Quantum and classical effects in scattering of fast electrons by the atomic planes of ultrathin crystal

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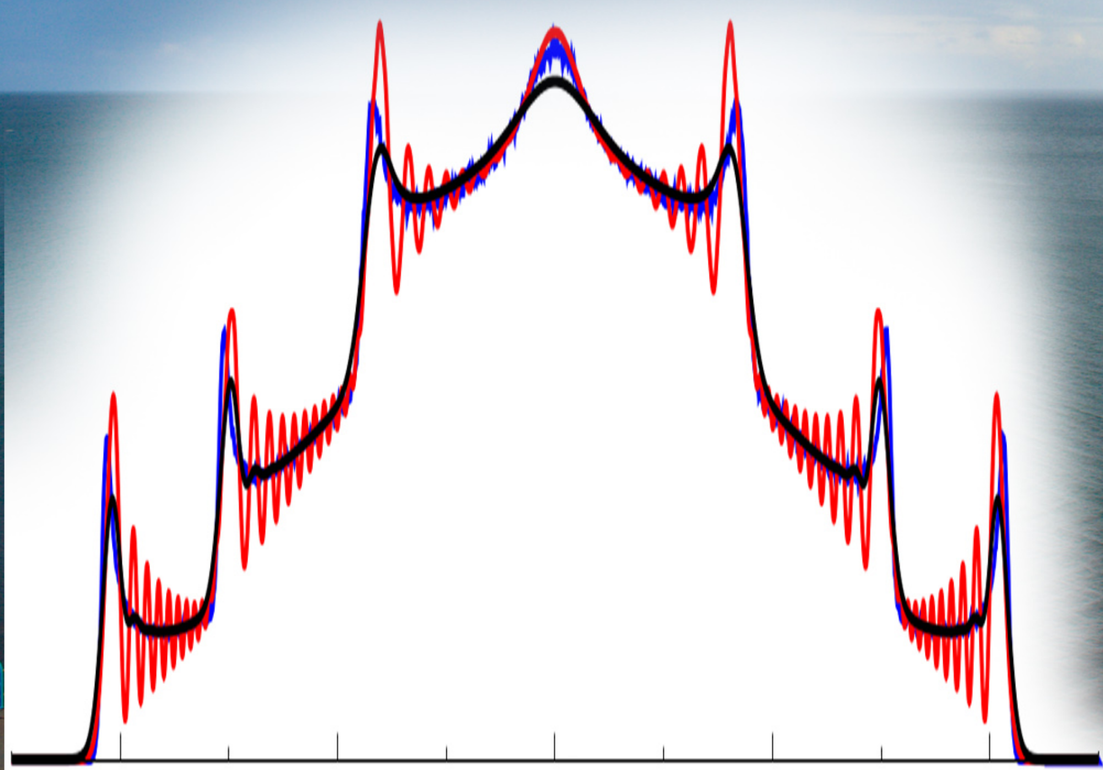
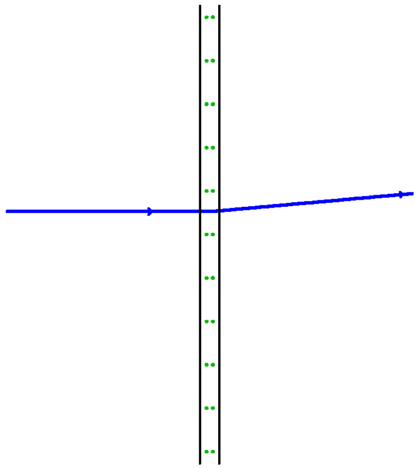
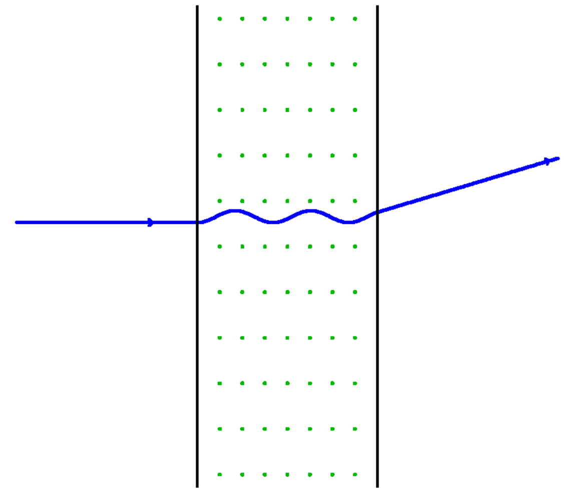


- Transitional region from ultrathin to thin crystals
- Scattering (rainbow, interference, …)
-
- ….

Ultrathin, Thin and Thick Crystals



~~Channeling~~



Channeling

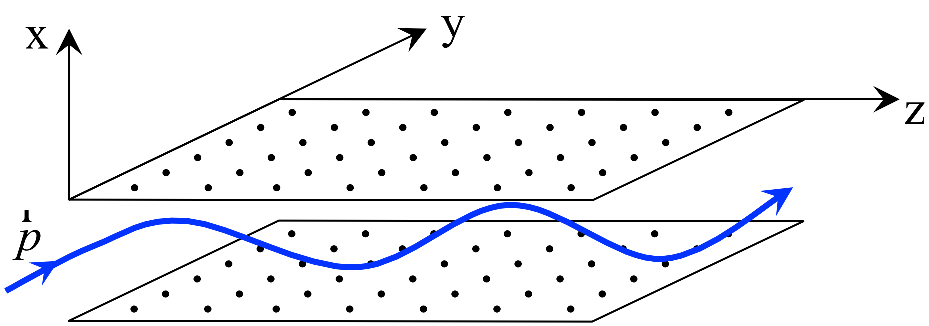
Recent experiments:

V. Guidi et al. Phys. Rev. Lett. (2012)

M. Mothapothula et al. NIM B283 (2012) 29

Phenomenon of Planar Channeling

J.Lindhard (1965)

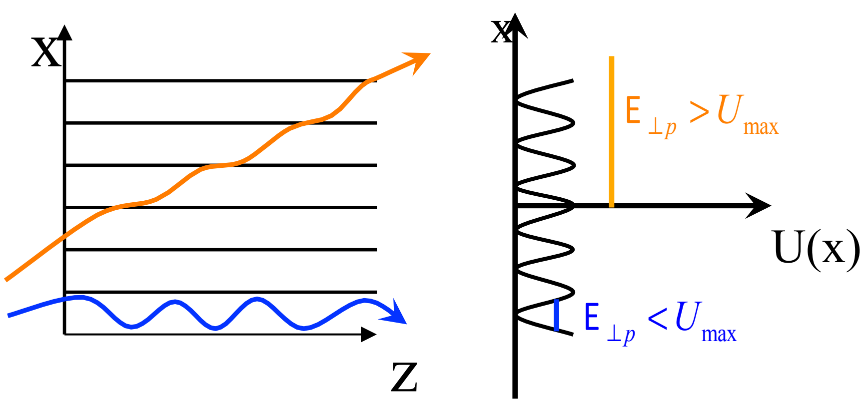


$$p_z = const \approx p$$

$$p_y = const \approx 0$$

$$\boxed{\begin{aligned} \ddot{x} &= -\frac{1}{E}\frac{\partial}{\partial x}U(x) \\ E_\perp &= \frac{E\dot{x}^2}{2} + U(x) \end{aligned}}$$

$$E_\perp = \frac{E\psi_c^2}{2} = U_{\max} \quad \Leftrightarrow \quad \boxed{\psi_c \sim \sqrt{2U_{\max}/E}}$$



