|^2)$$

$$\underbrace{\frac{k'}{k}|A|^2}_{T} + \underbrace{|B|^2}_{R} = 1$$

— — —

$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \,/\psi^*$ & conj $\qquad -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* = E\psi^* \,/\psi.$

$-\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + \psi^* V\psi = \psi^* E\psi \qquad -\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + \psi^* V\psi = \psi^* E\psi$

rozdíl

$$-\frac{\hbar^2}{2m}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right] = 0$$

$$\psi^*\nabla^2\psi - \psi\nabla^2\psi^* = 0$$

$$? \quad \nabla\cdot(\underbrace{\psi^*\nabla\psi - \psi\nabla\psi^*}_{j}) = 0 \to j = const$$

$\psi|0\rangle = \frac{1}{\sqrt{\alpha\sqrt{\pi}}} e^{-\frac{x^2}{2\alpha^2}} \qquad |1\rangle = \frac{1}{\sqrt{\alpha\sqrt{\pi}}}\frac{\sqrt{2}x}{\alpha} e^{-\frac{x^2}{2\alpha^2}} \qquad \to \alpha = 1$

$|0\rangle = \pi^{-1/4} e^{-x^2/2} \qquad |1\rangle = \pi^{-1/4}\sqrt{2}x\, e^{-x^2/2}$

$\frac{d\psi_0}{dx} = -x\,\pi^{-1/4} e^{-x^2/2} \qquad \frac{d\psi_1}{dx} = \pi^{-1/4}\sqrt{2}\, e^{-x^2/2} - \pi^{-1/4}\sqrt{2}\,x^2 e^{-x^2/2}$

$\frac{1}{4}\pi^{-1/2}\Big[\left(e^{-x^2/2}e^{i\phi} + \sqrt{2}x e^{-x^2/2}e^{3i\phi}\right)\left(-x e^{-x^2/2}e^{-i\phi} + \sqrt{2}e^{-x^2/2}e^{-3i\phi} - \sqrt{2}x^2 e^{-x^2/2}e^{-3i\phi}\right)$

$-\left(e^{-x^2/2}e^{-i\phi} + \sqrt{2}x e^{-x^2/2}e^{-3i\phi}\right)\left(-x e^{-x^2/2}e^{i\phi} + \sqrt{2}e^{-x^2/2}e^{3i\phi} - \sqrt{2}x^2 e^{-x^2/2}e^{3i\phi}\right)\Big]$

same state $\to 0$

$\frac{1}{4}\pi^{-1/2}\Big[\sqrt{2}e^{-x^2}e^{-2i\phi} - \cancel{\sqrt{2}x^2 e^{-x^2}e^{-2i\phi}} - \cancel{\sqrt{2}x^2 e^{-x^2}e^{2i\phi}} - \left(\sqrt{2}e^{-x^2}e^{2i\phi} - \cancel{\sqrt{2}x^2 e^{-x^2}e^{2i\phi}} - \cancel{\sqrt{2}x^2 e^{-x^2}e^{-2i\phi}}\right)\Big]$

$= -\frac{i}{2}\pi^{-1/2}\sqrt{2}\, e^{-x^2}\sin(2\phi)$

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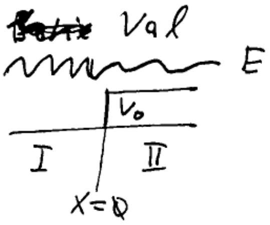
~~Barie~~ Val



$$\mathrm{I}: \ \psi = e^{ikx} + B e^{-ikx} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\mathrm{II}: \ \psi = A e^{ik'x} \qquad k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

· sešívací podmínky:

· $\psi|_{x\to 0-} = \psi|_{x\to 0+}$ spojitost fce

$\psi'|_{x\to 0-} = \psi'|_{x\to 0+}$ spojitost derivace (konečná změna potenciálu)

