Tok elektrického prúdu v nanoštruktúrach

Habilitačná prednáška

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Katedra fyziky, FEI STU

S T U

F E I

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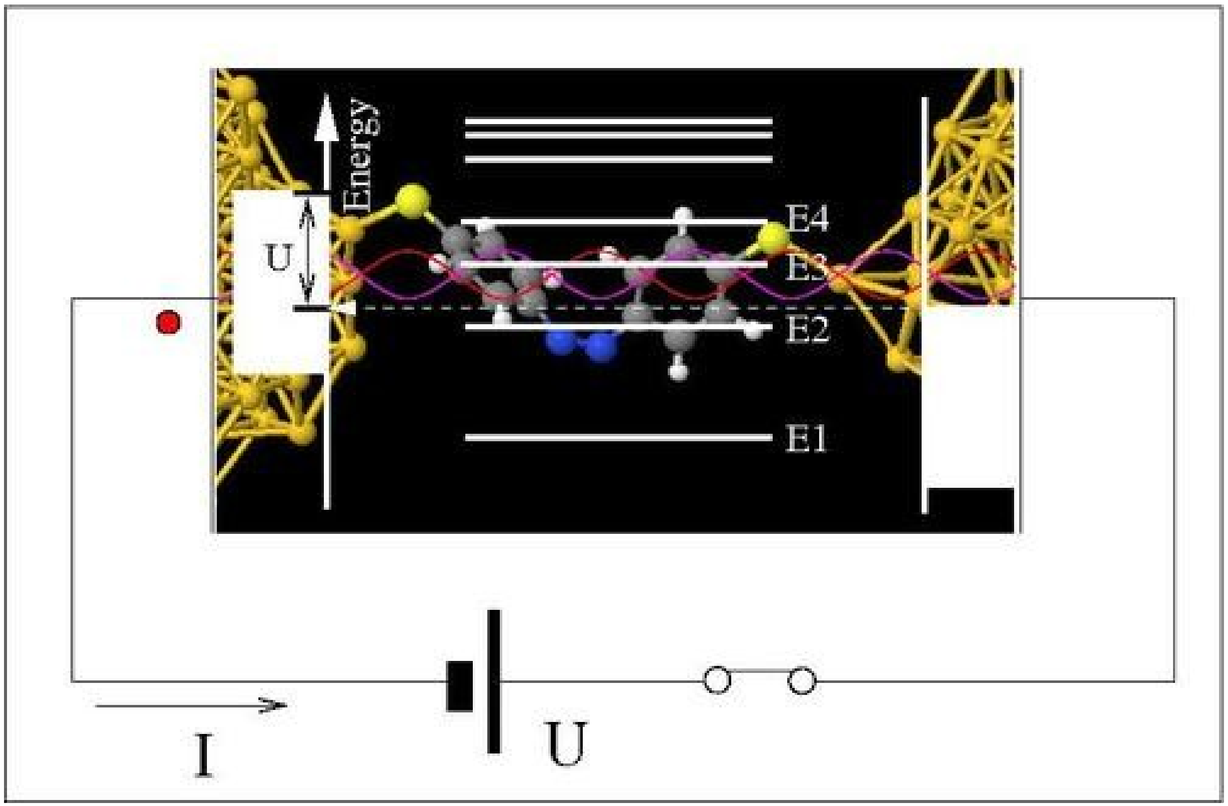


Ab-initio model

Nerovnovážny kvantový proces

Kvalitatívne porozumenie

Merateľné vlastnosti

$I(U), \ G = dI/dU|_{U=0}$

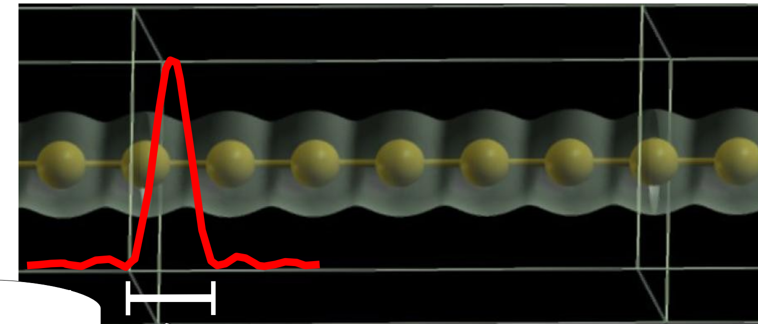
[Konduktancia]

Osnova prednášky

- Pohyb elektrónu a vlnová funkcia – vlnový balík
- Pravdepodobnosť prechodu cez nanoštruktúru - transmisia
- Pohyb mnohých elektrónov – ortogonálne vlnové balíky
- Landauerov vzťah pre elektrický prúd cez nanoštruktúru
- Transport cez realistické nanoštruktúry

Vlnový balík

- Časový vývoj stavu – Schrodingerova rovnica



$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} + u_e$$

$\Delta x \Delta k \geq 4\pi$ "Heisenbergov princíp neurčitosti"

- Stacionárne stavy:

$$\hat{H}\phi_k(\vec{r}) = E_k\phi_k(\vec{r})$$

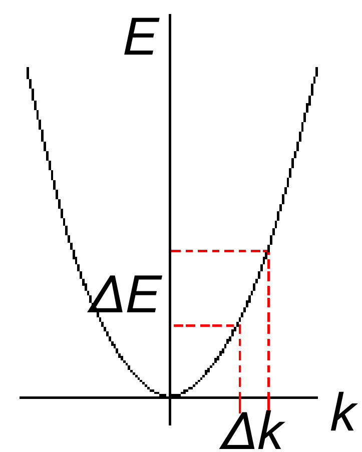
$$\phi_k(x) = Ae^{ikx}, \quad E_k = \frac{\hbar^2 k^2}{2m}, \; p = \hbar k$$

$$\psi_k(x,t) = \phi_k(x)e^{-iE_k t/\hbar}$$

$$P(x) = |\psi_k(x,t)|^2 = |A|^2$$

- **Vlnový balík:** súčet (integrál) vlastných stavov

$$\psi^{R/L}_{E,\Delta E}(x,t) = \int_{k-\Delta k/2}^{k+\Delta k/2} dk A e^{i(\pm kx - E_k t/\hbar)}$$



- lokalizovaný v priestore, a pohybuje sa **grupovou rýchlosťou**

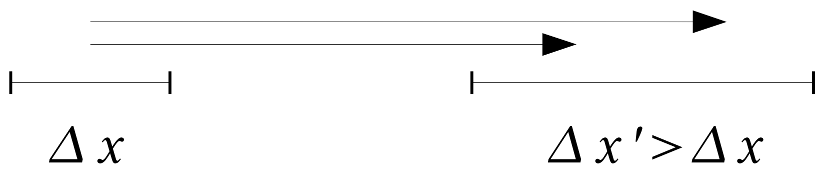
$$P(x) = |\psi^R_{E,\Delta E}(x,t)|^2 = 4|A|^2\frac{\sin^2(\frac{\Delta k}{2}(x-vt))}{(x-vt)^2}, v = \frac{1}{\hbar}\frac{dE_k}{dk}$$

- **normovateľný na 1** (pre každé *t>0)* ak

$$\int_{-\infty}^{\infty} dx P(x) = 1 \Rightarrow A = (2\pi\Delta k)^{-1/2}$$

Disperzia vlnového balíka

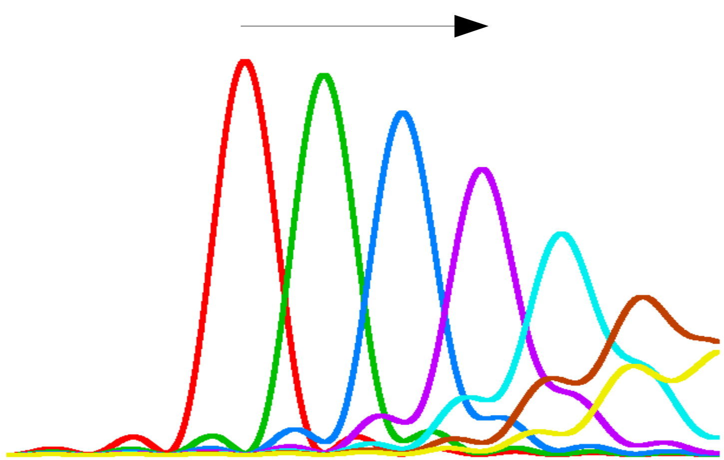
- **Disperzia** - nevyhnutná v dôsledku Heisenbergovho princípu neurčitosti:



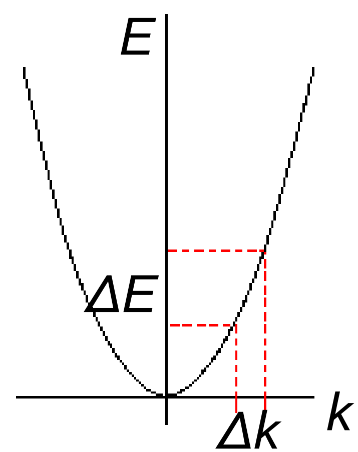
$$\Delta x \Delta p > \hbar$$

$$\Delta x' = \Delta x + \Delta v\, t\,, \Delta v = \frac{\hbar}{\Delta x\, m}$$

$$v = \frac{\partial E(k)}{\hbar \partial k}\,, \Delta v = \frac{\partial^2 E(k)}{\hbar \partial^2 k} \Delta k = \frac{\Delta p}{m}$$



keď E(k) nie je lineárna funkcia
alebo pre Δk/k >> 1

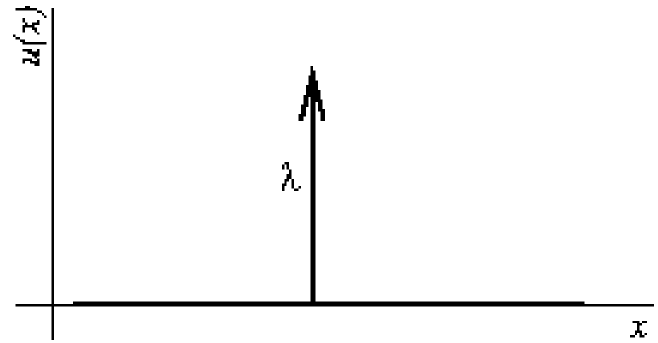


“Disperzný vzťah”

$$(p = \hbar k)$$

Transmisný koeficient, transmisia

- Hamiltonián: $\hat{H} = -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} + u_{eff}^{\lambda}(x)$



- Stacionárne riešenia pre $E_k = \hbar^2 k^2/(2m_e)$

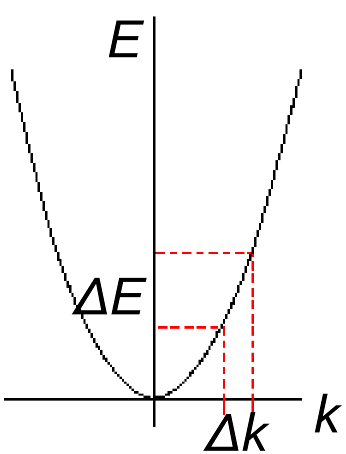
$$\phi_k^R(x) = A \begin{cases} e^{ikx} + r_k e^{-ikx} & x << 0 \\ t_k e^{ikx} & x >> 0 \end{cases} \qquad \phi_k^L(x) = A \begin{cases} \tilde{t}_k e^{-ikx} & x << 0 \\ \ldots \end{cases}$$

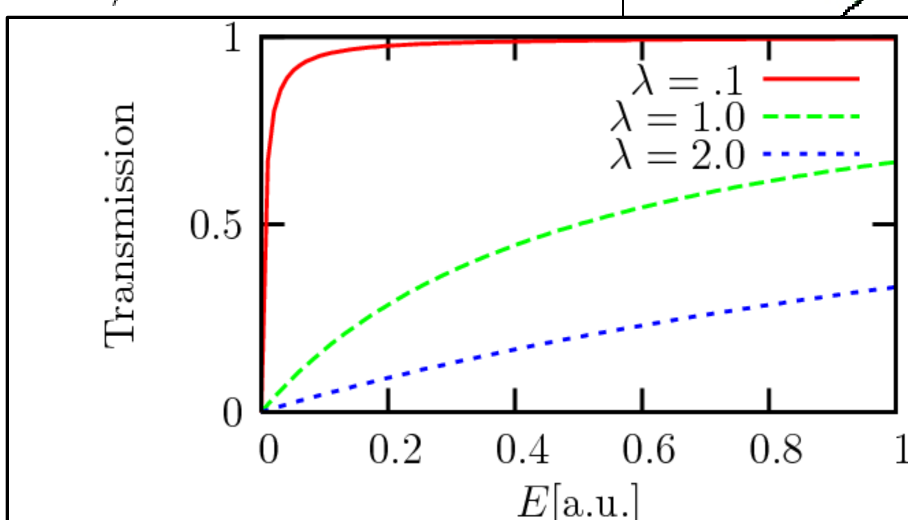
Transmisia: $T(E) = |t_k|^2$

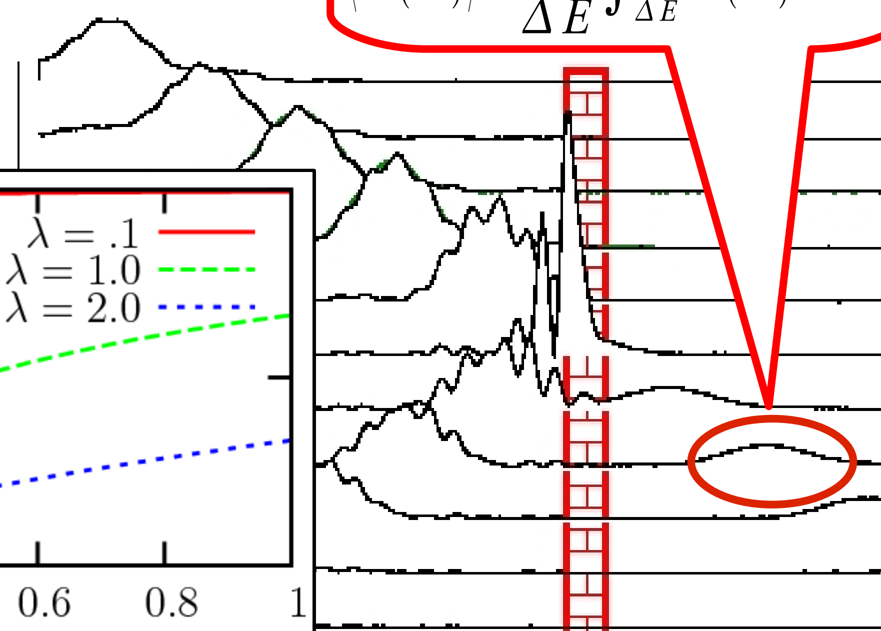
$$\langle T(E) \rangle = \frac{1}{\Delta E}\int_{\Delta E} T(E)\, dE$$

- Balík

$$\psi_{E,\Delta E}^R(x,t) = \int_{k-\Delta k/2}^{k+\Delta k/2} A\phi_k^R(x) e^{-iE_k t/\hbar}$$







Transmisný koeficient, rezonancia

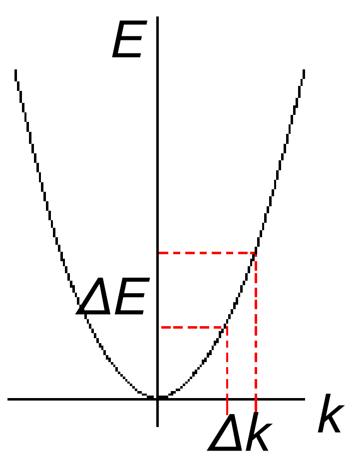
- Hamiltonián: $\hat{H} = -\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2} + u^{\lambda}_{eff}(x)$

