

Dva typy řešení stacionární Schrödingerovy rovnice

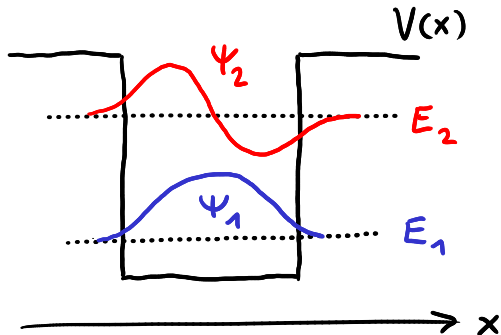
stacionární SR
$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi(x) = E \Psi(x)$$

→ soubor vlastních stavů $\Psi_n(x)$ a vlastních energií E_n

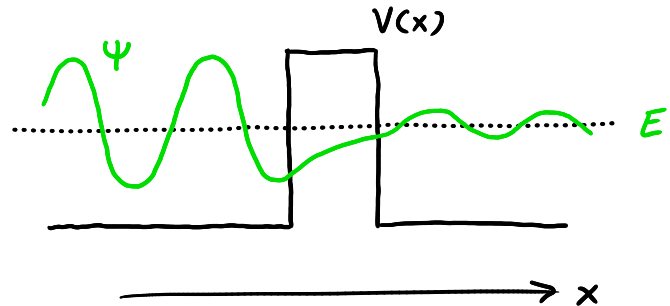
→ soubor stacionárních stavů $\psi_n(x,t) = \Psi_n(x) e^{-\frac{i}{\hbar} E_n t}$

nestacionární SR
$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

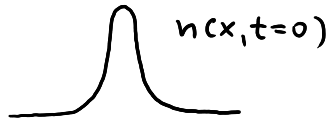
• vázané stavy



• rozptylové stavy



Připomínka difúze a rovnice kontinuity



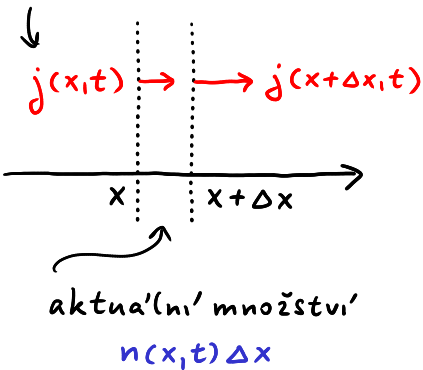
čas →



- koncentrační profil
difundující substance

- odvození rovnice kontinuity:

tok v místě x a čase t



změna množství substance $n\Delta x$ za čas Δt

$$n(x,t+\Delta t)\Delta x - n(x,t)\Delta x = j(x,t)\Delta t - j(x+\Delta x,t)\Delta t$$

↓

příteče oteče

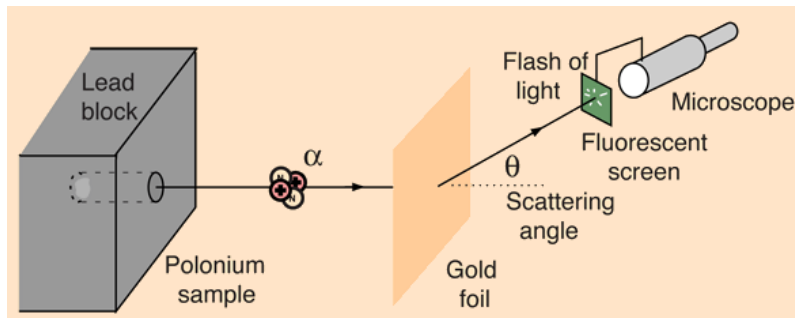
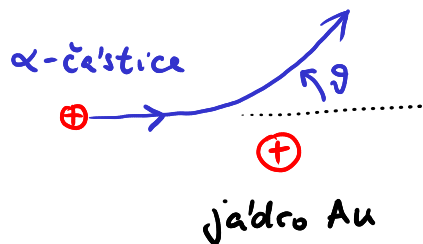
$$\left(\frac{\partial n}{\partial t} \Delta t\right) \Delta x = \left(-\frac{\partial j}{\partial x} \Delta x\right) \Delta t \rightarrow \frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0$$

(1D rovnice kontinuity)

- získali jsme 1D rovnici kontinuity, její 3D verze zní $\frac{\partial n}{\partial t} + \nabla \cdot \vec{j} = 0$

Rutherfordův experiment

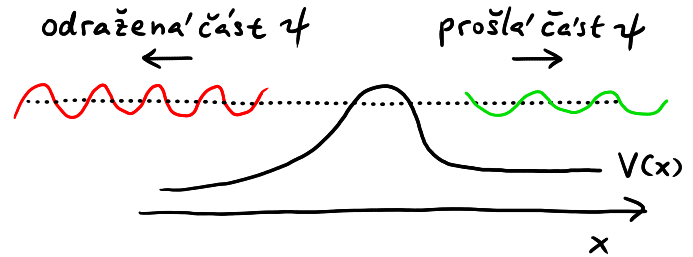
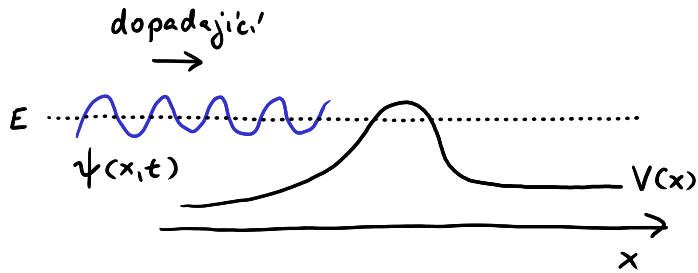
zkoumání atomů rozptylem α částic



kvantitativně popisováno dif. účinným průřezem:

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{tok částic rozptýlených do určitého směru vztažený na prostorový úhel}}{\text{plošný tok dopadajících částic}}$$

pro coulombovský potenciál jádra $\left(\frac{d\sigma}{d\Omega}\right) \sim \frac{1}{\sin^4 \frac{\vartheta}{2}}$

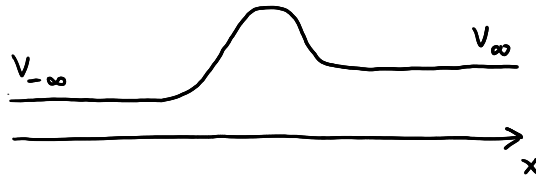


① pomocí stacionárního stavu $\psi(x,t) = \Psi(x) e^{-\frac{i}{\hbar} E t}$

dopadající' + odražená'

$$\Psi(x) \rightarrow e^{ikx} + R e^{-ikx}$$

$$k = \frac{\sqrt{2m(E - V_{-\infty})}}{\hbar}$$

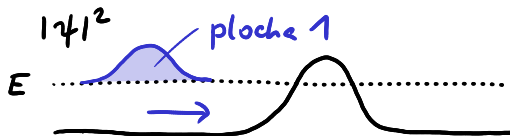


prošla'

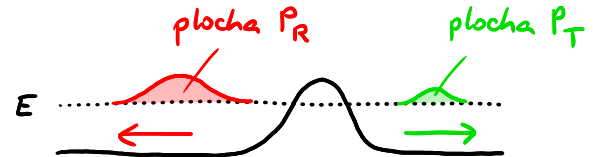
$$\Psi(x) \rightarrow T e^{ik'x}$$

$$k' = \frac{\sqrt{2m(E - V_{\infty})}}{\hbar}$$

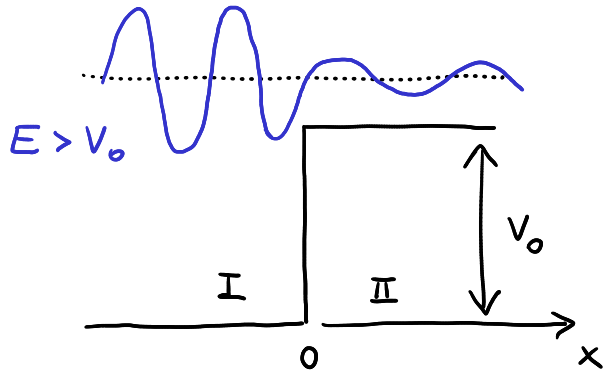
② pomocí balíků



pozdější čas :