1) v $x=0$: $e^{ikx} + B e^{-ikx} = A e^{ik'x}$

$$1 + B = A \qquad \to \ A - B = 1$$

2) derivace: v $x=0$: $ik e^{ikx} - ikB e^{-ikx} = ik' A e^{ik'x}$ $\qquad \to \sqrt{1-c}\,A + B = 1$

$$ik - ikB = ik'A$$

$$k(1-B) = k'A$$

definujme / uvažujme $V_0 = cE \quad 0<c<1$

$$k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \sqrt{\frac{2m(E-cE)}{\hbar^2}} = \sqrt{\frac{2mE}{\hbar^2}}\sqrt{1-c} = k\sqrt{1-c}$$

$$\to \quad 1 + B = A$$

$$\oplus \quad \cancel{k}(1-B) = \cancel{k}\sqrt{1-c}\,A$$

$$2 = A(1+\sqrt{1-c})$$

$$A = \frac{2}{1+\sqrt{1-c}}$$

$$B = A - 1 = \frac{2}{1+\sqrt{1-c}} - 1 = \frac{2-1-\sqrt{1-c}}{1+\sqrt{1-c}} = \frac{1-\sqrt{1-c}}{1+\sqrt{1-c}}$$

$$T = \frac{k'}{k}A^2 = \frac{k\sqrt{1-c}}{k}\,\frac{4}{(1+\sqrt{1-c})^2} = \frac{4\sqrt{1-c}}{1+1-c+2\sqrt{1-c}} = \frac{4\sqrt{1-c}}{2-c+2\sqrt{1-c}}$$

$$R = B^2 = \frac{(1-\sqrt{1-c})^2}{(1+\sqrt{1-c})^2} = \frac{1+1-c-2\sqrt{1-c}}{1+1-c+2\sqrt{1-c}} = \frac{2-c-2\sqrt{1-c}}{2-c+2\sqrt{1-c}}$$

$V = \frac{3}{4}E_0 \quad c = 3/4 \ \to \quad \sqrt{1-3/4} = 1/2$

$$T = \frac{4\sqrt{1-3/4}}{2-3/4+2\sqrt{1-3/4}} = \frac{2}{\frac{5}{4}+1} = \frac{8}{9}$$

$$R = \frac{2-3/4-2\cdot 1/2}{2-3/4+2\cdot 1/2} = \frac{5/4-1}{5/4+1} = \frac{1}{4}\cdot\frac{4}{9} = \frac{1}{9}$$

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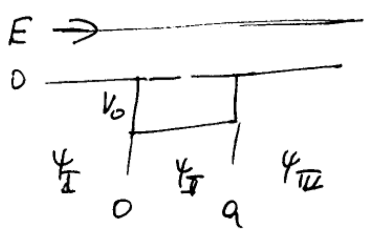


$$\psi_I = A e^{ikx} + B e^{-ikx}$$
$$\psi_{II} = C e^{ik'x} + D e^{-ik'x}$$
$$\psi_{III} = E e^{ikx}$$

bod 0: $\psi_I(0) = \psi_{II}(0)$ $\quad \psi_I'(0) = \psi_{II}'(0)$

$$1 + B = C + D \qquad ik - ikB = ik'C - ik'D$$

bod a: $\psi_{II}(a) = \psi_{III}(a)$ $\quad \psi_{II}'(a) = \psi_{III}'(a)$

$$Ce^{ik'a} + De^{-ik'a} = Ee^{ika} \qquad ik'Ce^{ik'a} - ik'De^{-ik'a} = ikEe^{ika}$$

$$B - C - D = -1$$
$$kB + k'C - k'D = k$$
$$Ce^{ik'a} + De^{-ik'a} - Ee^{ika} = 0$$
$$k'Ce^{ik'a} - k'De^{-ik'a} - kEe^{ika} = 0$$

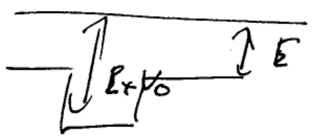
→ 4 rovnice 4 neznámé, 3 parametry: E, V_0, a