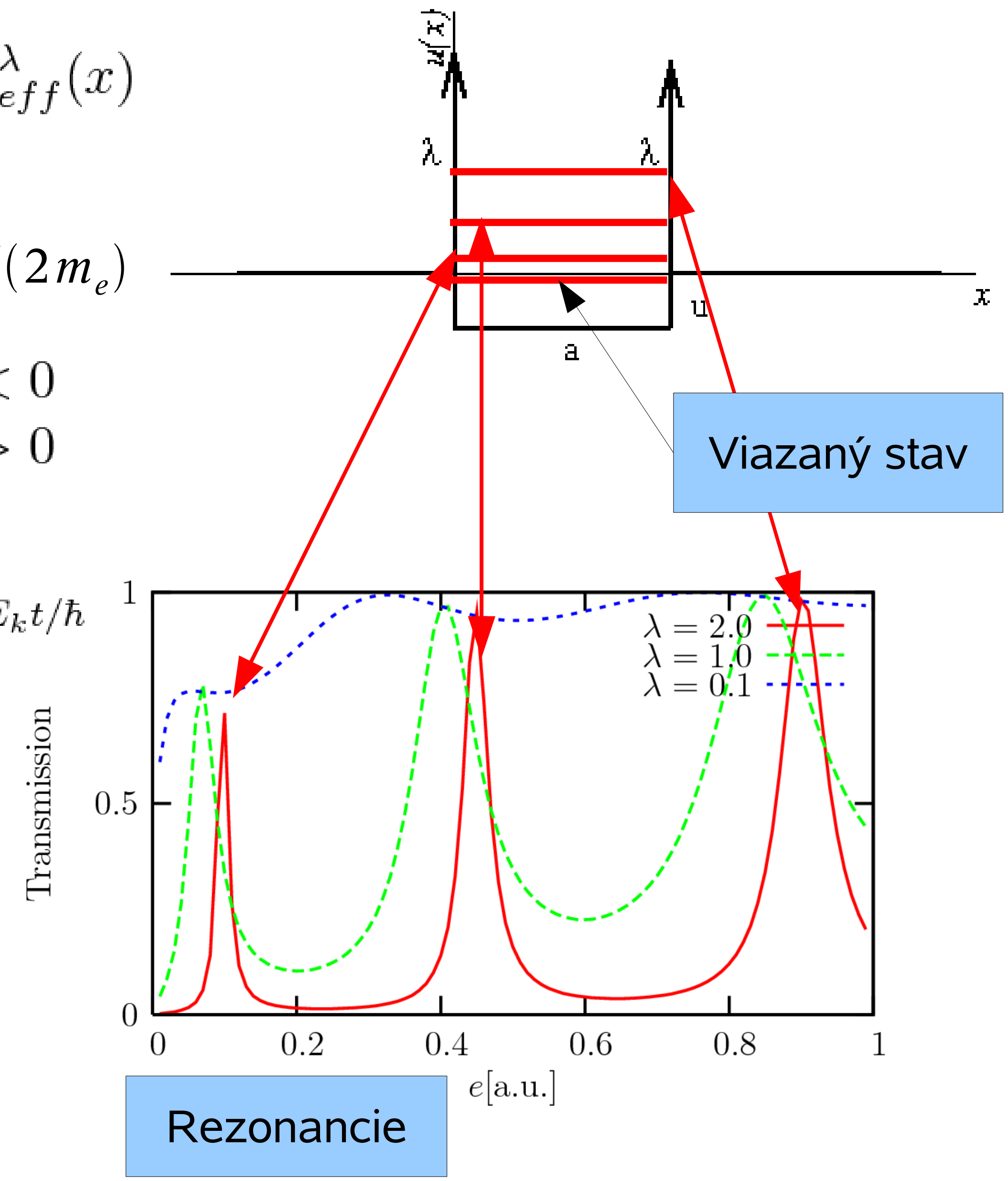
- Stacionárne riešenia pre $E_k = \hbar^2 k^2 / (2 m_e)$

$$\phi^R_k(x) = A \begin{cases} e^{ikx} + r_k e^{-ikx} & x << 0 \\ t_k e^{ikx} & x >> 0 \end{cases}$$

- Balík

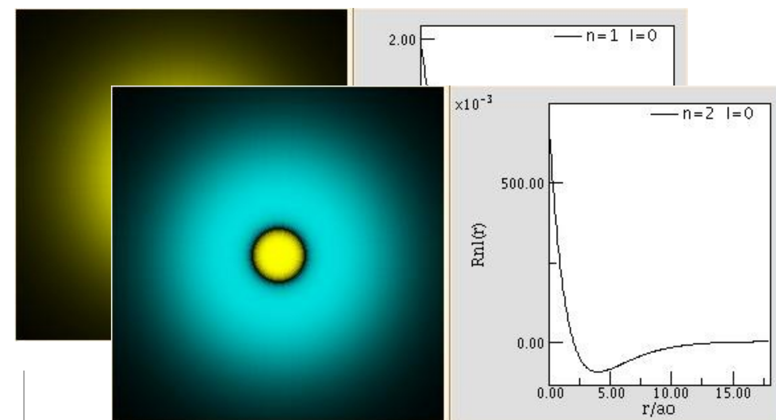
$$\psi^R_{E,\Delta E}(x,t) = \int_{k-\Delta k/2}^{k+\Delta k/2} A\phi^R_k(x) e^{-iE_k t/\hbar}$$





Kvantový popis mnoho elektrónov

- **Nestacionárna teória funkcionálu hustoty** [Time-dependent density-functional theory, TDDFT, E. Runge, E. K. U. Gross (1984)] – elektróny ako fiktívne neinteragujúce častice, pohybujúce sa v efektívnom potenciáli.

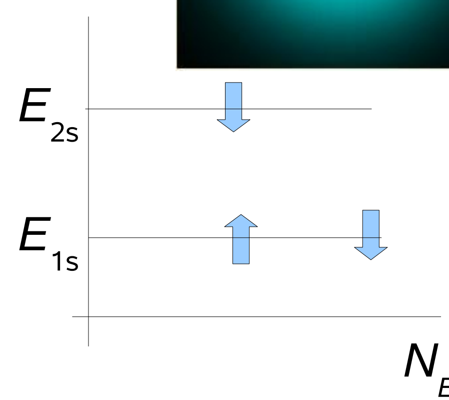


- Elektróny sa nachádzajú v stavoch daných **ortogonálnymi** vlnovými funkciami $\psi_n(\vec{r},t)$

$$\int_{-\infty}^{+\infty} dx \psi_n^*(x)\psi_m(x) = \delta_{nm}$$

- **Pauliho princíp** – najviac 2 elektróny v jednom stave, potom *exaktná* hustota bude

$$n(\vec{r},t) = \sum_n N_n |\psi_n(\vec{r},t)|^2, \quad N_n \in \{0,1,2\}$$



- Vlnové funckie sa menia s časom podľa rovnice

$$i\hbar\frac{\partial}{\partial t}\psi_n(\vec{r},t) = \hat{H}\psi_n(\vec{r},t), \quad \hat{H} = -\frac{\hbar^2}{2m_e}\Delta + u_{eff}[n(\vec{r}',t')](\vec{r},t)$$

1D kvantový vodič

- stacionárna Schrödingerova rovnica

$$\hat{H}\phi_n(\vec{r}) = E_n\phi_n(\vec{r}), \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

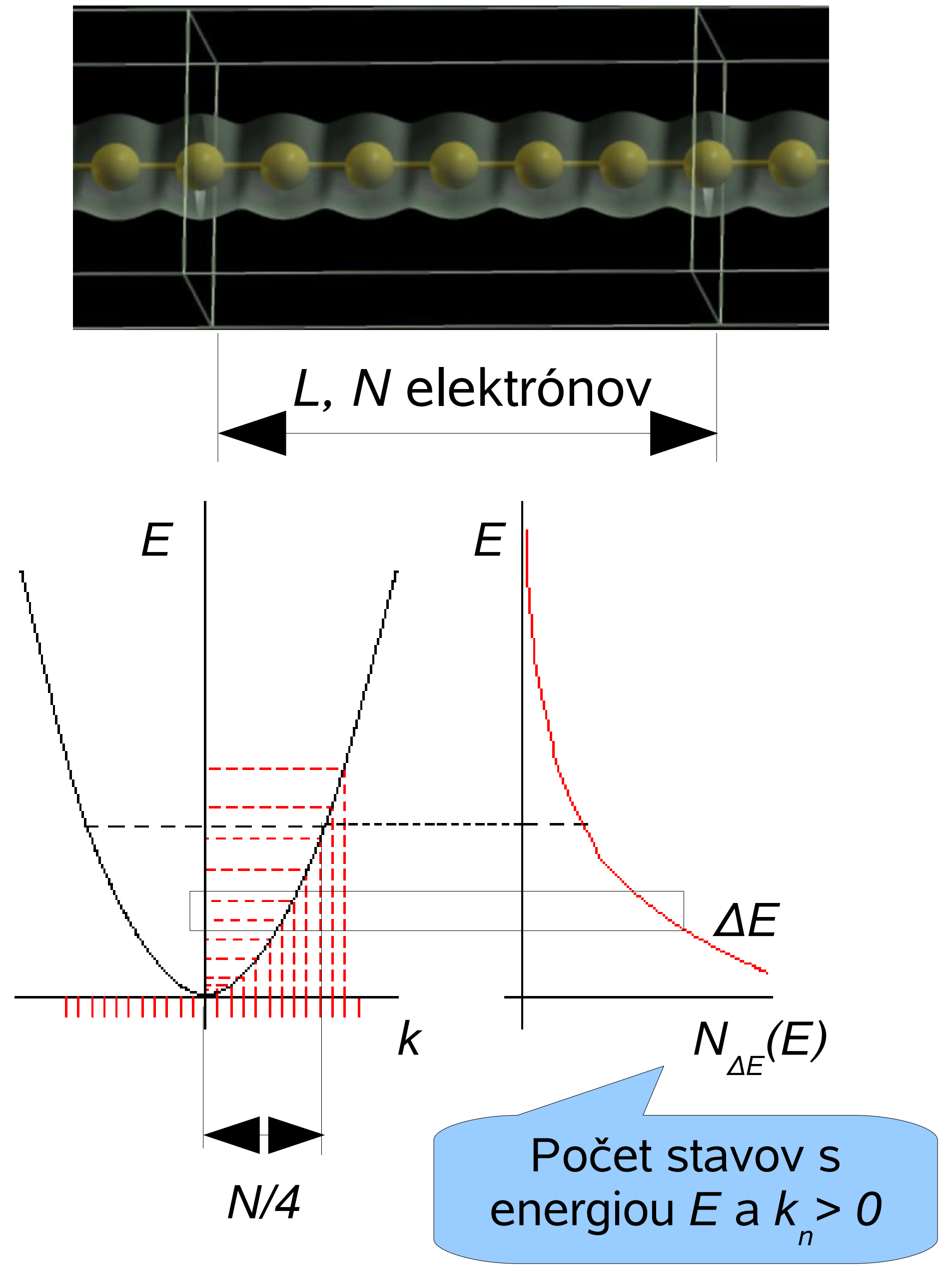
$$\phi_n(x) = \frac{1}{\sqrt{L}}e^{ik_nx}, \quad E_n = \frac{\hbar^2 k_n^2}{2m}$$