Quantum consideration

$$\psi = e^{i(pz-\varepsilon t)}\varphi(x,t)$$

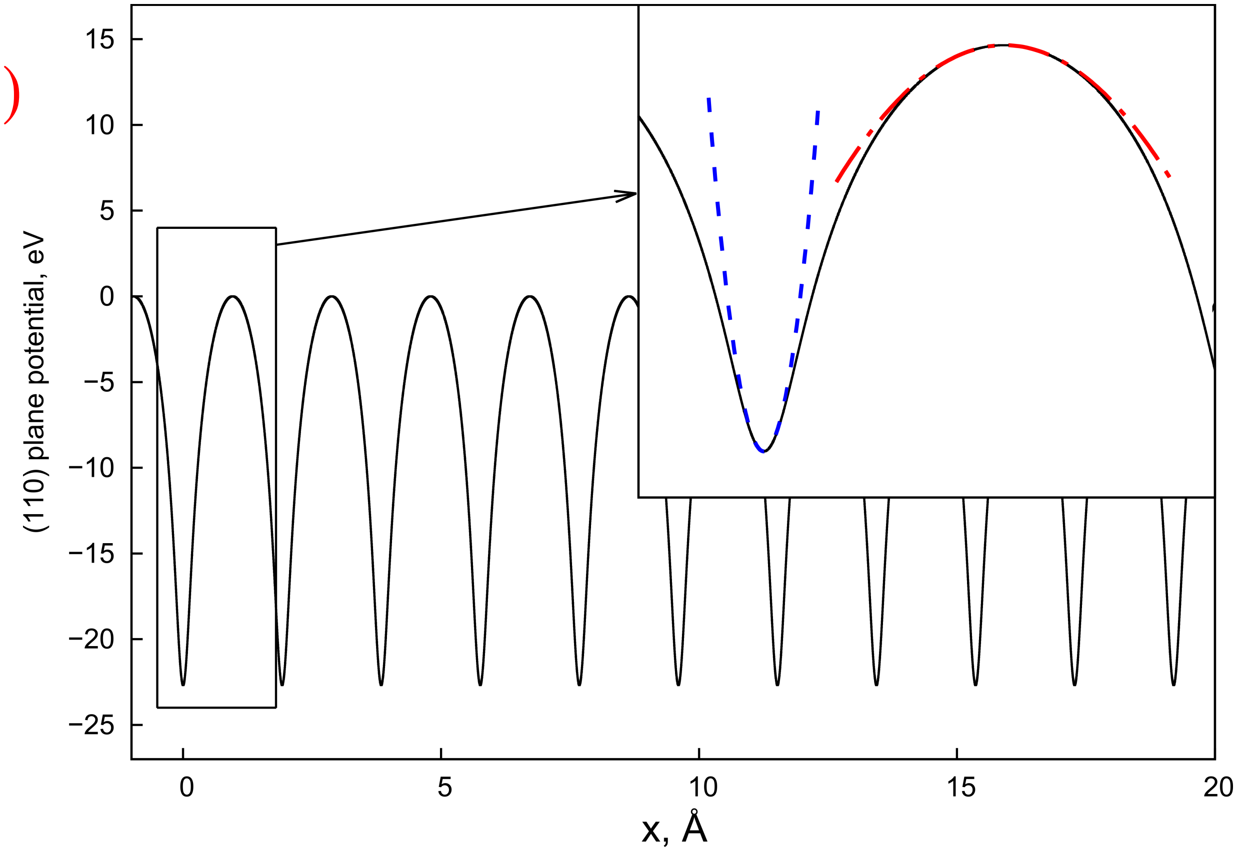
$$i\hbar\partial_t\varphi = \left(-\frac{\hbar^2}{2\varepsilon}\frac{\partial^2}{\partial x^2} + U(x)\right)\varphi(x,t)$$

$$\boxed{n_{levels} \sim \sqrt{E_{MeV}}}$$

Phenomenon of Above Barrier Motion: A. Akhiezer, N. Shul'ga (1978)

Continuous Planes Potential

$$U_{pl}(x) = \frac{1}{a_{pl}} \int_0^{a_{pl}} dy\, U_{ax}(x,y)$$



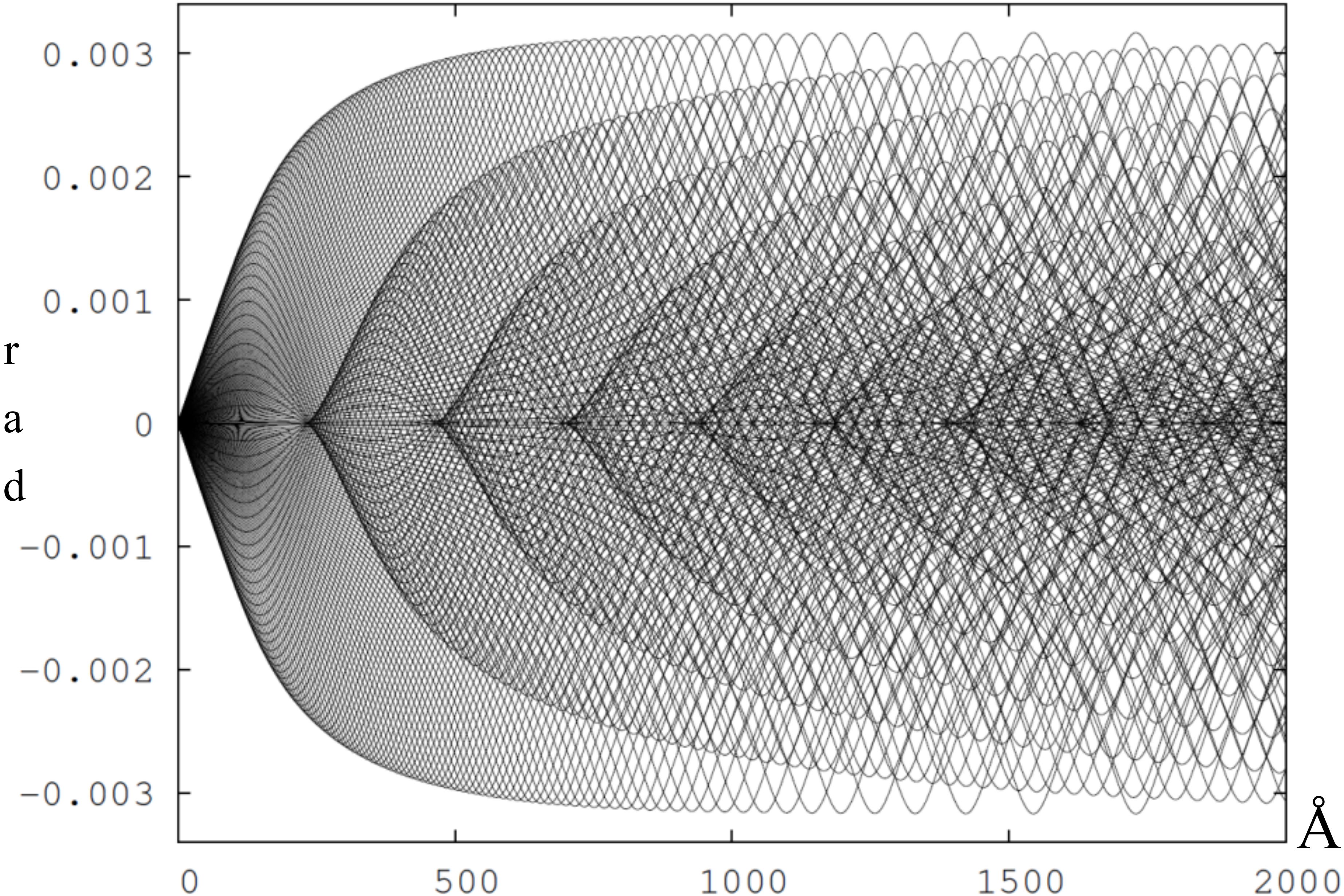
$$U_{ax}(\vec{\rho}) = \frac{1}{a_1 \bar{v}^2} \int d^2 v\, e^{-v^2/2\bar{v}^2} \int_{-\infty}^{\infty} dz\, u(\vec{\rho} + \vec{v}, z) \quad - \quad \text{string potential}$$