---

vak2: $\cancel{\psi_I = Ae^{ik}}$

$$\left(k^2 e^{2iak_p} - k^2 - k_p^2 e^{2iak_p} + k_p^2\right)^2 =$$
$$= k^4 e^{4iak_p} - 2k^4 e^{2iak_p} - 2k^2 k_p^2 e^{2iak_p} + 2k^2 k_p^2 e^{2iak_p}$$
$$+ k^4 + 2k^2 k_p^2 e^{2iak_p} - 2k^2 k_p^2 + k_p^4 e^{4iak_p} - 2k_p^4 e^{2iak_p} + k_p^4)$$

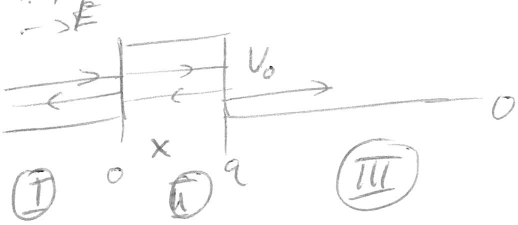
$\frac{k}{k'} \neq 1$ $\quad k' = k$



$k \sim \sqrt{E}$

$k' \sim \sqrt{E+V_0}$ $\quad \frac{k'}{k} = \frac{\sqrt{E-V_0}}{\sqrt{E}}$

21.11.4 X UKMTS.26



I: $\psi_I = c_1 e^{ikx} + c_2 e^{-ikx}$ $k = \frac{\sqrt{2mE}}{\hbar}$

$E > V_0$: II: $\psi_{II} = c_3 e^{ik'x} + c_4 e^{-ik'x}$ $k' = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

III: $\psi_{III} = c_5 e^{ikx}$ ← jen prošla

$\psi_I(0) = \psi_{II}(0)$: $c_1 + c_2 = c_3 + c_4$

$\psi_I'(0) = \psi_{II}'(0)$: $ik(c_1 - c_2) = ik'(c_3 - c_4)$

$\psi_{II}(a) = \psi_{III}(a)$: $c_3 e^{ik'a} + c_4 e^{-ik'a} = c_5 e^{ika}$

$\psi_{II}'(a) = \psi_{III}'(a)$: $ik'c_3 e^{ik'a} - ik'c_4 e^{-ik'a} = ikc_5 e^{ika}$

jeden koeficient volný – v podstatě normalizace $c_5 = 1$

$$c_1 + c_2 - c_3 - c_4 = 0$$
$$c_1 - c_2 - \frac{k'}{k}c_3 + \frac{k'}{k}c_4 = 0$$
$$e^{ik'a}c_3 + e^{-ik'a}c_4 = e^{ika}$$
$$k'e^{ik'a}c_3 - k'e^{-ik'a}c_4 = ke^{ika} \quad \leftarrow e^{ik'a}c_3 - e^{-ik'a}c_4 = \frac{k}{k'}e^{ika}$$

$$2e^{ik'a}c_3 = e^{ika}\left(1 + \frac{k}{k'}\right) \qquad c_3 = \frac{1}{2}e^{i(k-k')a}\left(1 + \frac{k}{k'}\right)$$
$$2e^{-ik'a}c_4 = e^{ika}\left(1 - \frac{k}{k'}\right) \qquad c_4 = \frac{1}{2}e^{i(k+k')a}\left(1 - \frac{k}{k'}\right)$$

$$c_1 + c_2 - \frac{1}{2}e^{i(k-k')a}\left(1 + \frac{k}{k'}\right) - \frac{1}{2}e^{i(k+k')a}\left(1 - \frac{k}{k'}\right) = 0$$
$$c_1 - c_2 - \frac{1}{2}\frac{k'}{k}e^{i(k-k')a}\left(1 + \frac{k}{k'}\right) + \frac{1}{2}\frac{k'}{k}e^{i(k+k')a}\left(1 - \frac{k}{k'}\right) = 0$$

$$\cancel{c_1 + c_2 - e^{i(k-k')a} = 0}$$
$$\cancel{c_1 - c_2 - \frac{k'}{k}e^{i(k-k')a}\frac{k}{k'} = 0}$$