$$k_n = \frac{2\pi}{L}n, \quad n = 0, \pm 1, \pm 2, \ldots$$

- hustota, energia

$$n(x) = \sum_{|n|<N/4} 2|\phi_n(x)|^2 = N/L$$

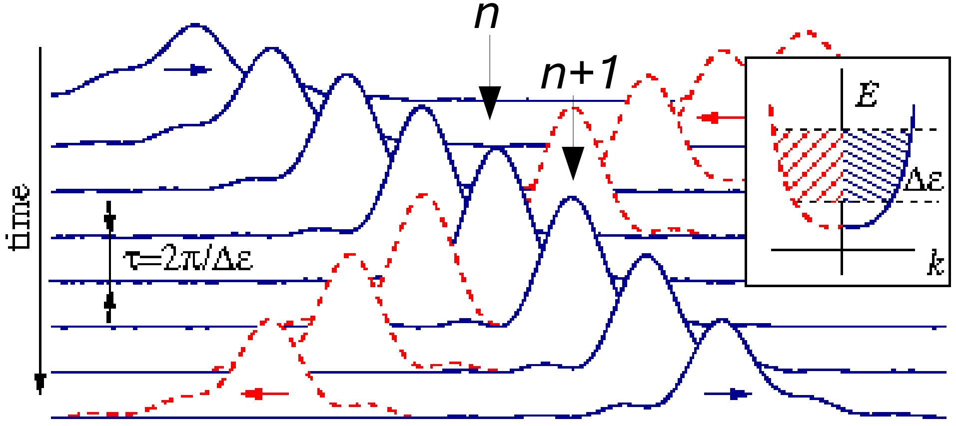
$$E = \sum_{|n|<N/4} 2E_n = \ldots$$



Ortogonálne vlnové balíky

- Balíky $$\psi^{R/L}_{E,\Delta E,n}(x) = \frac{\hbar}{\sqrt{2\pi m_e \Delta E}} \int_{k-\Delta k/2}^{k+\Delta k/2} dk \sqrt{k}\,\phi_k^{R/L}(x)\; e^{-iE_k t/\hbar}\Big|_{t=n\tau}$$

"Stroboskopické balíky"



s časovým krokom $\tau = \dfrac{2\pi\hbar}{\Delta E}$

sú ortogonálne:

$$\int_{-\infty}^{+\infty} dx\, \psi^*_{E,\Delta E,n}(x)\psi_{E,\Delta E,m}(x) = \delta_{nm}$$

- "Princíp neurčitosti": $\Delta E\,\tau \sim 2\pi\hbar$

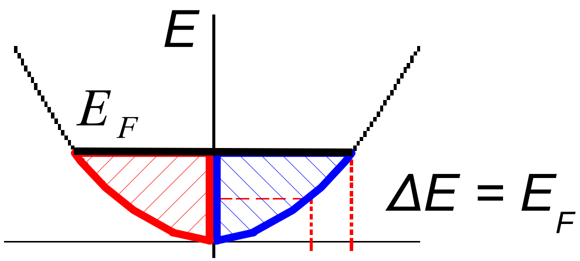
- Navzájom ortogonálne sú aj balíky
  - s disjunktných intervalov energií
  - naopak idúce ["*R*" s "*L*"]

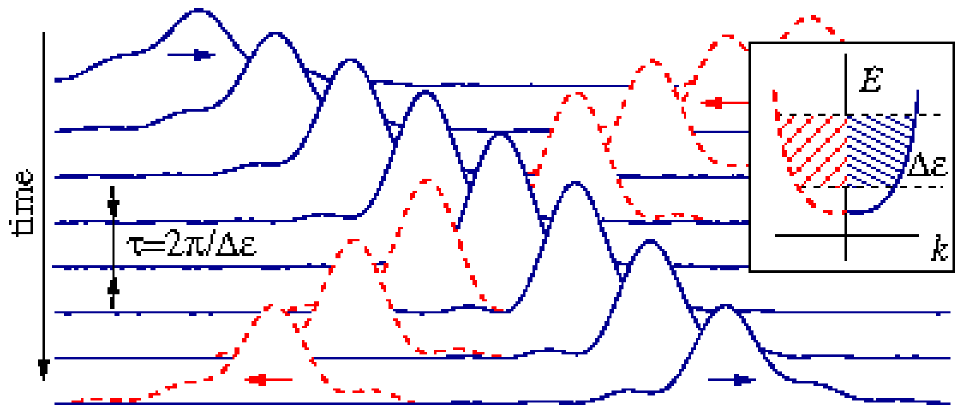
- Všetky balíky dokopy tvoria **úplný systém funkcií**

Obsadenie balíkov

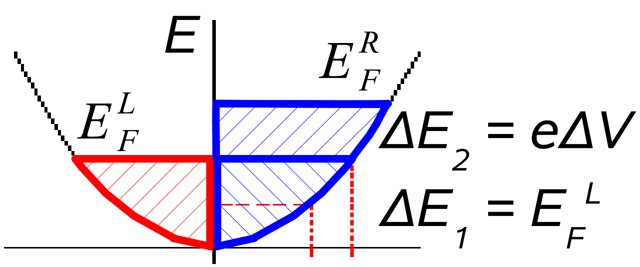
- **Fermiho energia** - rezervoár elektrónov naplní všetky stavy s $E<E_F$

$$n(\vec{r},t) = \sum_{occ} 2|\psi_n(\vec{r},t)|^2$$



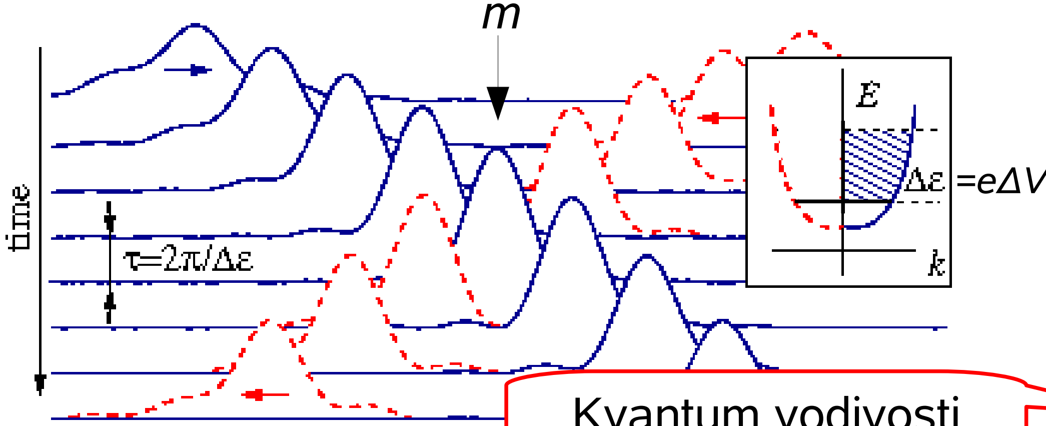


- **Aplikované napätie** – rozdiel Fermiho energií rezervoárov pripojených na vodič zľava a zprava $\Delta V = (E_F^R - E_F^L)/e$



Landauerov vzťah pre elektrický prúd

Čistý vodič:



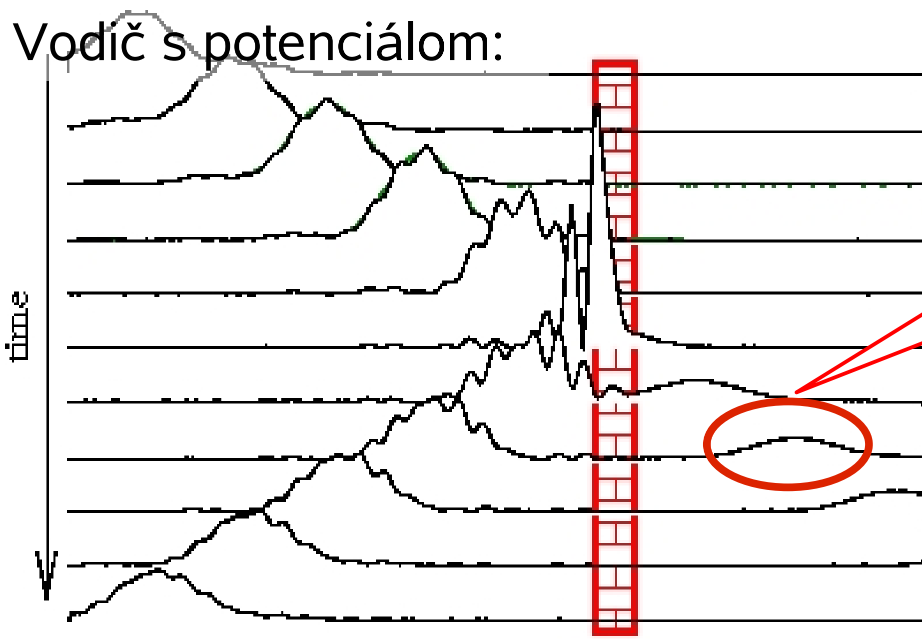
$$I_m(t) = \frac{e}{\tau} N_m(t)$$

$$I = \frac{e}{2\pi\hbar/(eV)} N_m(t) = \frac{2e^2}{h} V$$

Kvantum vodivosti

$$G_0 = \frac{2e^2}{h}, R_0 = \frac{h}{2e^2} \approx 12.9\text{k}\Omega$$

Vodič s potenciálom:



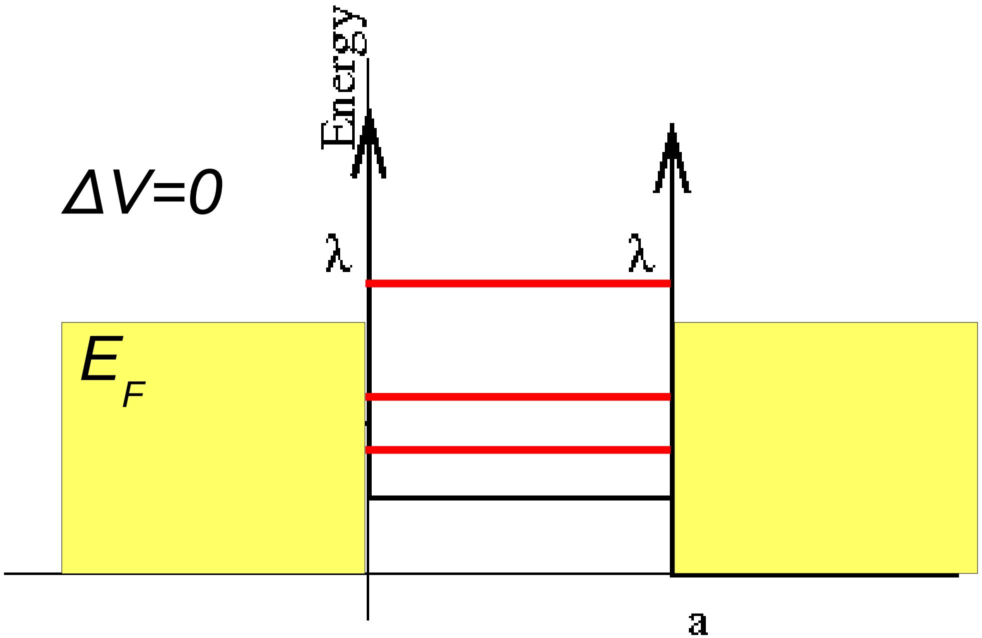
Transmisia dá obsadenie:
$N_m(t)$ = 2<T(E)>