v - heat oscillations of atom coordinates

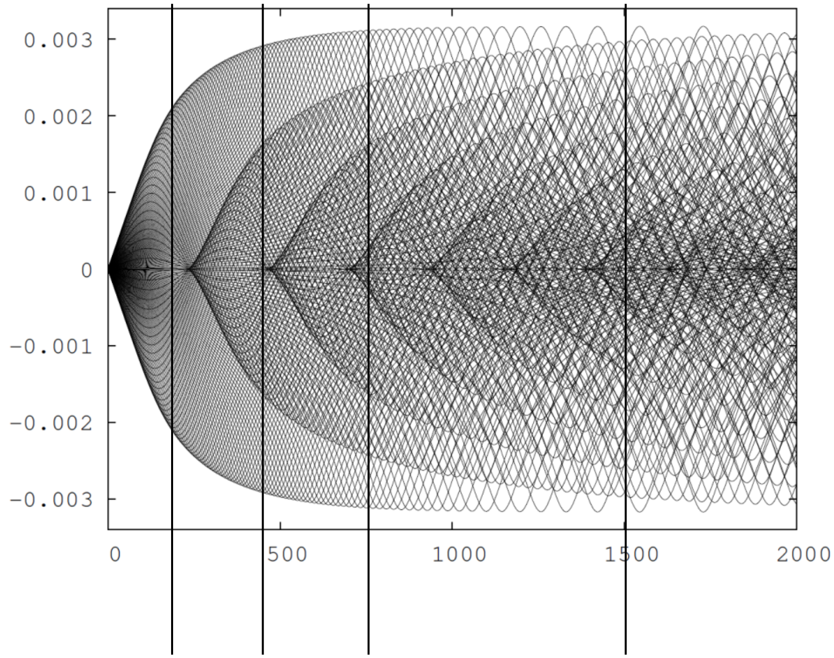
$$u_m(r) = \sum_i \alpha_i \exp(-\beta_i r / R) \quad - \quad \text{Moliere approximation for single atoms}$$

$$\dot{\theta} = -\frac{1}{E}\frac{\partial}{\partial x}U(x)$$

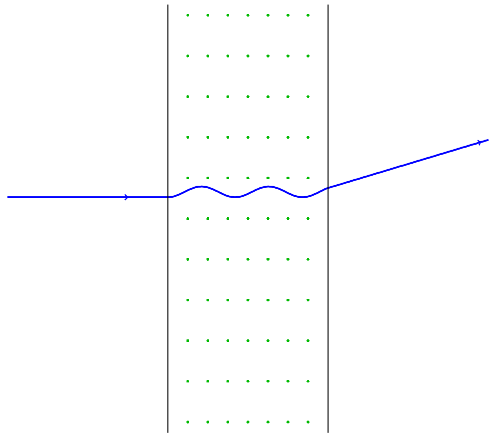
Classical scattering angles of 4 MeV electrons in (110) Planes of Si crystal as function of impact parameter and crystal tickness

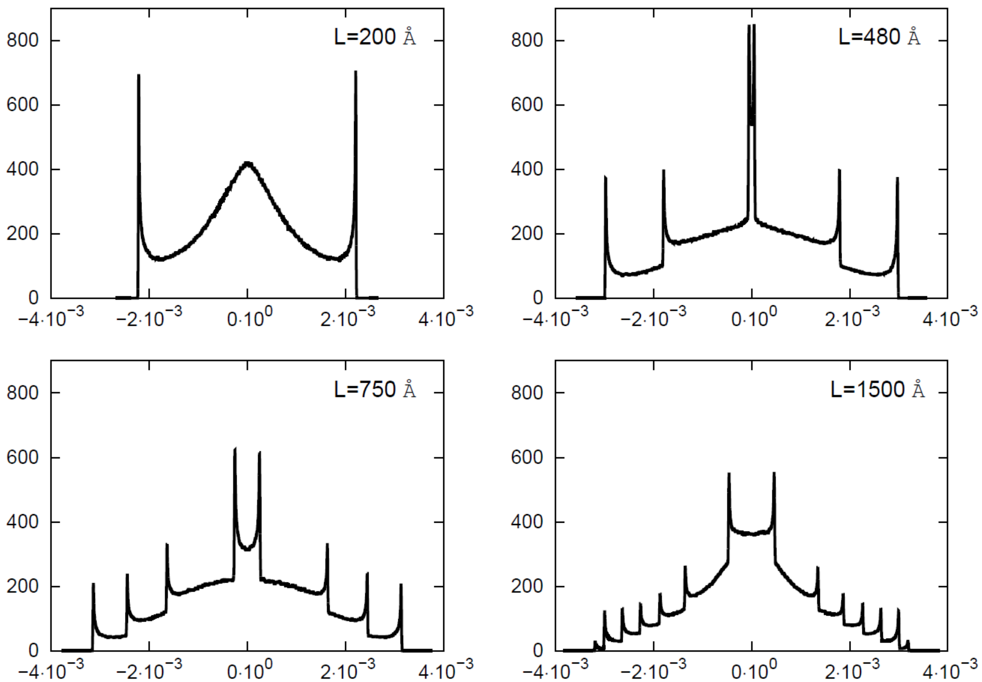


1D-classical scattering of 4 MeV electrons channeled by (110) Plane in Si crystal