"Propustnost" pravouhelného potenciálového schodu

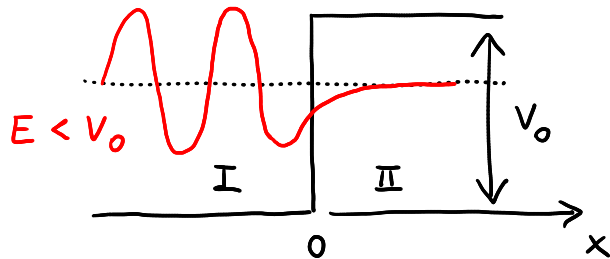


$$\Psi_{\text{I}}(x) = e^{ikx} + R e^{-ikx}$$

$$\Psi_{\text{II}}(x) = T e^{ik'x}$$

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

$$k' = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$



$$\Psi_{\text{I}}(x) = e^{ikx} + R e^{-ikx}$$

$$\Psi_{\text{II}}(x) = A e^{-\alpha x}$$

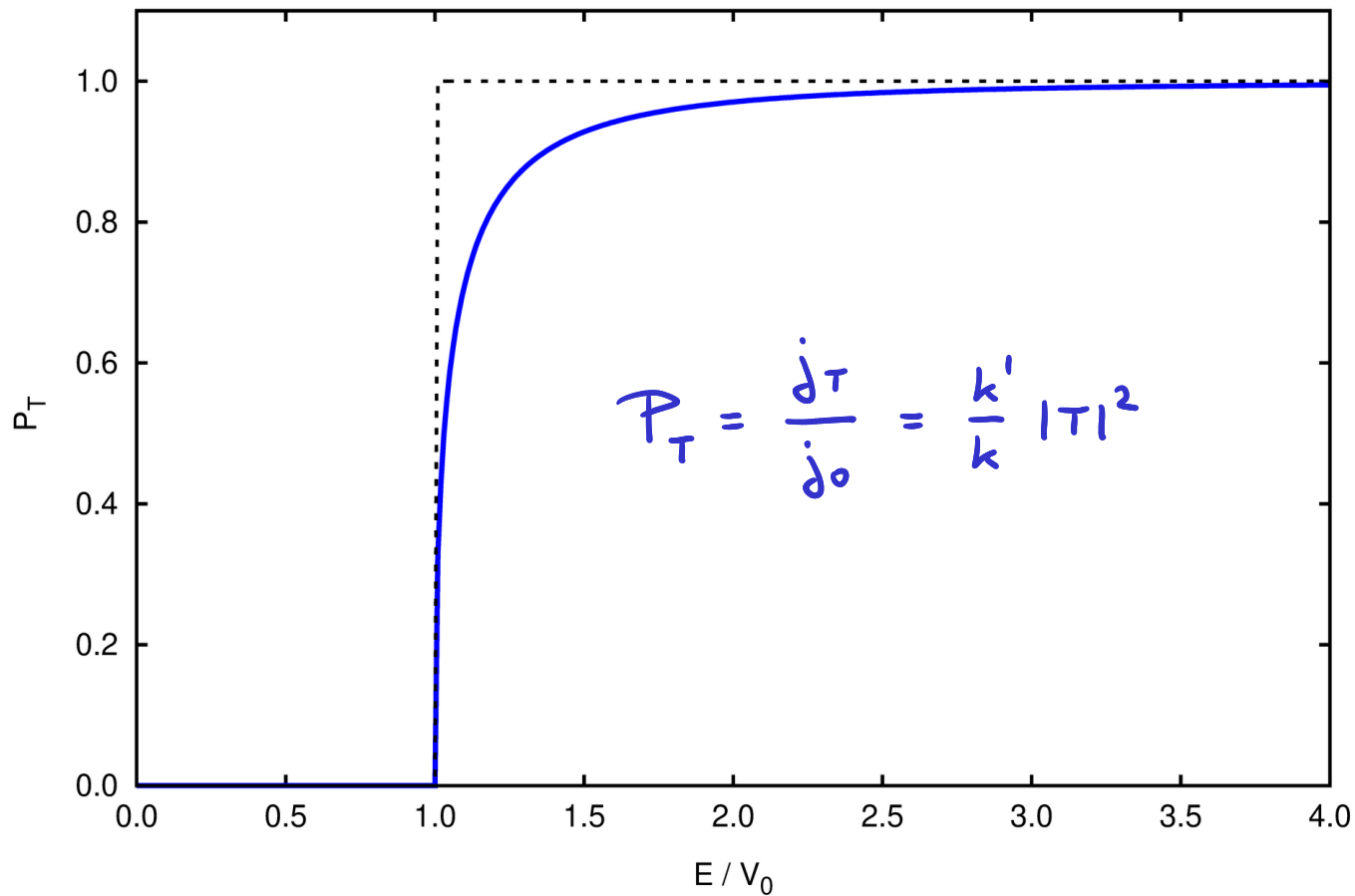
$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

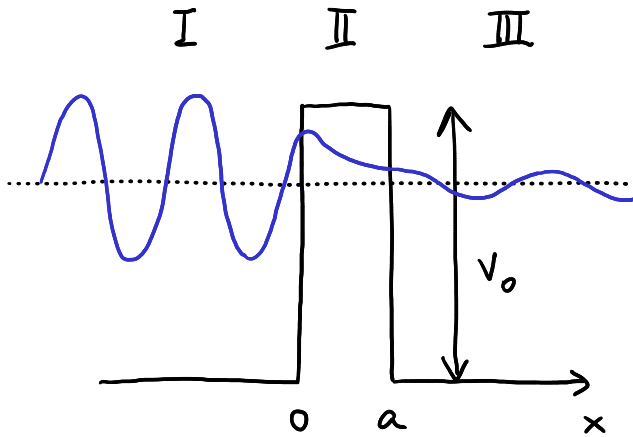
v obou případech „sešívací“ podmínky : $\Psi_{\text{I}}(0) = \Psi_{\text{II}}(0)$ spojitost