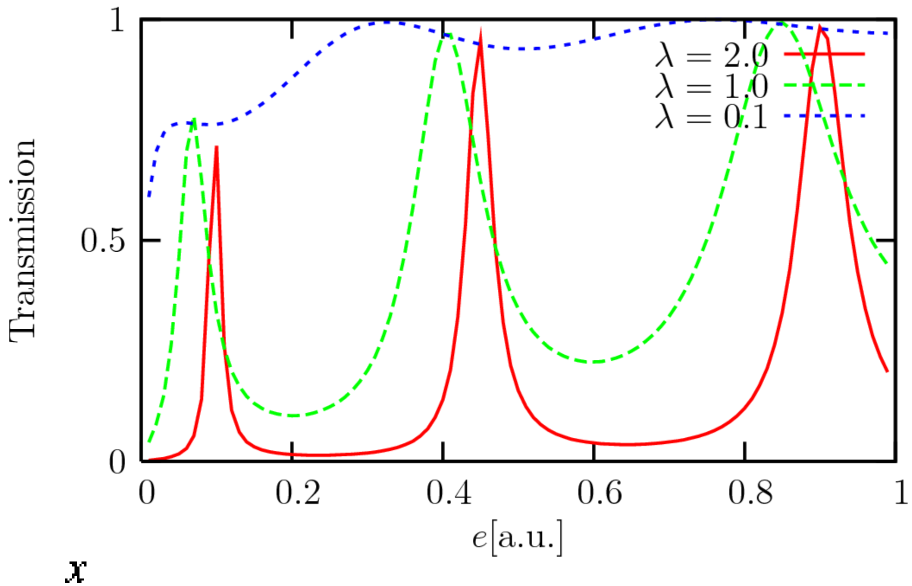
Viac kanálov

=> Landauerov vzťah

$$I = \frac{2e}{h} \int_{e\Delta V} \sum_i T_i(E) dE$$

Rezonančné tunelovanie, *I/V*

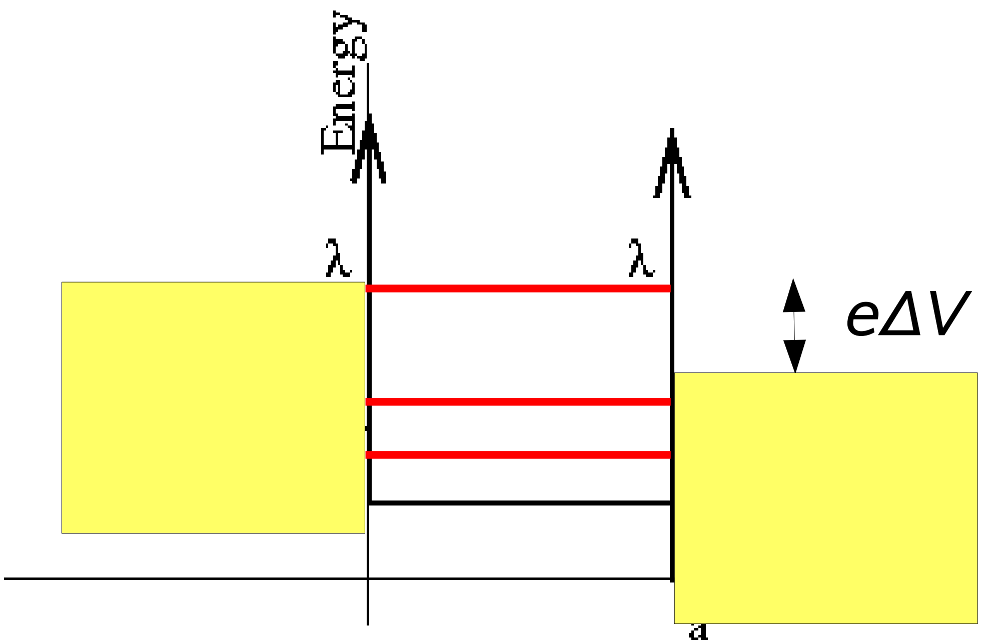


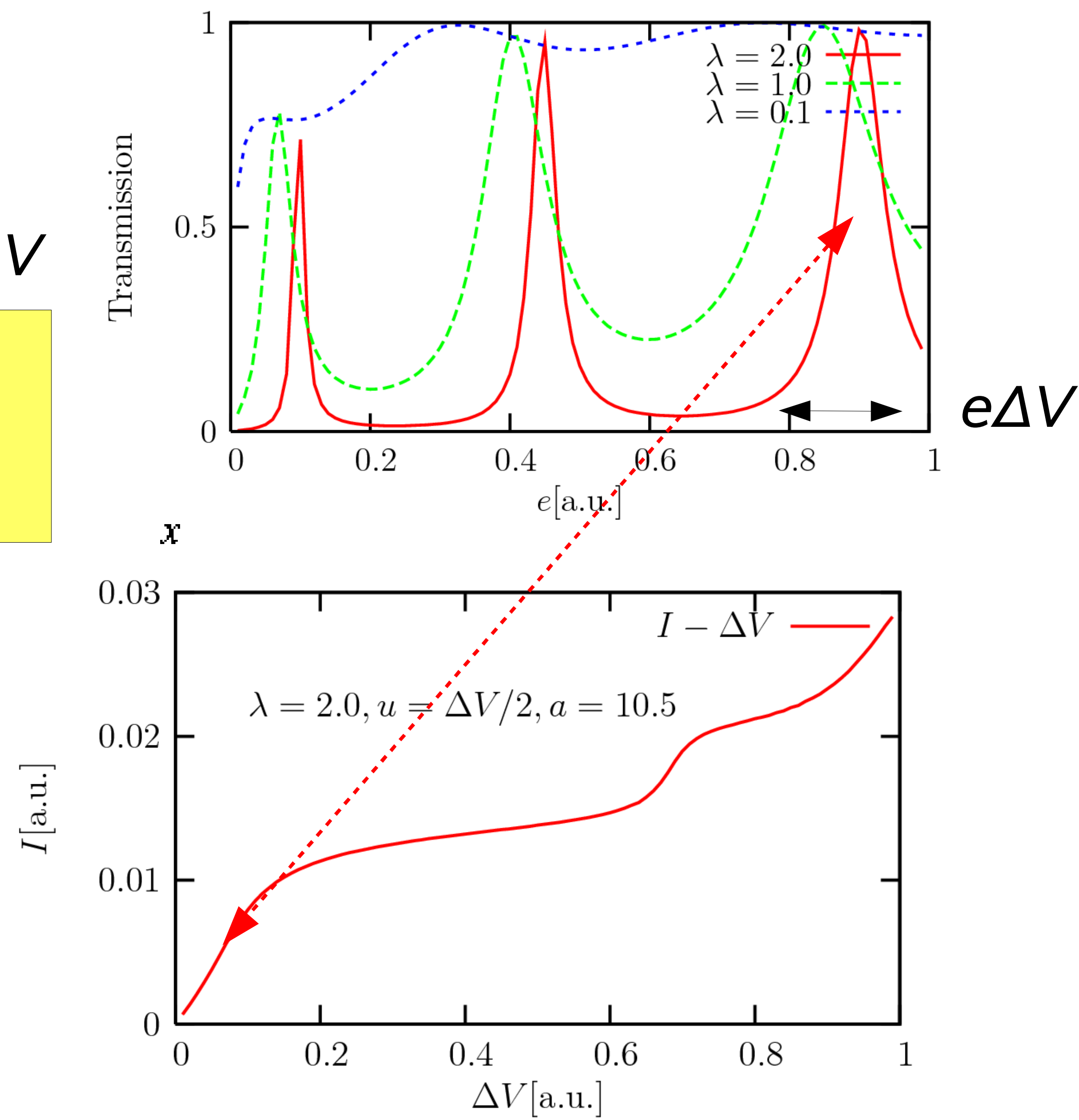


Stacionárny prúd:

$$I = \frac{2e}{h}\int_{e\Delta V} T(E)dE$$

Rezonančné tunelovanie, *I/V*





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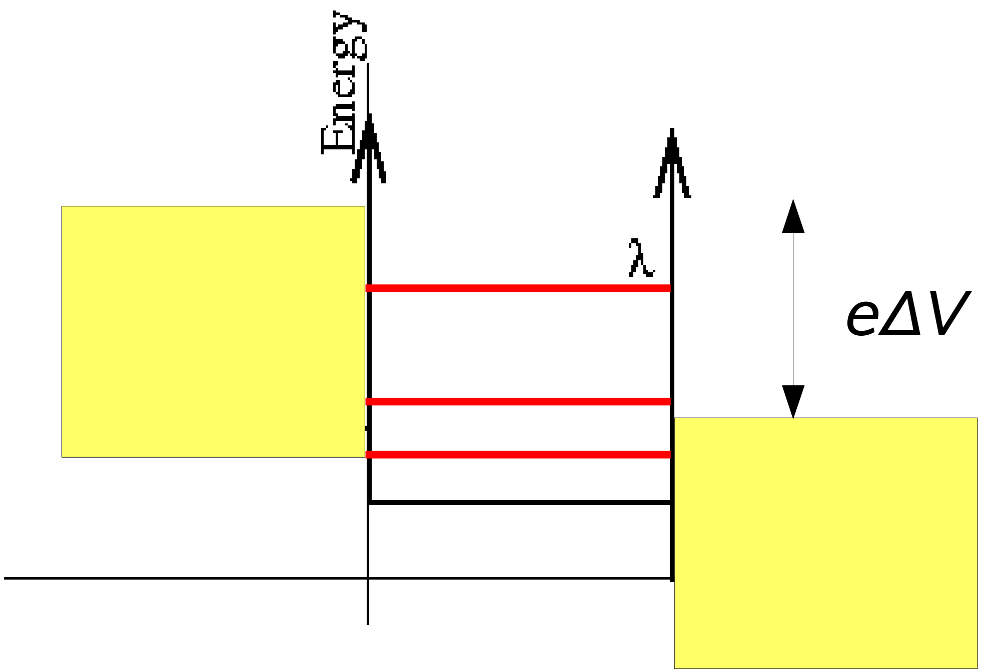
Rezonančné tunelovanie, *I/V*