21.11.4 contn'd X UKMTS.3

$$c_3 = \frac{1}{2} e^{i(k-k')a}\left(1+\frac{k}{k'}\right)$$

$$c_4 = \frac{1}{2} e^{i(k+k')a}\left(1-\frac{k}{k'}\right)$$

$$c_1 + c_2 - \frac{1}{2} e^{i(k-k')a}\left(1+\frac{k}{k'}\right) - \frac{1}{2} e^{i(k+k')a}\left(1-\frac{k}{k'}\right) = 0$$

$$c_1 - c_2 - \frac{1}{2}\frac{k'}{k} e^{i(k-k')a}\left(1+\frac{k}{k'}\right) + \frac{1}{2}\frac{k'}{k} e^{i(k+k')a}\left(1-\frac{k}{k'}\right) = 0$$

$$\cancel{2c_1 - \frac{1}{2} e^{i(k-k')a}\left(1+\frac{k}{k'}\right) - \frac{1}{2}\frac{k'}{k} e^{i(k-k')a}\left(1+\frac{k}{k'}\right) = 0}$$

$2c_2$

$$2c_1 - \frac{1}{2}\left(1+\frac{k'}{k}\right)\left(1+\frac{k}{k'}\right) e^{i(k-k')a} - \frac{1}{2}\left(1-\frac{k'}{k}\right)\left(1-\frac{k}{k'}\right) e^{i(k+k')a} = 0$$

$$2c_2 - \frac{1}{2}\left(1-\frac{k'}{k}\right)\left(1+\frac{k}{k'}\right) e^{i(k-k')a} - \frac{1}{2}\left(1+\frac{k'}{k}\right)\left(1-\frac{k}{k'}\right) e^{i(k+k')a} = 0$$

$$2c_1 - \frac{1}{2}\left(1+\frac{k'}{k}+\frac{k}{k'}+1\right) e^{i(k-k')a} - \frac{1}{2}\left(1-\frac{k'}{k}-\frac{k}{k'}+1\right) e^{i(k+k')a} = 0$$

$$2c_2 - \frac{1}{2}\left(1-\frac{k'}{k}+\frac{k}{k'}-1\right) e^{i(k-k')a} - \frac{1}{2}\left(1-\frac{k}{k'}+\frac{k'}{k}-1\right) e^{i(k+k')a} = 0$$

$$2c_1 - \frac{1}{2}\left(2+\frac{k'^2+k^2}{kk'}\right) e^{i(k-k')a} - \frac{1}{2}\left(2-\frac{k'^2+k^2}{k'k}\right) e^{i(k+k')a} = 0$$

$$2c_2 + \frac{1}{2}\frac{k'^2-k^2}{k'k} e^{i(k-k')a} + \frac{1}{2}\frac{k^2-k'^2}{k'k} e^{i(k+k')a} = 0$$

$$2c_1 - e^{i(k-k')a} - e^{i(k+k')a} - \frac{k'^2+k^2}{2kk'} e^{i(k-k')a} + \frac{k'^2+k^2}{2k'k} e^{i(k'+k)a} = 0$$

$$2c_2 + \frac{1}{2}\frac{k'^2-k^2}{k'k}\left[e^{i(k-k')a} - e^{i(k+k')a}\right] = 0$$

$$2c_1 = e^{ika}\left[e^{-ik'a} + e^{ik'a} + \frac{k'^2+k^2}{2kk'} e^{-ik'a} - \frac{k'^2+k^2}{2kk'} e^{ik'a}\right]$$

$$2c_2 = \frac{1}{2}\frac{k'^2-k^2}{k'k} e^{ika}\left[e^{ik'a} - e^{-ik'a}\right]$$