$\Psi'_{\text{I}}(0) = \Psi'_{\text{II}}(0)$ hladkost

"Propustnost" pravouhého potenciálového schodu



"Propustnost" pravouhlé bariéry



$$\Psi_I(x) = e^{ikx} + R e^{-ikx}$$

$$\Psi_{II}(x) = A e^{\alpha x} + B e^{-\alpha x}$$

$$\Psi_{III}(x) = T e^{ik(x-a)}$$

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

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

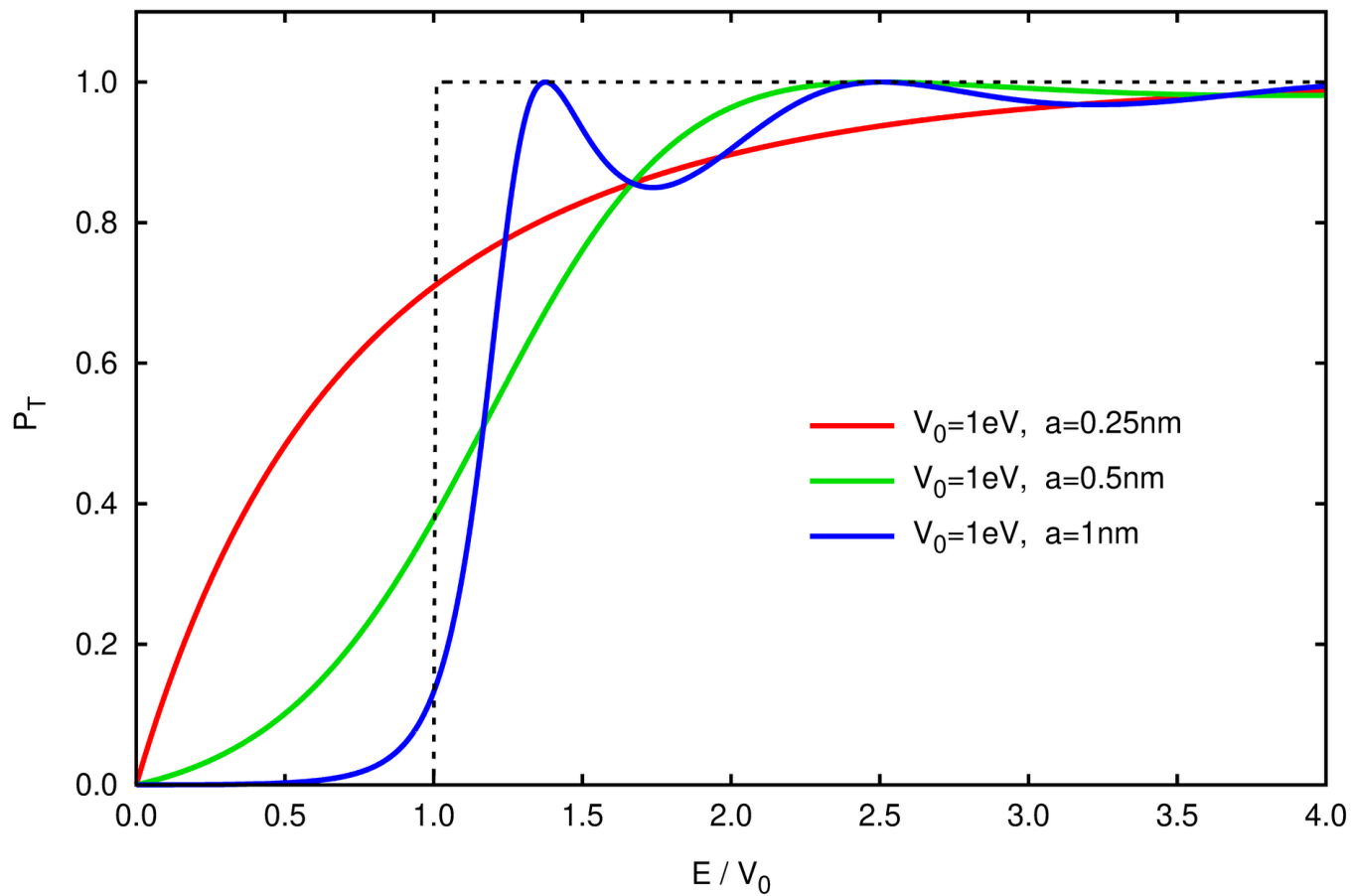


pravděpodobnost tunelování

$$P_T = |T|^2 = \frac{1}{1 + \frac{1}{4} \left(\frac{\alpha}{k} + \frac{k}{\alpha} \right)^2 \sinh^2 \alpha a}$$

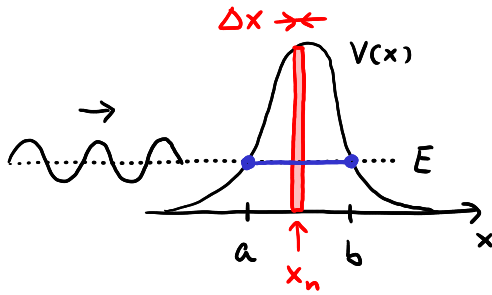
$$\sim e^{-2\alpha a}$$

"Propustnost" pravouhlé bariéry



Gamowova formule

(odhad, ale pro malé propustné' barier' poměrně uspokojivý)



barieru v klasicky nedostupne' oblasti: ($E < V(x)$)

nahradíme sadou N tenkých pravouhly'ch barier s výškami kopírujícími $V(x)$

šířka elem. barier středy barier

$$\Delta x = \frac{b-a}{N}$$

$$x_n = a + (n - \frac{1}{2}) \Delta x \quad n = 1, 2, 3, \dots, N$$

propustnost sady barier odhadneme jako součin jednotlivých propustností' aproximovaných $e^{-2\alpha\Delta x}$

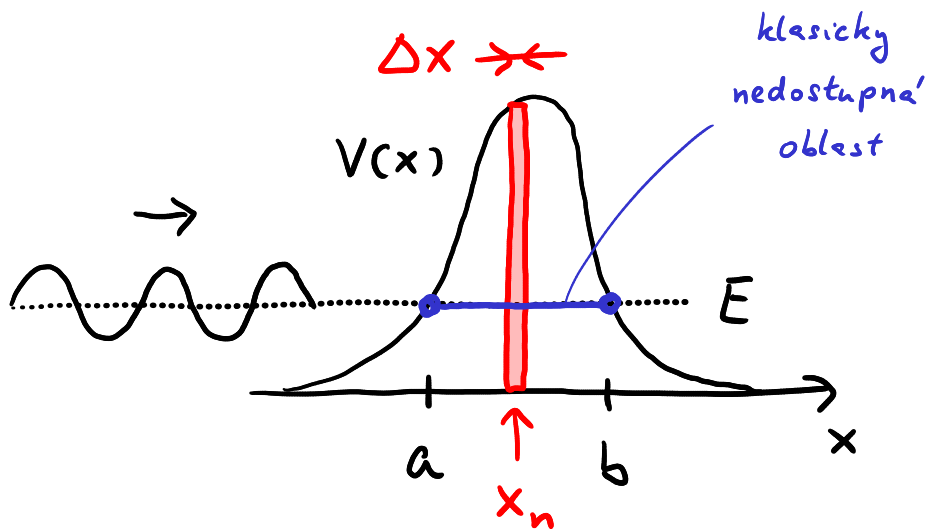
$$P_T \approx \prod_{n=1}^N P_T \left(x_n - \frac{\Delta x}{2}, x_n + \frac{\Delta x}{2} \right) \approx \prod_{n=1}^N e^{-2\alpha_n \Delta x} = \prod_{n=1}^N e^{-\frac{2}{\hbar} \sqrt{2m[V(x_n) - E]} \Delta x}$$

$$= \exp \left\{ -\frac{2}{\hbar} \sum_{n=1}^N \sqrt{2m[V(x_n) - E]} \Delta x \right\}$$

$$\rightarrow P_T \approx \exp \left\{ -\frac{2}{\hbar} \int_a^b \sqrt{2m[V(x) - E]} dx \right\} = e^{-G}$$

Gamowův Faktor G

Gamowova formule



šířka elem. bariér

$$\Delta x = \frac{b-a}{N}$$

středý bariér

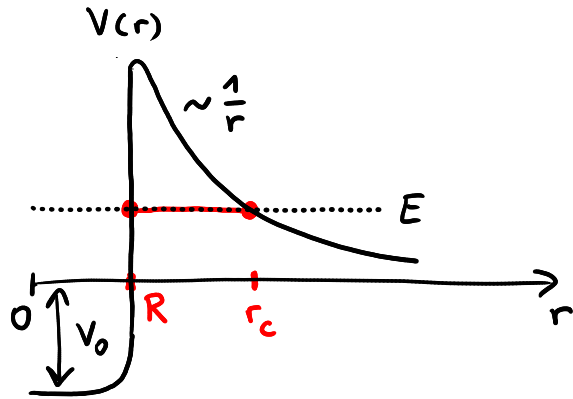
$$x_n = a + (n - \frac{1}{2}) \Delta x$$

$$n = 1, 2, 3, \dots, N$$

$$P_T \approx \exp \left\{ -\frac{2}{\hbar} \int_a^b \sqrt{2m [V(x) - E]} dx \right\} = e^{-G}$$