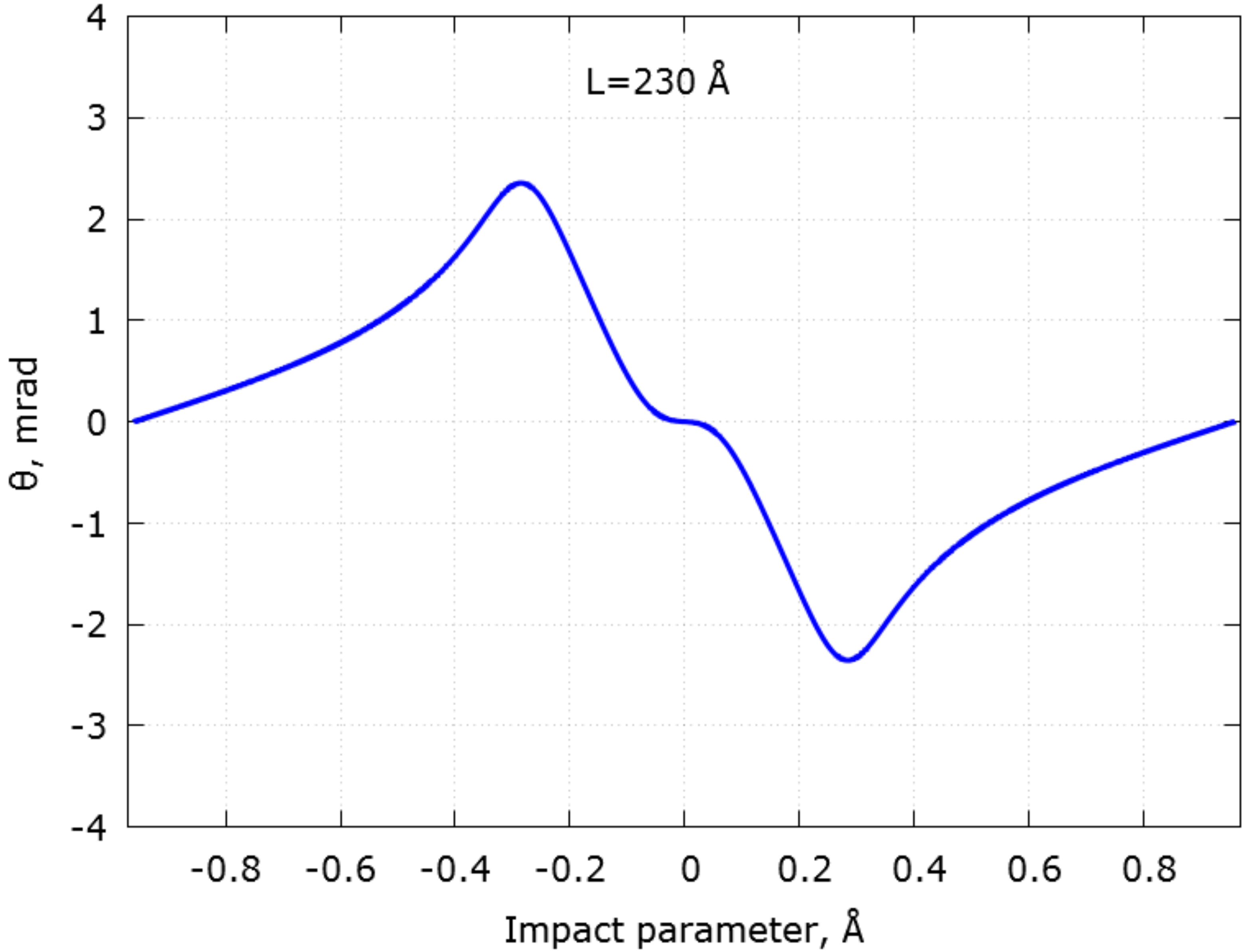
$L = 200\,A \quad 480\,A \quad 750\,A \quad 1500\,A$





1D-classical scattering of 4 MeV positrons channeled by (110) Plane in Si crystal

Deflection function
of 4 MeV electrons in ultrathin Si (110) crystal planes



Deflection function
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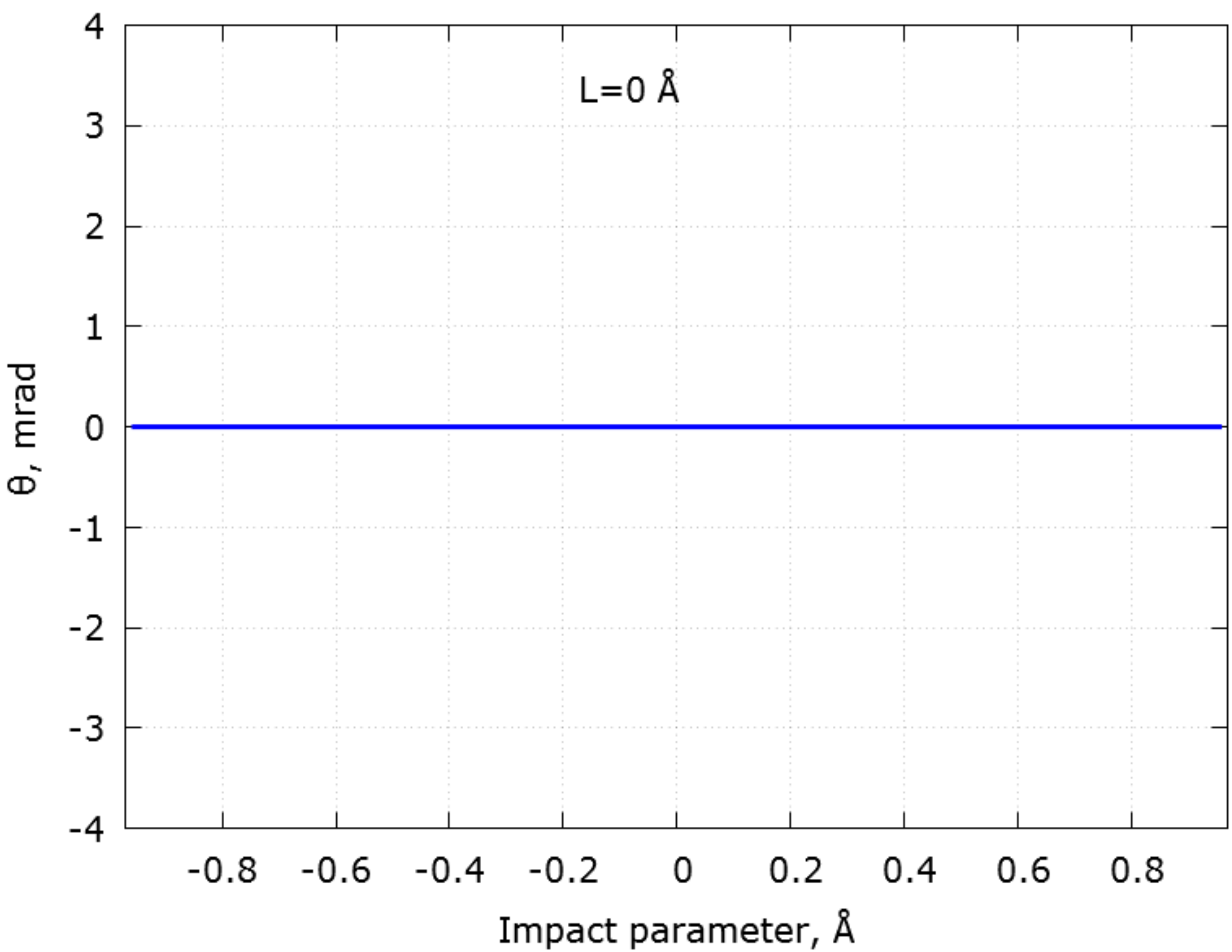
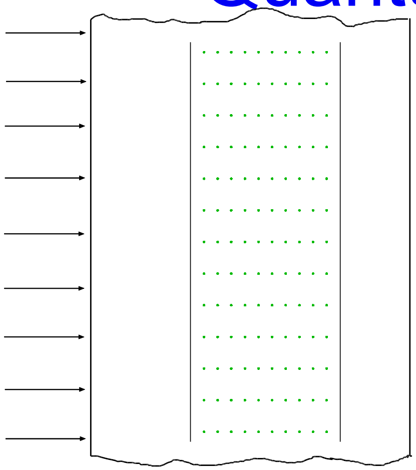


Quantum consideration: Spectral Method



$\psi_{in} = e^{i\vec{p}\vec{r}}$ $\qquad$ $\psi_f = e^{i\vec{p}'\vec{r}}\varphi(\vec{r})$

$$\psi = e^{i(pz-\varepsilon t)}\varphi(x,t)$$

Schrödinger type equation

$$\boxed{i\hbar\partial_t\varphi = \left(-\frac{\hbar^2}{2\varepsilon}\frac{d^2}{dx^2} + U(x)\right)\varphi}$$