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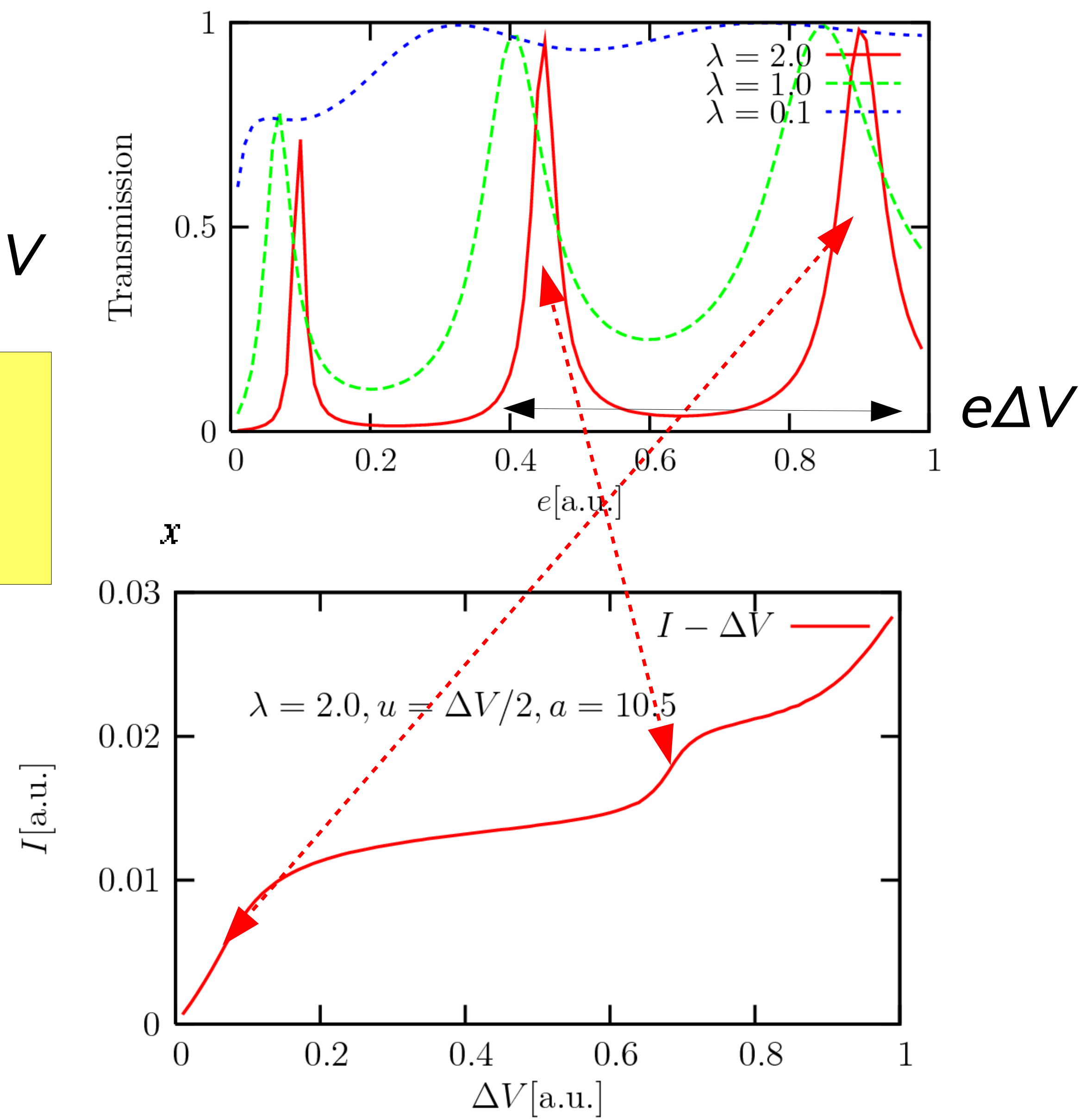
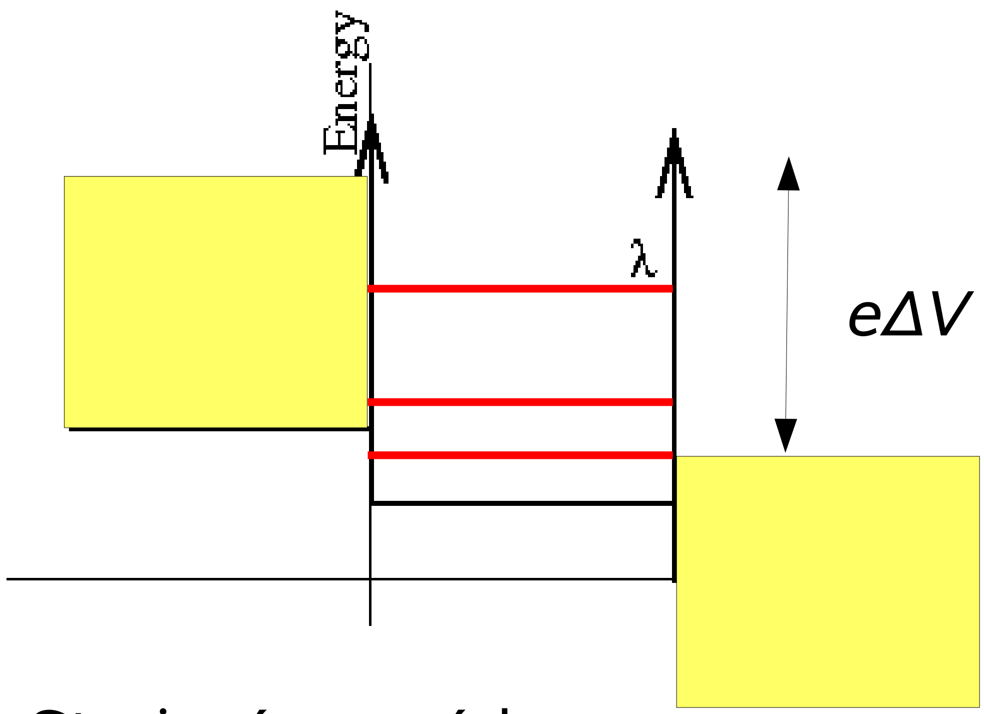
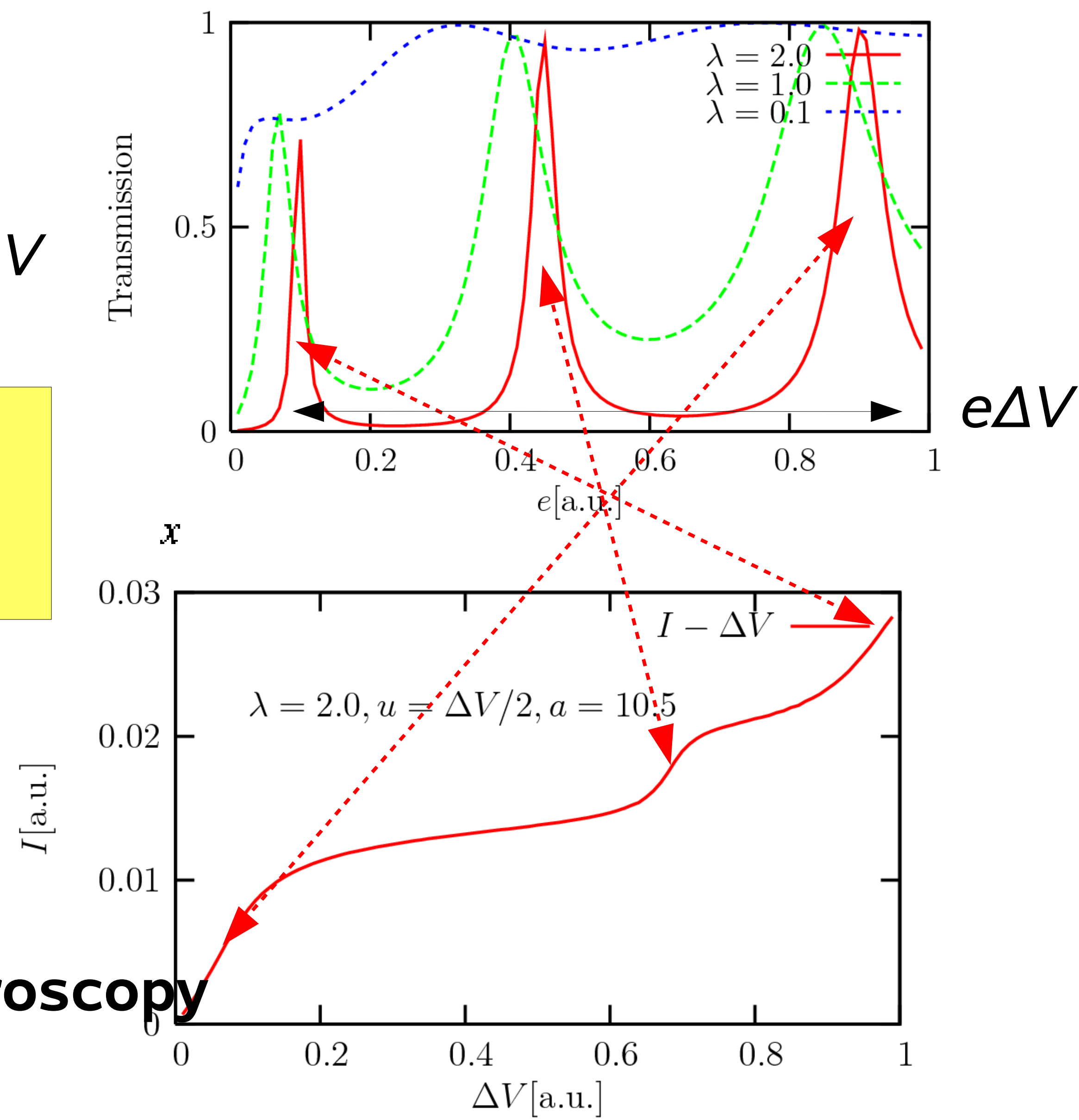


Rezonančné tunelovanie, *I/V*





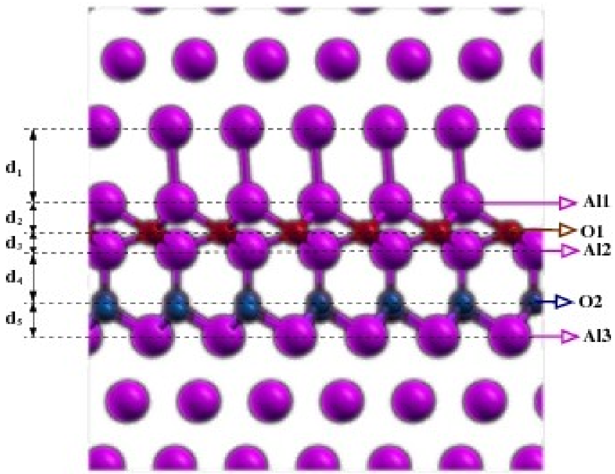
Stacionárny prúd:

$$I = \frac{2e}{h} \int_{e\Delta V} T(E) dE$$

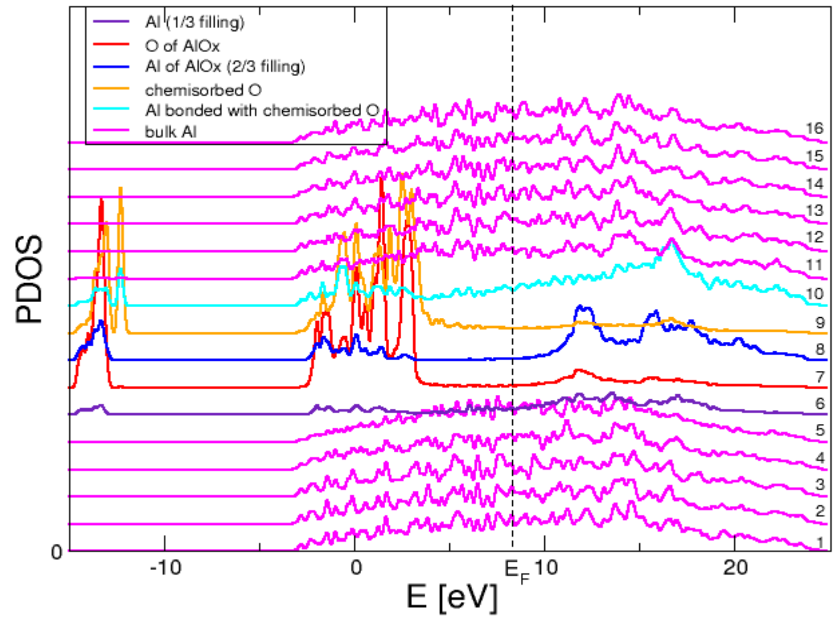
=> Scanning Tunneling Spectroscopy (STS/STM)