Gamowův Faktor G

α -rozpad jader



1) velikost jádra $R \approx R_0 Z^{1/3}$

$$R_0 \approx 1.6 \text{ fm } (10^{-15} \text{ m})$$

2) potenciál vně $V(r) = \frac{\gamma}{r}$,

$$\text{kde } \gamma = \frac{2(Z-2)e^2}{4\pi\epsilon_0} \approx \frac{2Ze^2}{4\pi\epsilon_0}$$

3) r_c - klasický bod obrátu

přiletaující částice: $r_c = \frac{\gamma}{E}$

pravděpodobnost tunelování α -částice ven z jádra podle Gamowovy Formule

$$P_T = e^{-G} \quad G = \frac{2}{\hbar} \int_R^{r_c} \sqrt{2m\left(\frac{\gamma}{r} - E\right)} dr = \frac{2r_c}{\hbar} \sqrt{2mE} \left[\frac{\pi}{2} - \arcsin \sqrt{\frac{R}{r_c}} - \sqrt{\frac{R}{r_c} \left(1 - \frac{R}{r_c}\right)} \right]$$

pro $R \ll r_c$:

$$G \approx \frac{2r_c}{\hbar} \sqrt{2mE} \left(\frac{\pi}{2} - 2\sqrt{\frac{R}{r_c}} \right) =$$

$$\frac{2}{\hbar} \frac{2Ze^2}{4\pi\epsilon_0 E} \sqrt{2mE} \left(\frac{\pi}{2} - 2\sqrt{R_0 Z^{1/3} E \frac{4\pi\epsilon_0}{2Ze^2}} \right) = \beta_1 \sqrt{\frac{Z}{E}} - \beta_2 Z^{3/2}$$

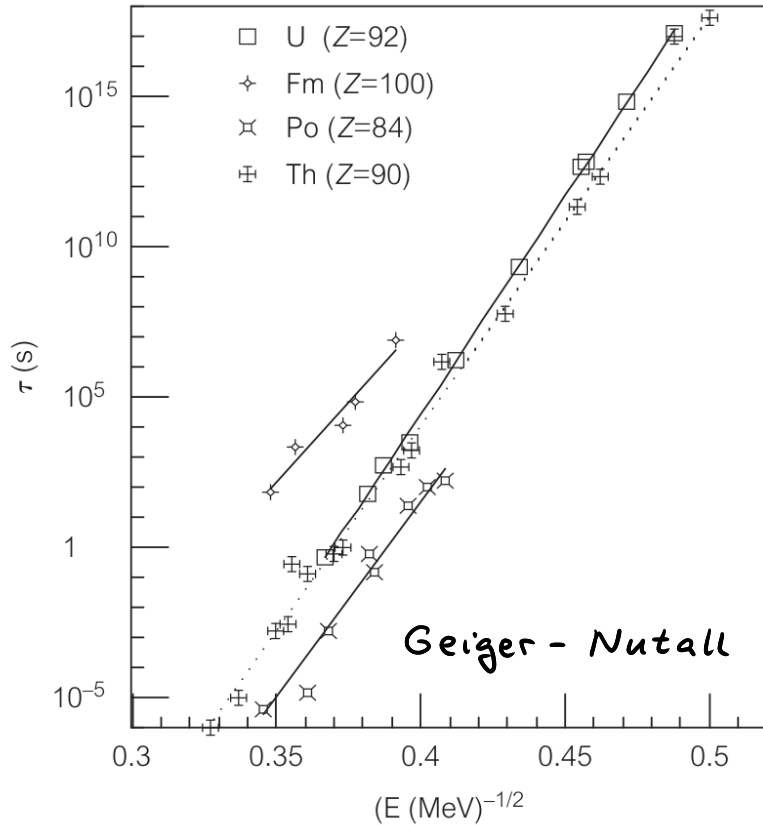


Figure 11.17. Semilog plot of α -decay lifetime (τ in seconds) versus $1/\sqrt{E_\alpha}$ (in MeV) for four different radioactive decay series, the so-called Geiger–Nuttall plot. The data are taken from a recent edition of the Chart of the Nuclides (Walker (1983).)

rozpadový zákon

$$\frac{dN}{dt} = -\frac{1}{\tau} N \rightarrow N(t) = N_0 e^{-t/\tau}$$

$\frac{1}{\tau}$ = pravděpodobnost
rozpadu za jednotku času

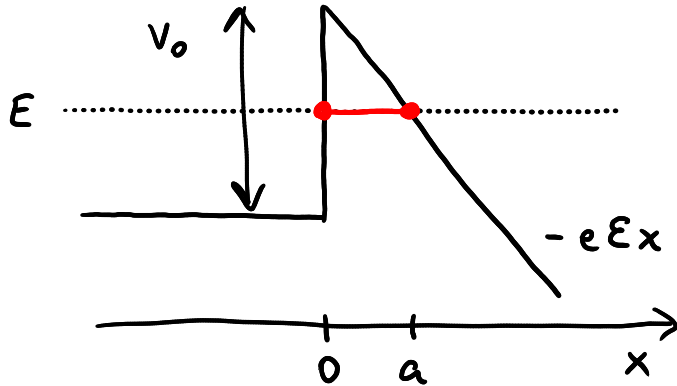
$$= P_T \times \text{frekvence nárazů } f_0 = \left(\frac{2R}{v}\right)^{-1}$$

$$\tau = \frac{1}{f_0} e^G \quad v = \frac{p}{m} = \frac{\sqrt{2mE}}{m}$$

↓

$$\ln \tau = \beta_1 \frac{Z}{\sqrt{E}} - \beta_2 Z^{\frac{2}{3}} - \ln f_0$$

Studená emise (autoemise)



V_0 - výstupní práce

\mathcal{E} - intenzita elektrického pole

klasicky zakázaná oblast

$$x \in [0, a = \frac{V_0 - E}{e\mathcal{E}}]$$

$$P_T = e^{-G} \quad G = \frac{2}{\hbar} \int_0^a \sqrt{2m(V_0 - e\mathcal{E}x - E)} dx = \frac{4\sqrt{2m} (V_0 - E)^{3/2}}{3\hbar e \mathcal{E}} = \frac{\mathcal{E}_0}{\mathcal{E}}$$

→ pravděpodobnost tunelování $P_T \approx e^{-\frac{\mathcal{E}_0}{\mathcal{E}}}$

→ tunelový proud $I \sim e^{-\frac{\mathcal{E}_0}{\mathcal{E}}}$ (Fowler & Nordheim, 1928)