- wave function iteration $\varphi(x,t+\Delta t) = e^{-\frac{i}{\hbar}\left(\hat{H}_0 + U(x)\right)\Delta t}\varphi(x,t)$
- recurrent relation $\varphi(x,t+N\Delta t)$
- Correlation function. **Scattering cross - section**

Optics (resonant frequencies in waveguides and optical fibers)
M. Feit et al. J. Comp. Phys. 47 (1982) 412.
Nuclear Physics
Yu. Bolotin et al. Phys. Lett. A 323 (2004) 218.
Channeling
S. Dabagov et al. NIM B30 (1988) 185 (ε~MeV)
A. Kozlov, N. Shul'ga, et al. Phys. Lettl A374 (2010) 4690 (levels and zone structure)
N. Shul'ga. V. Syshchenko et al. NIM B309 (2010) 153 (levels for dynamical chaos in thick crystals)
S. Shul'ga, N. Shul'ga et al. arXiv:1512.04601v1 (2015) (scattering)

Wave function calculation in Spectral Method

$$\varphi(x,t+\Delta t)=e^{-\frac{i}{\hbar}\left(\hat{H}_0+U(x)\right)\Delta t}\varphi(x,t):\ \text{non-commuting operators in exp}$$

$$e^{-\frac{i}{\hbar}\left(\hat{H}_0+U(x)\right)\Delta t}\neq e^{-\frac{i}{\hbar}\hat{H}_0\Delta t}e^{-\frac{i}{\hbar}U(x)\Delta t}$$

Zassenhaus formula

$$e^{\delta(C+D)}=e^{\delta C}e^{\delta D}e^{\delta^2[C,D]}e^{\frac{1}{6}\delta^3\left(2[D,[C,D]]+[C,[C,D]]\right)}\cdot O\left(e^{\delta^4}\right)$$

$$\boxed{e^{-\frac{i}{\hbar}\hat{H}\Delta t}=e^{\frac{1}{2}B\Delta t}e^{A\Delta t}e^{\frac{1}{2}B\Delta t}},\qquad A=-\frac{i\hbar}{2E_P/c^2}\frac{d^2}{dx^2},\qquad B=-\frac{i}{\hbar}eU(x)$$

presision up to $\sim\Delta t^3$

$$\varphi_n=\frac{1}{N}\sum_{k=0}^{N-1}e^{i\frac{2\pi}{N}nk}\sum_{m=0}^{N-1}e^{-i\frac{2\pi}{N}km}\varphi_m\quad -\ \text{Fourier expansion}$$

$$G(x)\equiv\frac{eU(x)}{2\hbar},\qquad \zeta\equiv\frac{\hbar\Delta t}{2E_P/c^2}$$

$$\boxed{\begin{aligned}&\psi(t+\Delta t);\\&=\exp\left(-iG(x)\Delta t\right)\cdot\frac{1}{N}\sum_{k=0}^{N-1}e^{i\frac{2\pi}{N}nk}\left\{\underbrace{\exp\left[-i\zeta\left(\frac{2\pi}{N\Delta x}k\right)^2\right]\cdot\sum_{m=0}^{N-1}e^{-i\frac{2\pi}{N}km}\underbrace{\exp\left(-iG_m\Delta t\right)\psi_m}_{1}}_{2}\right\}\end{aligned}}$$

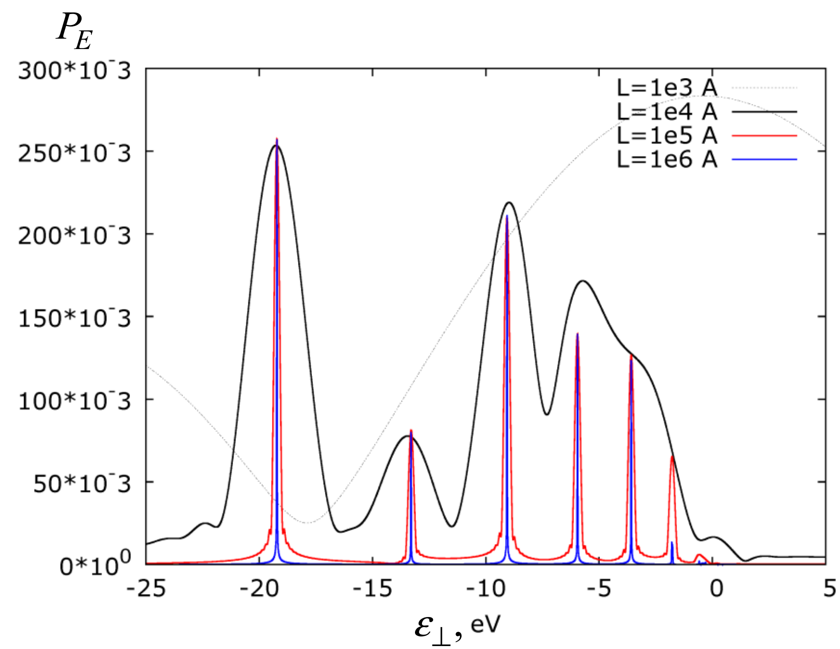
On Zassenhaus formula - D. Scholz, M. Weyrauch, J. Math. Phys. 47 (2006).

Calculation of Energy Spectrum of Channeling Radiation by the Spectral Method

$$P(t) = \int_{-\infty}^{\infty} dx\, \psi^*(x, t=0)\, \psi(x,t)$$

$$P_E = \frac{1}{T}\int_0^T dt\, \exp(iEt/h)\, P(t)\, w(t)$$

$$h\omega \xrightarrow[\text{Lorentz Transf.}]{\text{Doppler eff.}} 2\gamma^2 \cdot h\omega$$



Levels of transversal energy of 50MeV electrons in Si crystal (planar scattering)

PHIL	$\varepsilon \sim 5\text{MeV}$	$h\omega_{obs} \sim 1keV$
ThomX	$\varepsilon \sim 50\text{MeV}$	$h\omega_{obs} \sim 100keV$
PRAE	$\varepsilon \sim 140\text{MeV}$	$h\omega_{obs} \sim 500keV$

planar scattering $N_{levels} \sim \sqrt{\varepsilon[MeV]}$

axial scattering $N_{levels} \sim \varepsilon[MeV]$

What radiation should we get at scattering by ultrathin crystal?
Possible application for study of quantum chaos

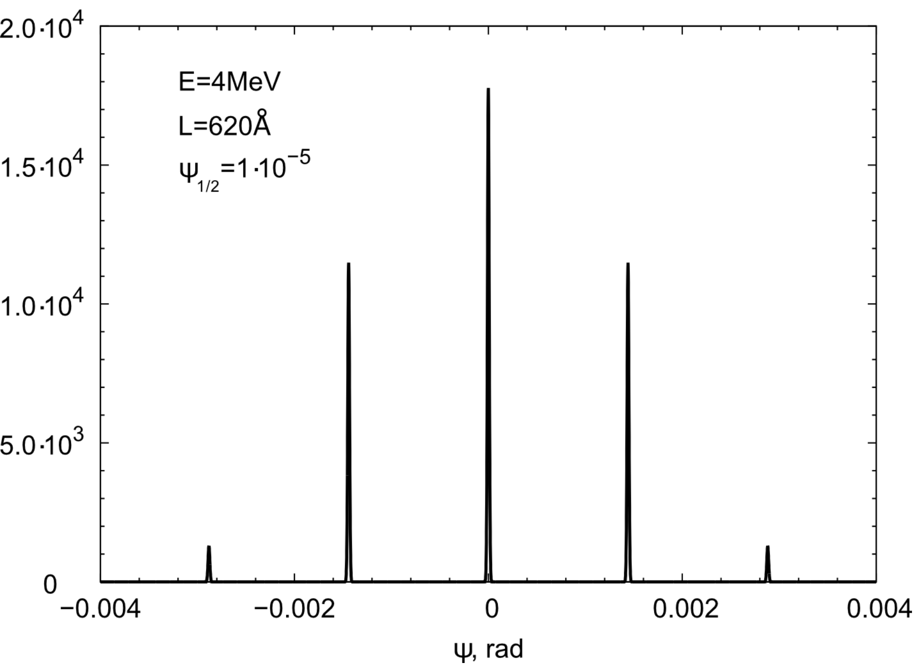
Scattering of electrons by crystal plane. Quantum case