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$$c_1 = \frac{e^{ika}}{2}\left[e^{-ik'a} + e^{ik'a} + \frac{k'^2+k^2}{2k'k}\left(-e^{ik'a} + e^{-ik'a}\right)\right]$$

$$c_2 = \frac{1}{4}\,\frac{k'^2-k^2}{k'k}\,e^{ika}\left(e^{ik'a} - e^{-ik'a}\right)$$

$$c_1 = e^{ika}\left[\cos(k'a) + i\frac{k'^2+k^2}{2k'k}\sin(k'a)\right]$$

$$c_2 = ie^{ika}\,\frac{k'^2-k^2}{2k'k}\sin(k'a)$$

$$R = \left|\frac{c_2}{c_1}\right|^2 = \frac{\left(\frac{k'^2-k^2}{2k'k}\right)^2\sin^2(k'a)}{\left[\cos(k'a) + i\frac{k'^2+k^2}{2k'k}\sin(k'a)\right]\left[\cos(k'a) - i\frac{k'^2+k^2}{2k'k}\sin(k'a)\right]}$$

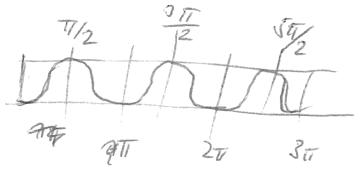
$$= \frac{(k'^2-k^2)\sin^2(k'a)}{\left[4k'^2k^2\cos^2(k'a) + \left(\frac{k'^2+k^2}{\cancel{\ }}\right)^2\sin^2(k'a)\right]}$$

$$T = \left|\frac{c_5}{c_1}\right|^2 = \frac{1}{\left[\cos(k'a) + i\frac{k'^2+k^2}{2k'k}\sin(k'a)\right]\left[\cos(k'a) - i\frac{k'^2+k^2}{2k'k}\sin(k'a)\right]}$$

$$= \frac{4k'^2k^2}{4k'^2k^2\underbrace{\cos^2(k'a)}_{1-\sin^2} + (k^2+k'^2)^2\sin^2(k'a)} = \frac{4k'^2k^2}{4k'^2k^2 + (k^2-k'^2)^2\sin^2(k'a)}$$

$$\frac{R}{T} \overset{?}{=} \left|\frac{c_2}{c_5}\right|^2 = \frac{(k'^2-k^2)^2}{4k'^2k^2}\sin^2(k'a)$$ ← above step/well energy

$\sin^2$:

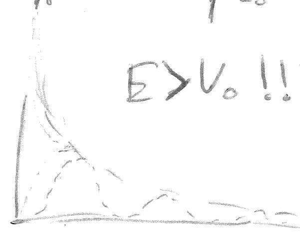


$$= \frac{\left(2m(E_0-V) - 2mE_0\right)^2}{4\,2^2m^2(E_0-V)^2E_0^2}\sin^2(k'a) =$$

$$k' = \frac{\sqrt{2m(E_0-V)}}{\hbar} = k\cdot\sqrt{\frac{E_0-V}{E_0}}$$

$$= \frac{(E_0 - V - E_0)^2}{(E_0-V)^{\cancel{2}}E_0^{\cancel{2}}}\sin^2(k'a) = \frac{V^2}{(E_0-V)E_0}\sin^2(k'a)$$

$E > V_0$!!!



$V>0$ $$\lim_{E_0\to V+}\frac{V^2}{(E_0-V)E_0}\sin^2(k'a) = \lim_{E_0\to V+}\frac{V^2}{\delta V}\sin^2\left(\frac{\sqrt{2m(E_0-V)}}{\hbar}a\right) =$$

$$= \lim_{E_0\to V+}\frac{V}{\delta}\,\cancel{\sin^2}\,\frac{2m(E_0-V)}{2\hbar}a^2 = V\frac{2ma^2}{2\hbar}$$ OK – výška bariéry · délka²

$V<0$ $$\lim_{E_0\to 0+}\underbrace{\frac{V^2}{(E_0-V)}}_{\text{konečné}}\frac{1}{E_0}\sin^2(k'a) \to C\cdot\frac{1}{E_0}\sin^2(k'a)$$ OK – nekonečno, pokud $\sin(k'a)=0$