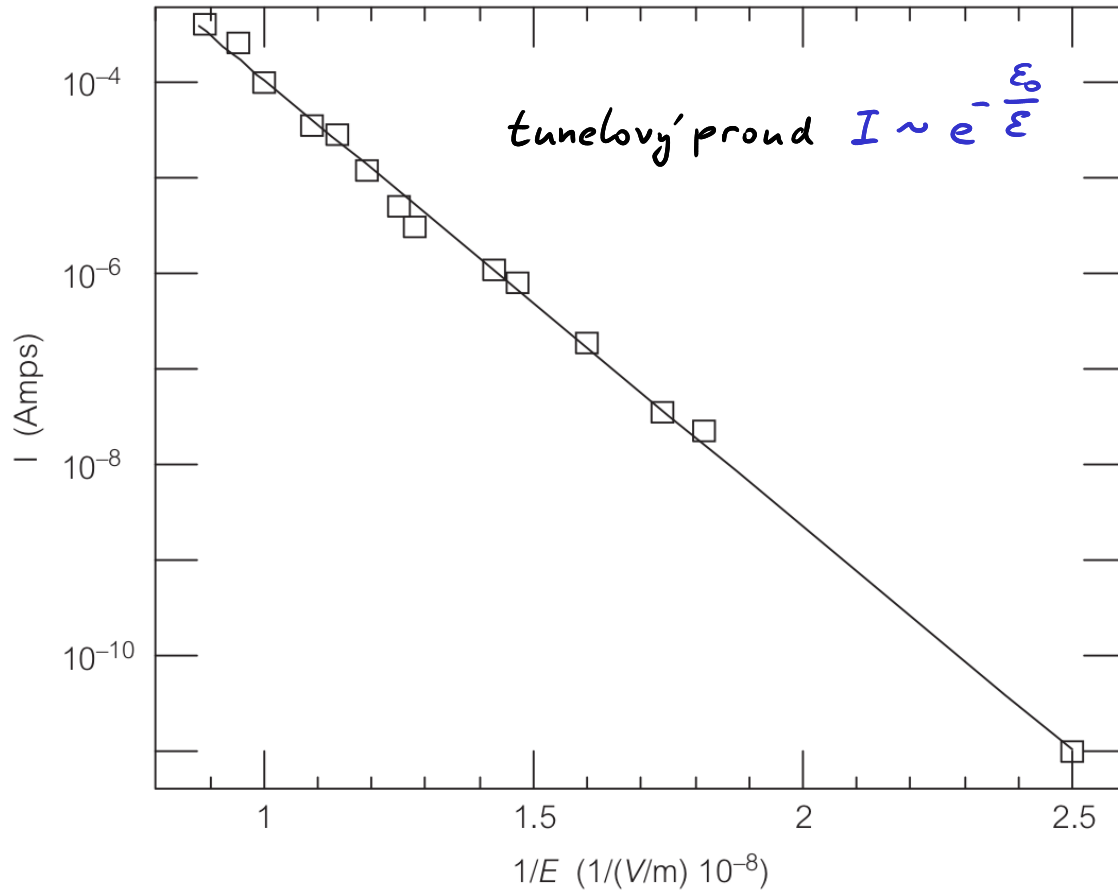
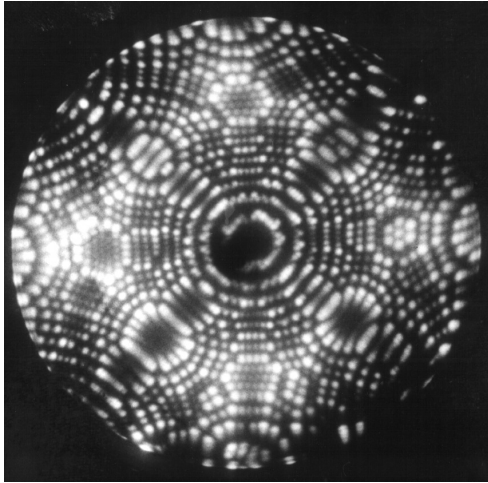


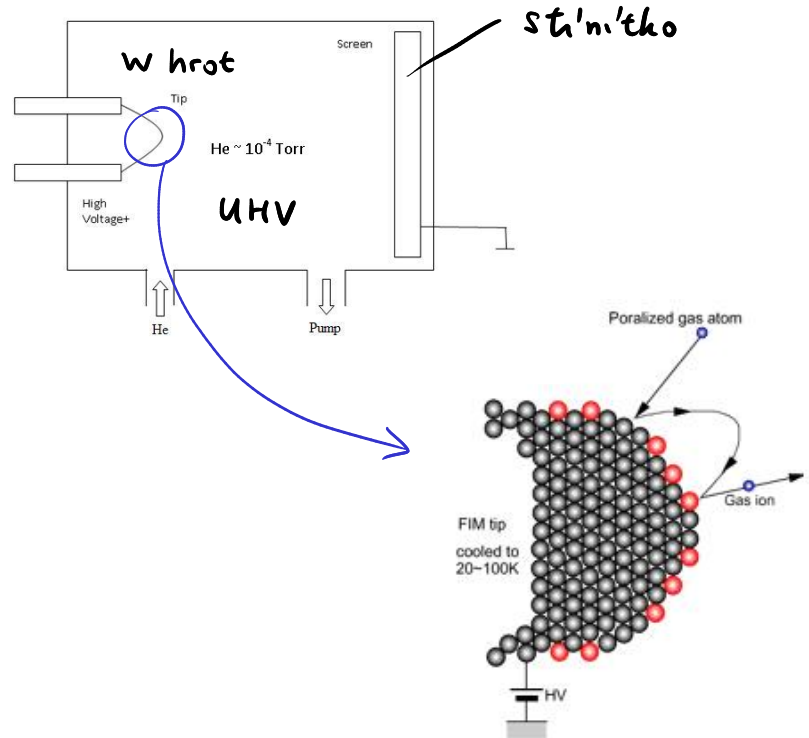
Figure 11.11. Semilog plot of tunneling current, I , versus $1/\mathcal{E}$ where \mathcal{E} is the applied electric field, illustrating field emission. The data are taken from Millikan and Eyring (1926).

Iontová autoemisní mikroskopie



FIM obrázek Pt hrotu

Tatsuo Iwata, z wikipedie



- do UHV vpuštěny ionty pracovního plynu (He, Ne)
- usedají na chlazený hrot (20-100K), ionizují se elektrickým polem u hrotu ($\sim 10^{11} \text{ V m}^{-1}$) a odletějí zanechat stopu na stínítku

výstupní práce pro W: $V_0 - E = 4.5 \text{ eV}$, určit \mathcal{E} , protože $P_T = \frac{1}{e} \rightarrow G = 1$

$$P_T = e^{-G} \quad G = \frac{4\sqrt{2m}(V_0 - E)^{\frac{3}{2}}}{3\hbar e \mathcal{E}} \quad \mathcal{E} = \frac{4\sqrt{2m}(V_0 - E)^{\frac{3}{2}}}{3\hbar e G} \approx 6.52 \times 10^{10} \text{ V m}^{-1}$$



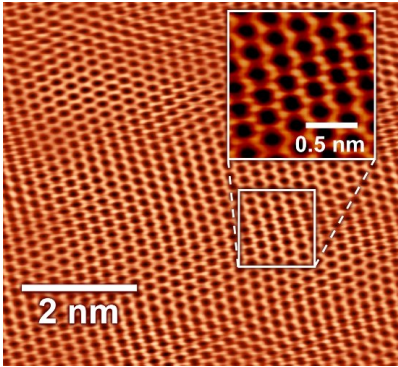
Erwin Wilhelm Müller

- 1911: Born June 13.
- 1936: Engineering Degree with Gustav Hertz.
- 1937: Invented the Field Emission Microscope.
- 1941: Discovered Field Desorption.
- 1951: Invented the Field Ion Microscope.
- 1952: Joined the Penn State Faculty.
- 1956: First observation of individual atoms.
- 1967: Invented the Atom-Probe.
- 1975: Elected, National Academy of Science and National Academy of Engineering.
- 1976: Under consideration (with Ernst Ruska) for the 1986 Nobel Prize in Physics.
- 1977: Died May 17 of a heart attack.
- 1977: Awarded the National Medal of Science (Posthumously from President Carter).