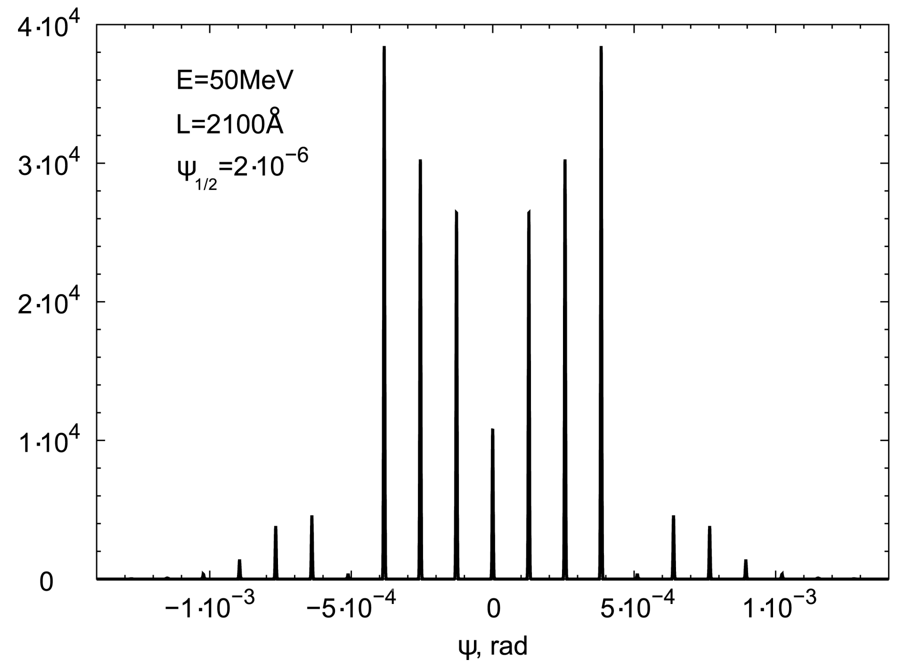
Electrons are considered as plane waves

Expansion over reciprocal lattice vectors

d_x – lattice period

$$\boxed{\psi_n = \frac{2\pi\hbar n}{d_x}\frac{1}{p_P}}$$



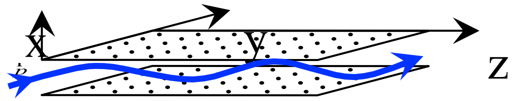


Convolution over different incidence angles corresponding to different electrons of a beam with divergence σ_{beam}

$$\overline{w_{beam}(\psi)} = \frac{1}{\sigma_{beam}\sqrt{\pi}}\int e^{-i\psi_i^2/\sigma_{beam}^2}\, w(\psi_i,\psi)\, d\psi_i$$

Classical and quantum angular distributions of 4 MeV electrons in ultrathin Si crystal

classical consideration



quantum consideration

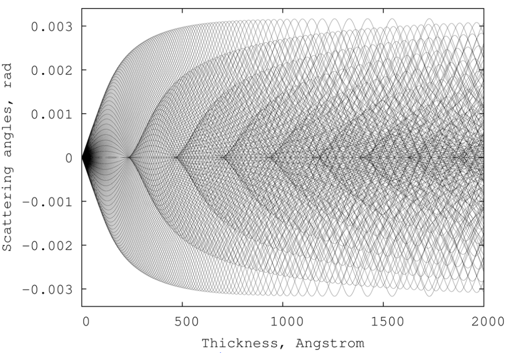
$$d\sigma_{cl} = d^2 b = \left| \frac{\partial (b_x, b_y)}{\partial (\vartheta_x, \vartheta_y)} \right| d\vartheta_x d\vartheta_y$$

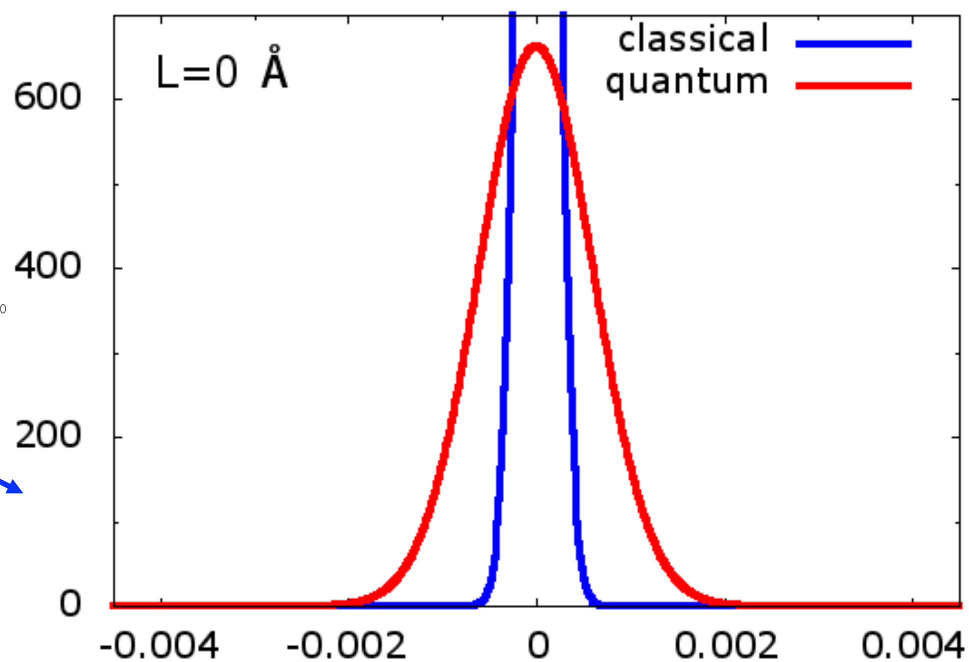
scattering on (110) plane

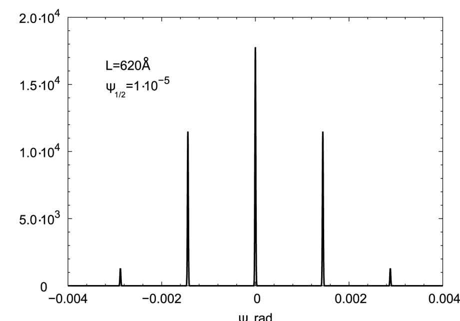
$$\Psi(x, t=0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \exp\left(-\frac{x^2}{2\sigma^2} + i \frac{p_x x}{\hbar} \right)$$