Transport cez rozhranie *Al/AlO$_x$/Al*

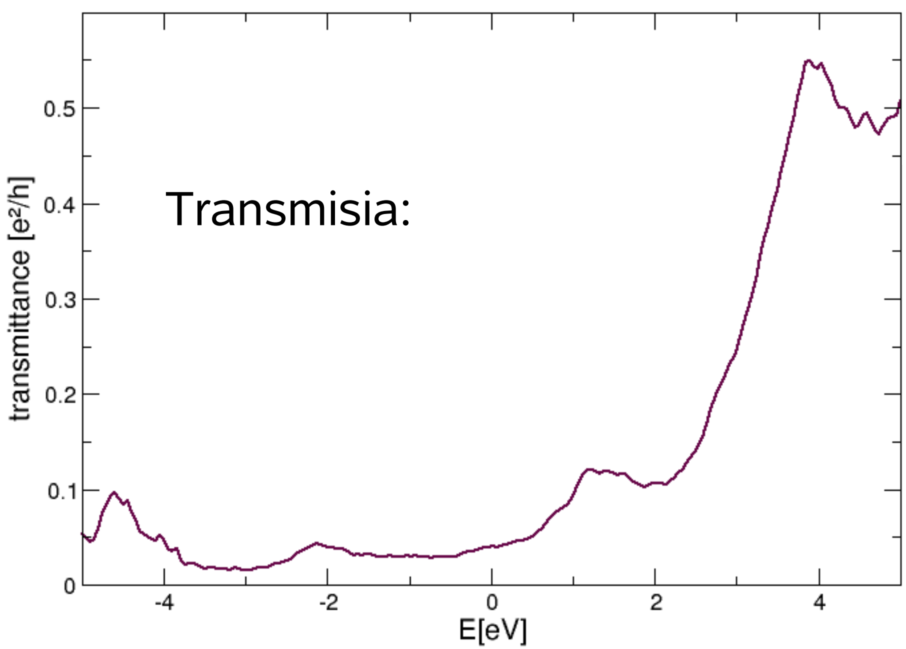
Atomárna geometria:

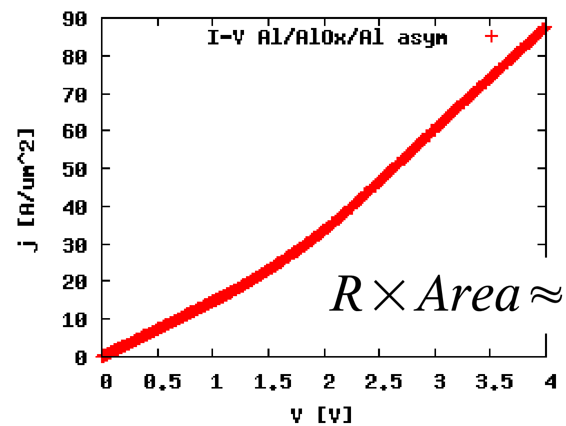


Lokálna hustota stavov:



Transmisia:

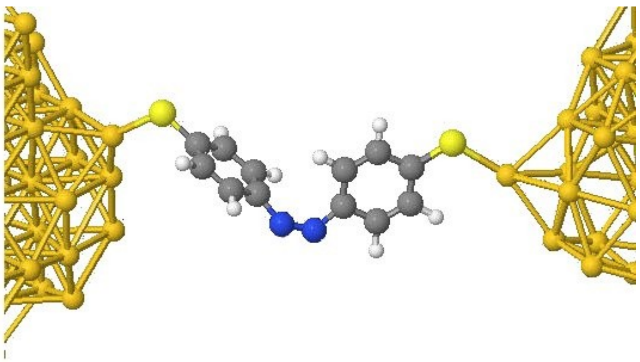




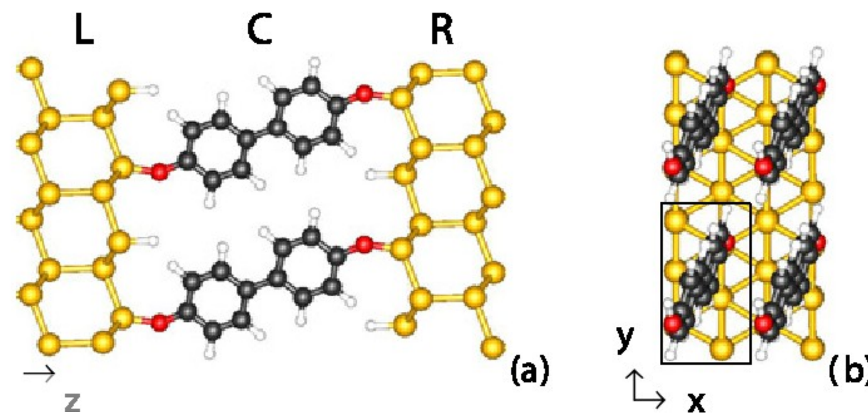
$$R \times Area \approx 0.04\,\Omega\,\mu m^2$$

M. Diešková, A. Ferretti, PB (2009),
M. Diešková, M. Konôpka, PB (2007)

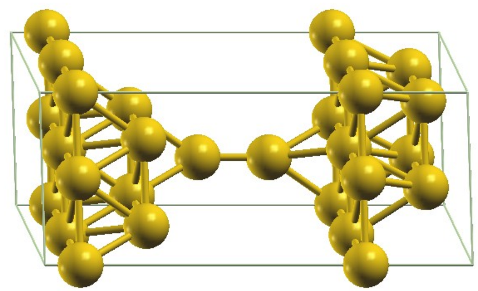
...a iné reálne nanokontakty



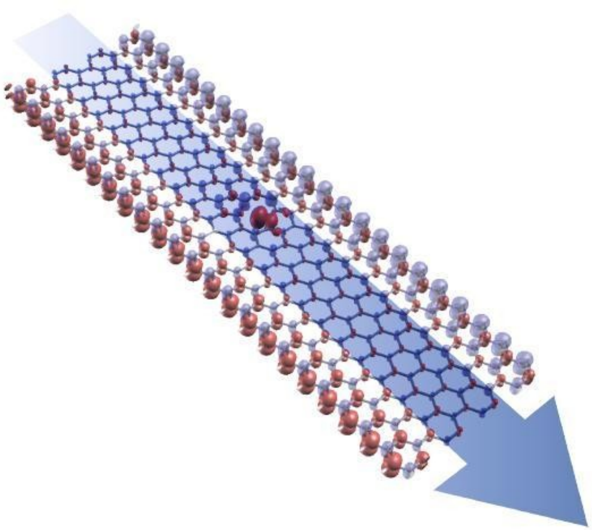
Au-Azobenzen-Au
Konôpka, Turanský, Štich (2008)



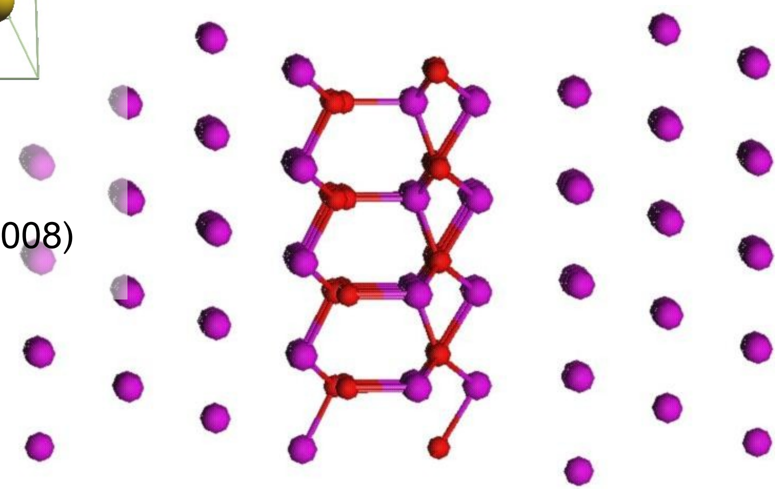
Si-$C_{12}H_{10}O_2$-Si
Bonferroni, Ferretti, Molinari (2008).



Au kontakt,
Verstraete, PB, Godby (2008)



Graphene
Rignanese, Charlier (2008)



Al-AlO_x-Al rozhranie
Diešková, Konôpka, PB (2007)

Zhrnutie

- Vlnový balík – vlnová funkcia dostáva zmysel
- Ortogonálne vlnové balíky pre mnoho elektrónov
- Landauerov vzorec pre elektrický prúd
- Reálne nanoštruktúry