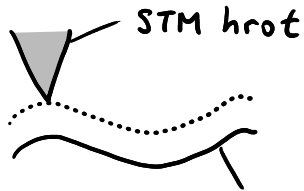
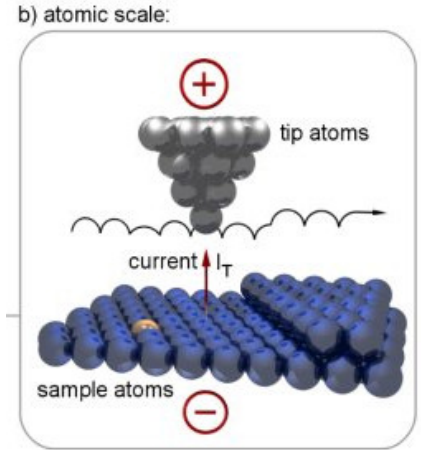
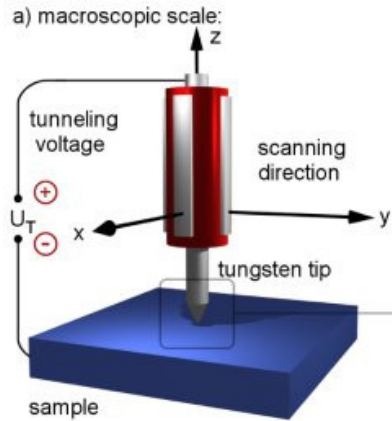
STM - Scanning Tunneling Microscopy

1981 Gerd Binnig & Heinrich Rohrer @ IBM

NC 1986

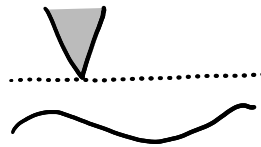


STM snímek povrchu grafítu



vodivý povrch

constant
current
mode



constant
height
mode

Tunelový proud v STM mikroskopu

M. Komai et al. / Applied Surface Science 146 (1999) 158–161

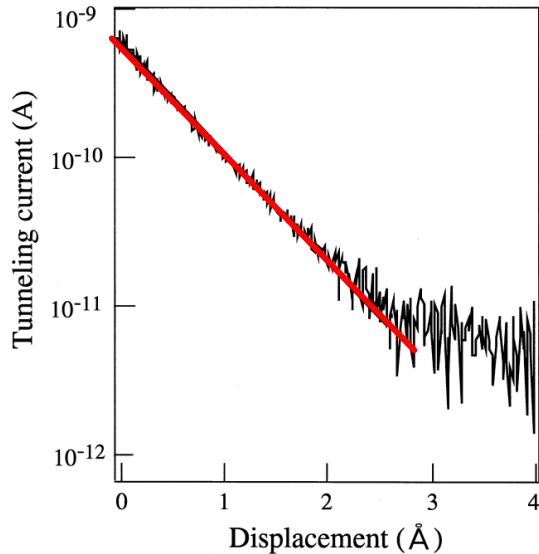


Fig. 4. Tunneling current obtained from the static measurement for Ba-deposited Si(111)-(3×1) surfaces as a function of the tip-sample distance. The tunneling current exponentially decays with the tip-sample distance over two orders of magnitude. The gradient of the $\ln I_T - s$ plot is $1.77 \text{ (\AA}^{-1}\text{)}$.

$$P_T \approx e^{-2\kappa a}$$

$$I_T \approx I_0 e^{-2\kappa a}$$

$$\rightarrow \ln I_T = \ln I_0 - 2\kappa a$$

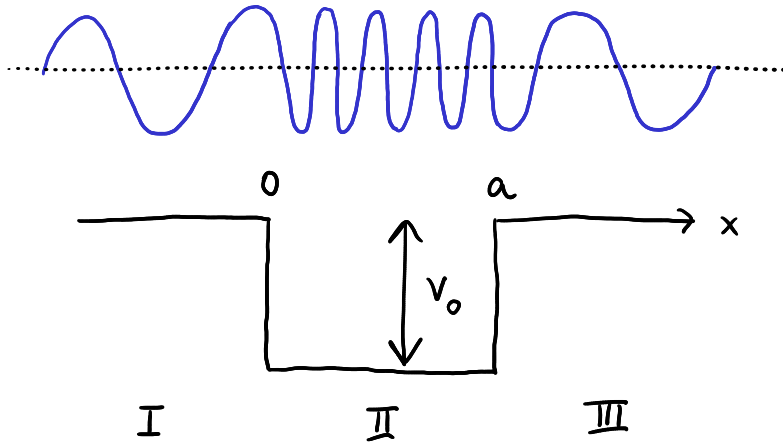
říkají, že 2κ je 1.77 \AA^{-1}

$$2\kappa = \frac{2\sqrt{2m}}{\hbar} \sqrt{V_0 - E}$$

výstupní práce

$$V_0 - E = \left(\frac{\hbar 2\kappa}{2\sqrt{2m}} \right)^2 \approx 2.98 \text{ eV}$$

Rezonanční průchod nad kvantovou jámou



$$\Psi_{\text{I}}(x) = e^{ikx} + R e^{-ikx}$$

$$\Psi_{\text{II}}(x) = A e^{ik'x} + B e^{-ik'x}$$

$$\Psi_{\text{III}}(x) = T e^{ik(x-a)}$$

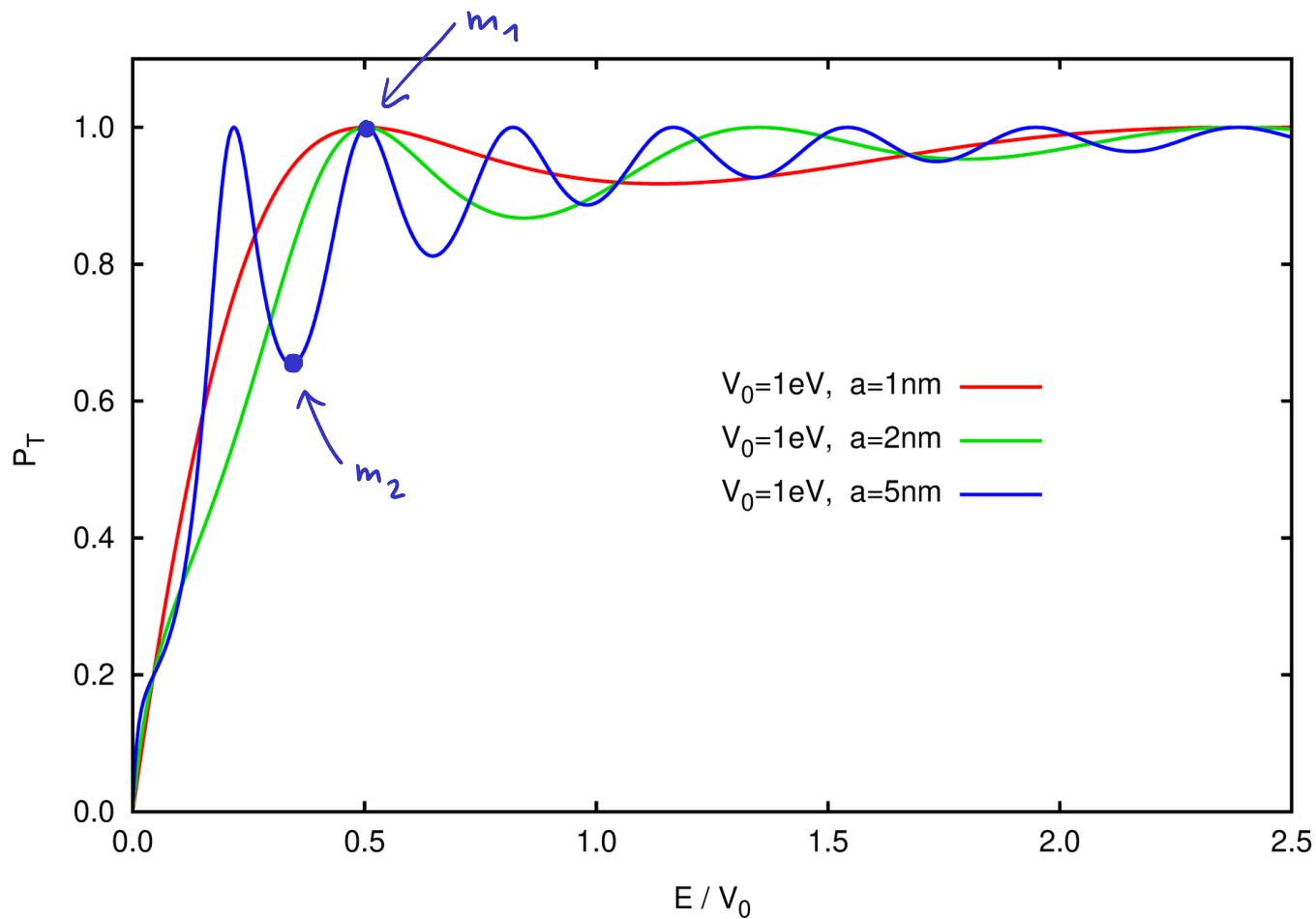
$$k = \frac{\sqrt{2mE}}{\hbar} \quad k' = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

pravděpodobnost průchodu $P_T = |T|^2 = \frac{1}{1 + \frac{1}{4} \left(\frac{k'}{k} - \frac{k}{k'} \right)^2 \sin^2 k'a}$