$$\dot{\vec{\rho}} = -\frac{c^2}{E} \nabla U(\vec{\rho})$$

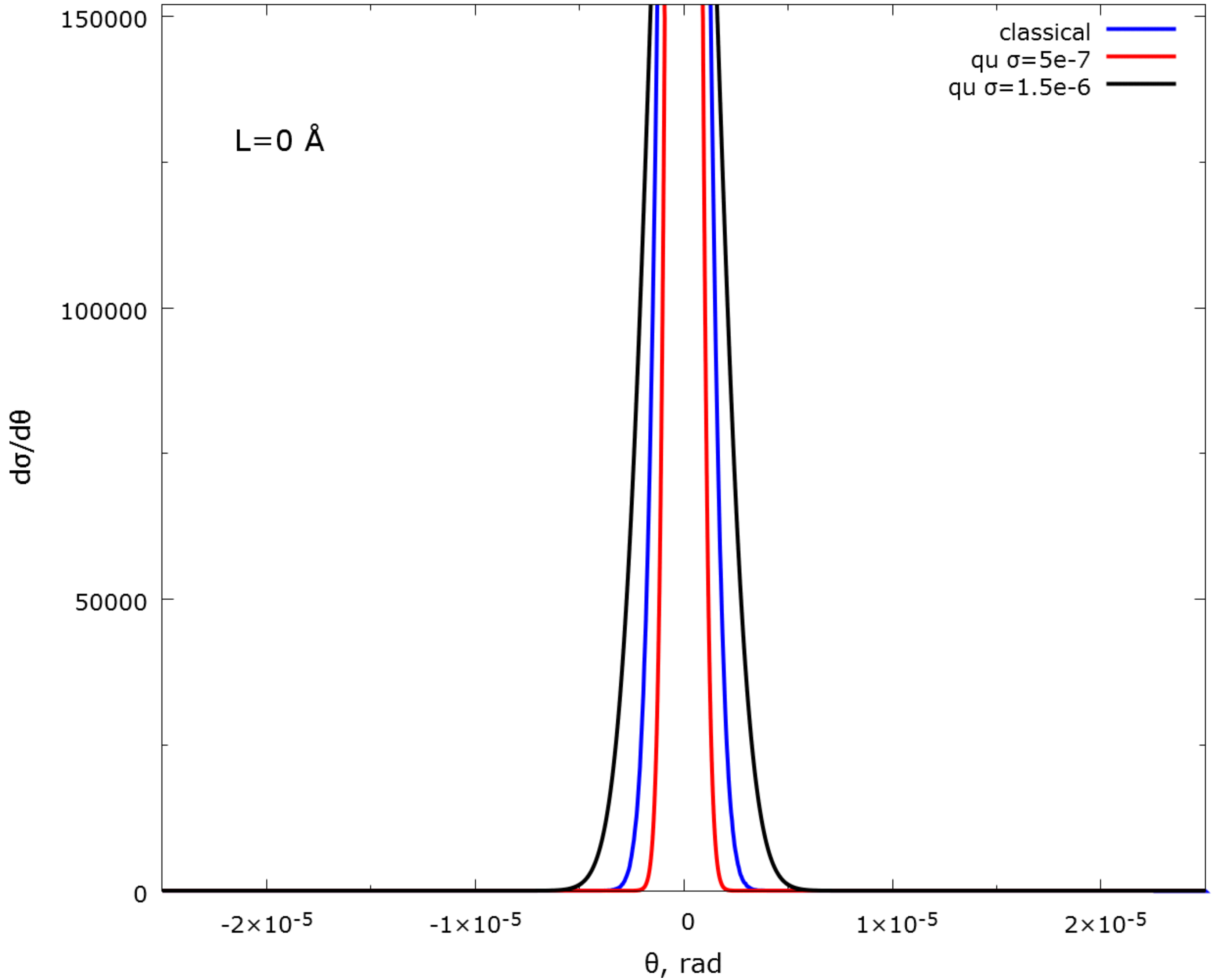
$$\Psi(x, t+\delta t) = \exp\left(-\frac{i}{\hbar} \delta t \, \hat{H} \right) \Psi(x, t)$$





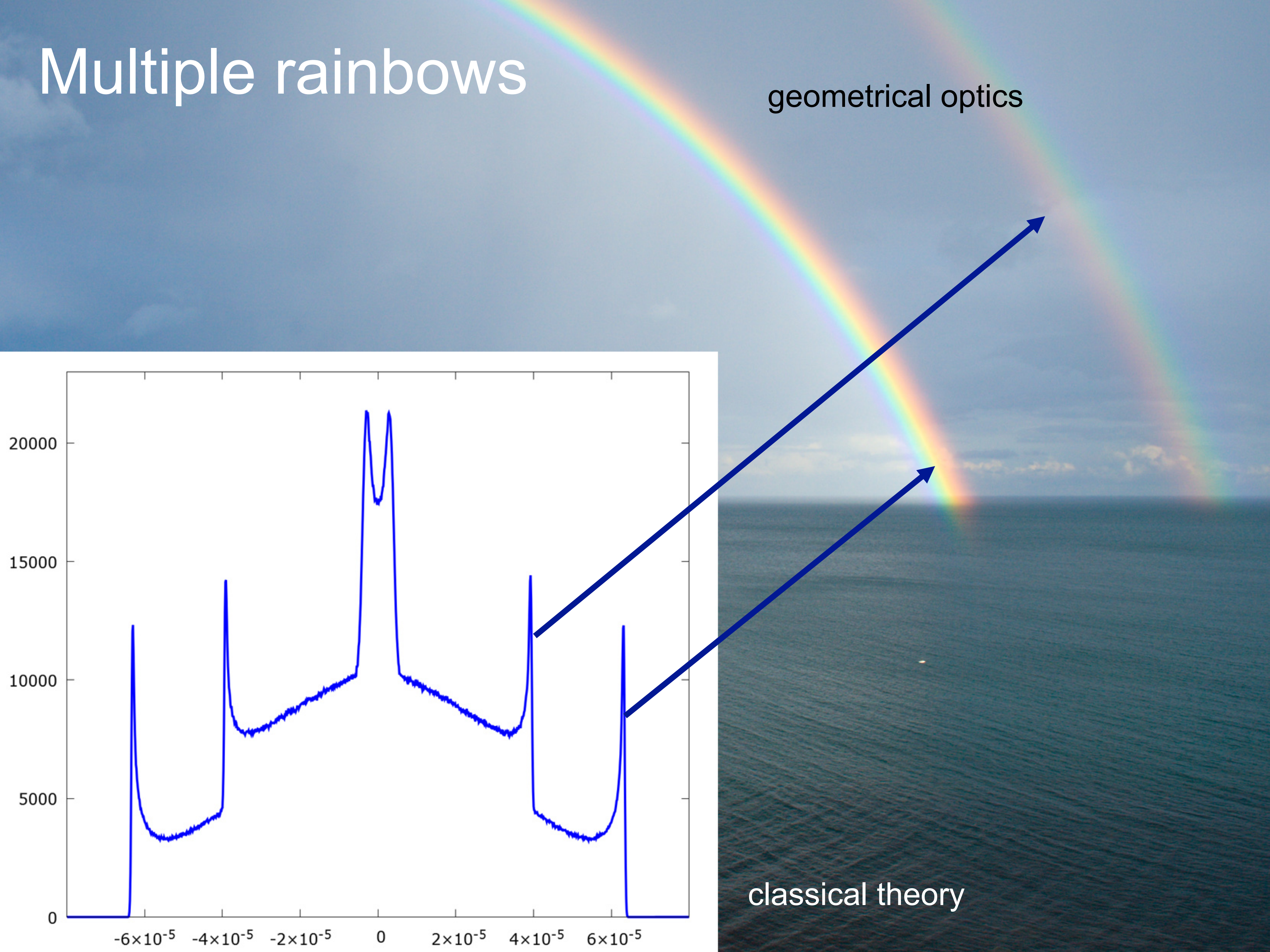


S.N. Shul'ga, N.F. Shul'ga, S. Barsuk, I. Chaikovska, R. Chehab. arXiv:1512.040601v1