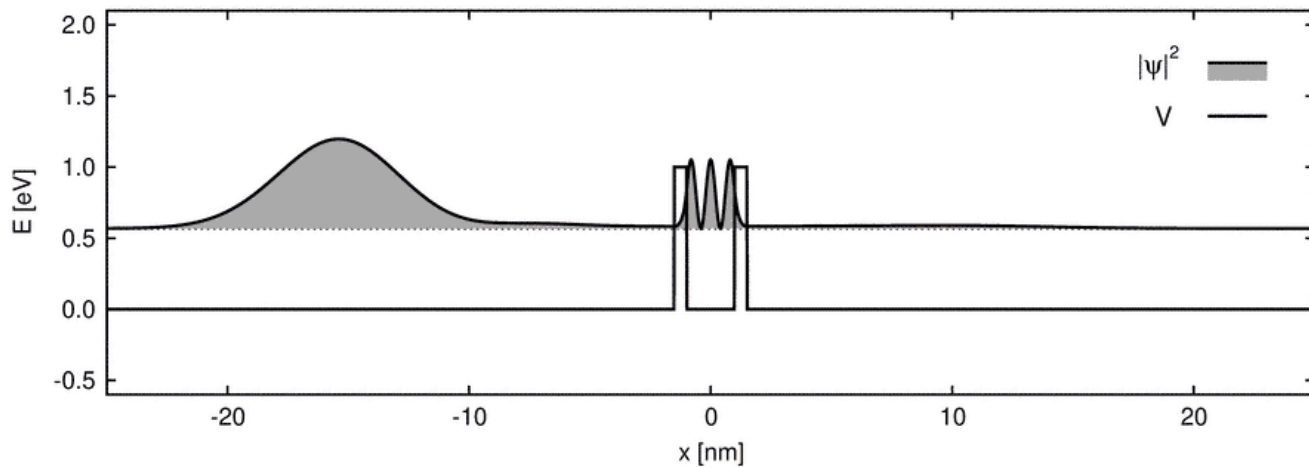
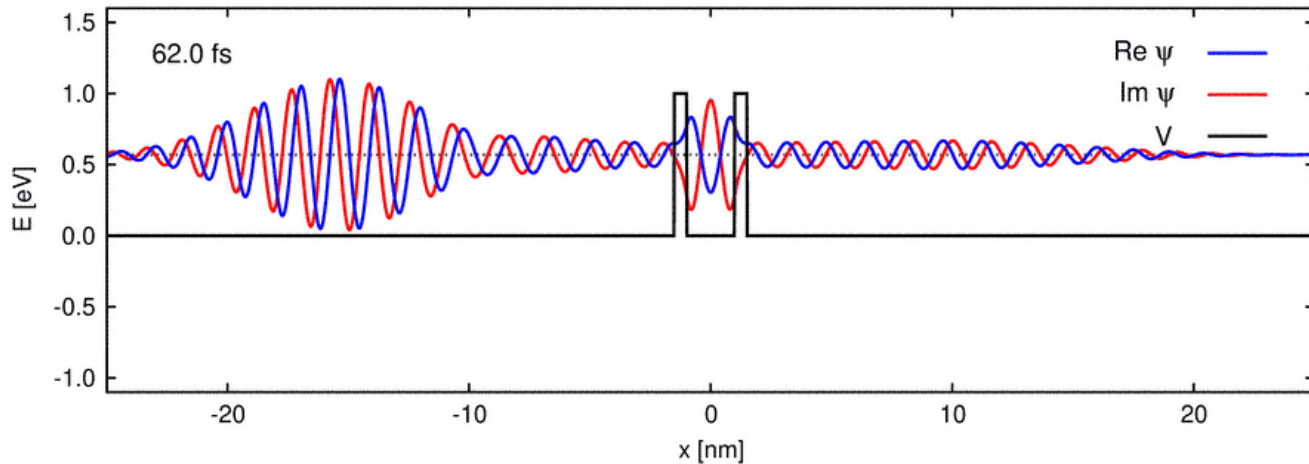
maxima $P_T = 1$ pro $k'a = n\pi \rightarrow E_0 + V_0 = \frac{\hbar^2 \pi^2}{2ma^2} n^2$

(rezonance při $E+V_0$ rovné energiím v ∞ hluboké jámě)

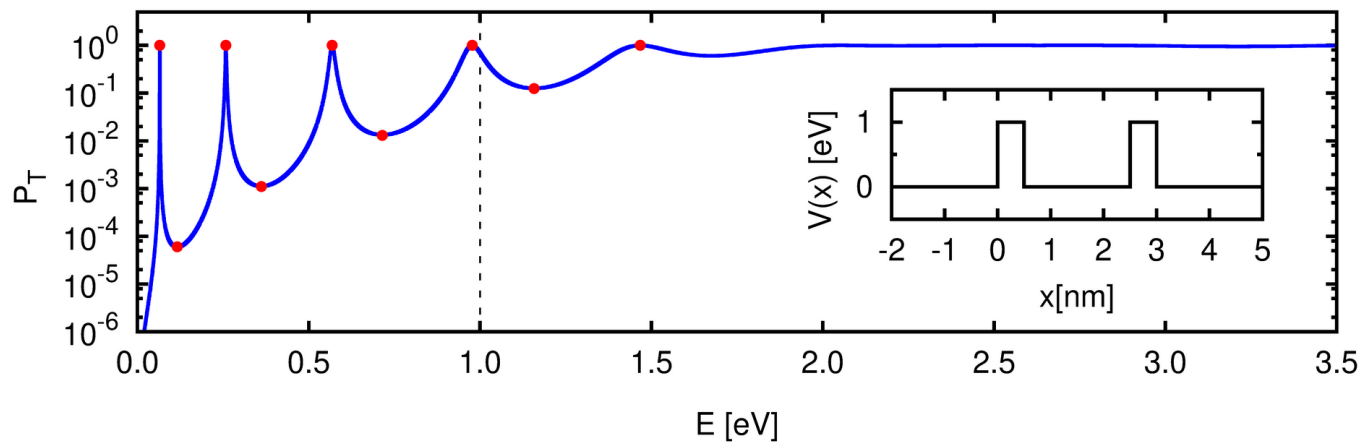
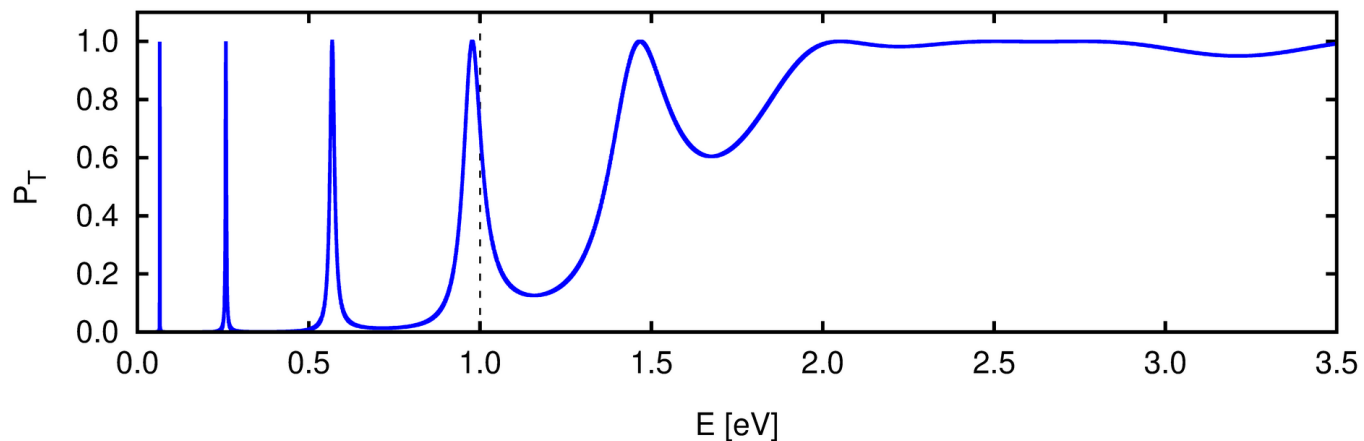
Rezonanční průchod nad kvantovou jámou



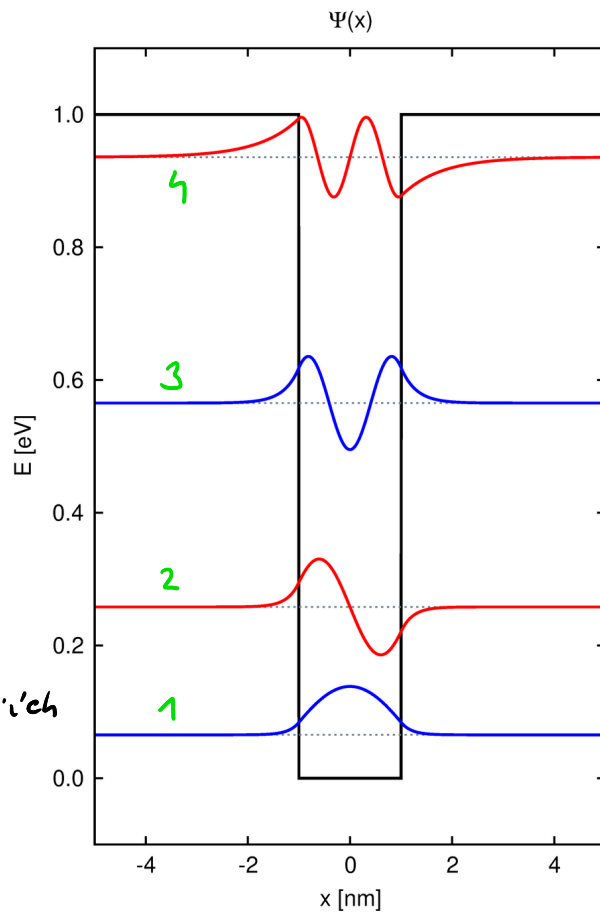
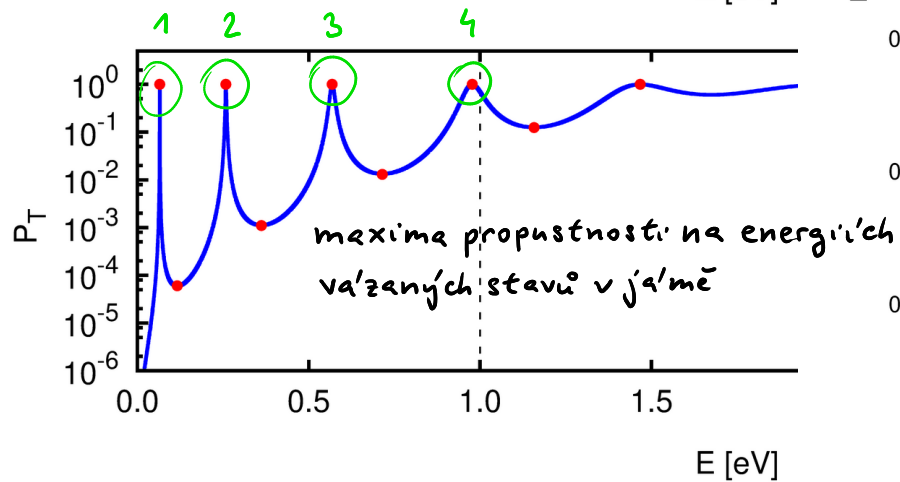
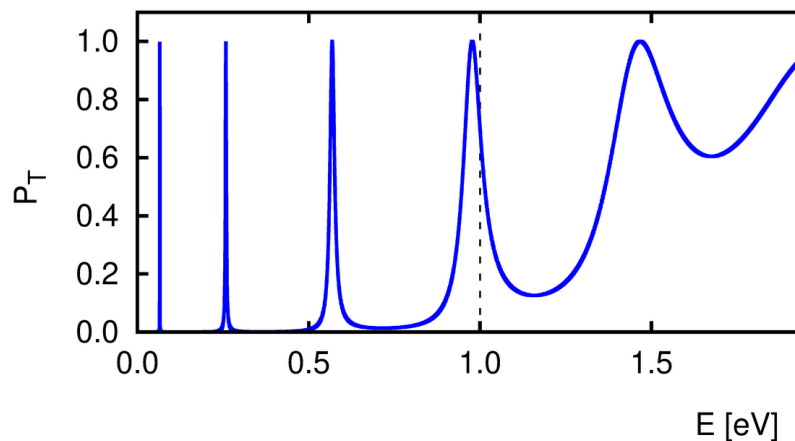
Metastabilní stavy



"Propustnost" pravoúhlé dvojbariéry

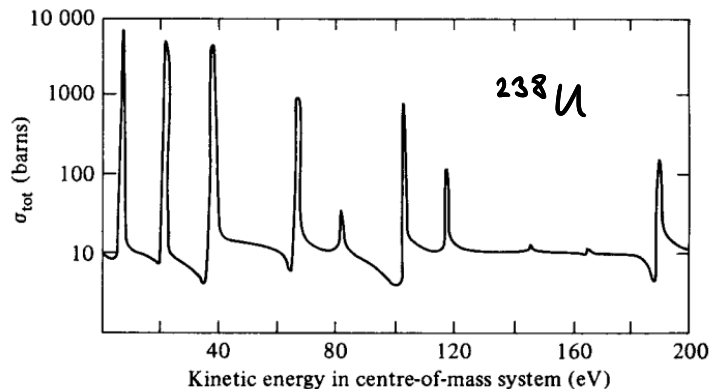
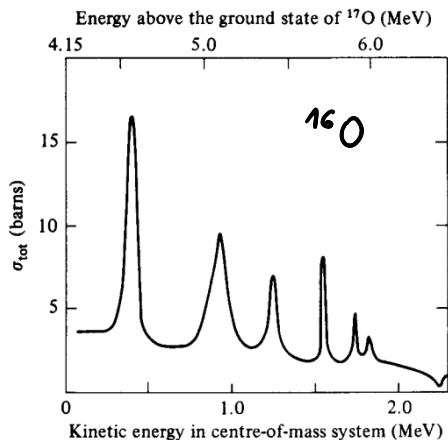


"Propustnost" pravoúhlé dvojbariéry



Rezonanční záchyt neutronů (volná analogie)

- účinný průřez záchytu neutronů v jádrech ^{16}O a ^{238}U



- úzké rezonance odpovídají utváření excitovaných stavů jader ^{17}O a ^{239}U