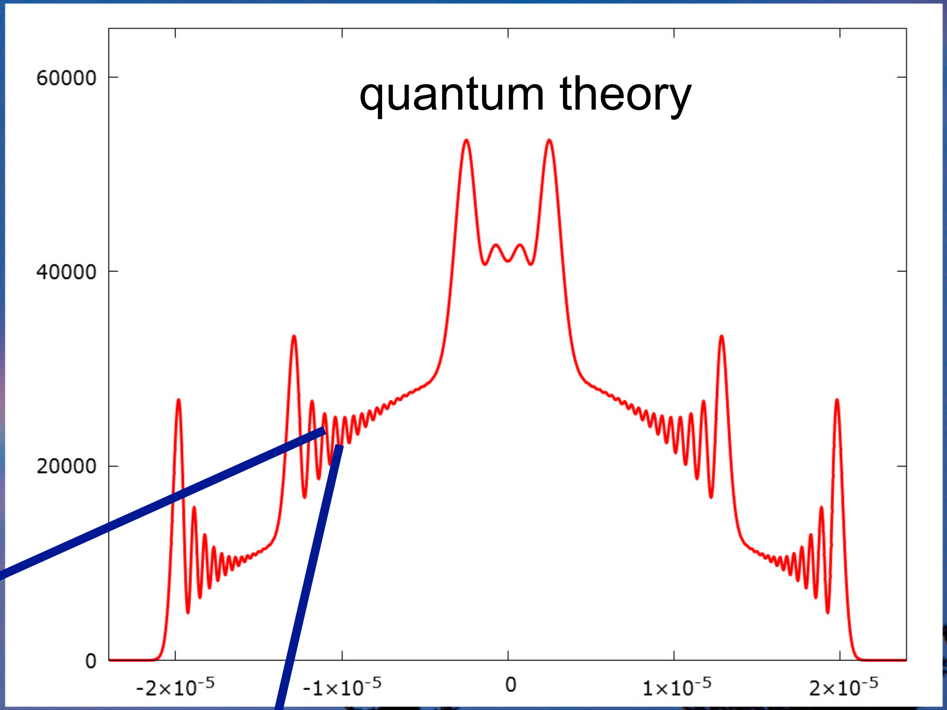


500 MeV electrons

Multiple rainbows



Supernumerary rainbows



wave optics

Conclusions

- Transitional region from ultrathin to thin crystals, recent experimens on ultrathin crystals
- Scattering (rainbow, interference, …)
- Quantum scattering picture is substantially different from the classical one at MeV energies but is close to it at 100s GeV
    - although, quantum effects are still present at such energies
- Sharp maxima in classical (trajectories thickening) and quantum (**interference from different channels**) scattering pictures have different nature
- Possibility of experimental observation

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Grazie!

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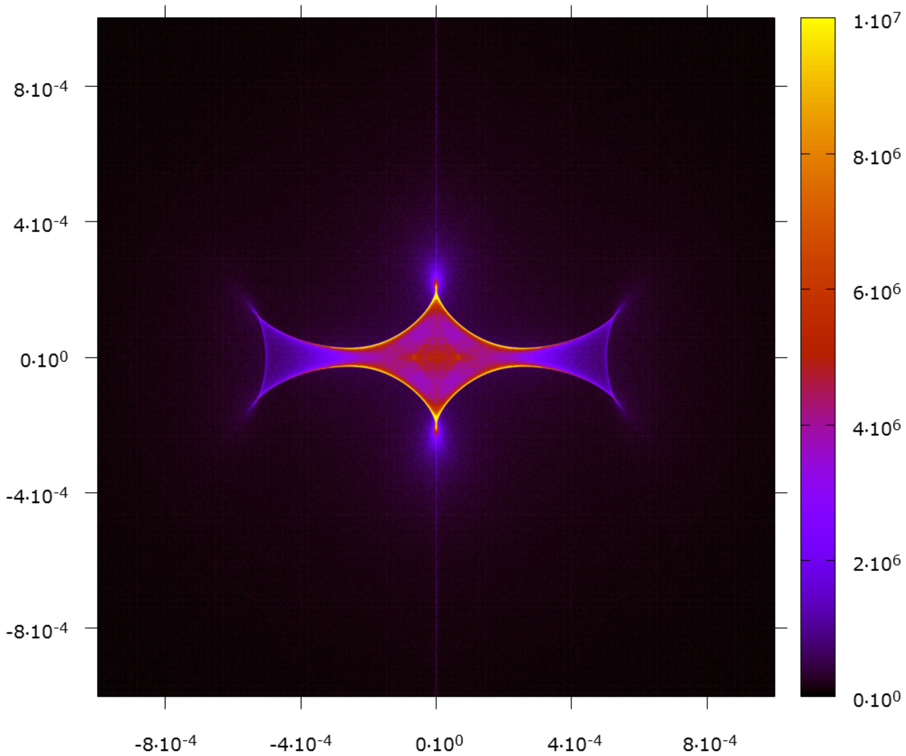
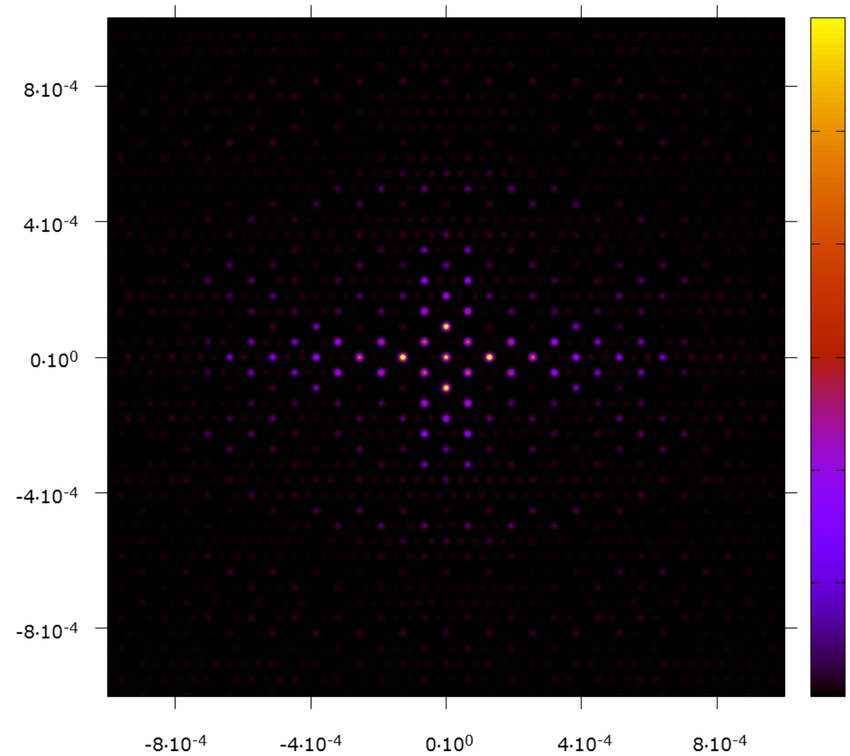
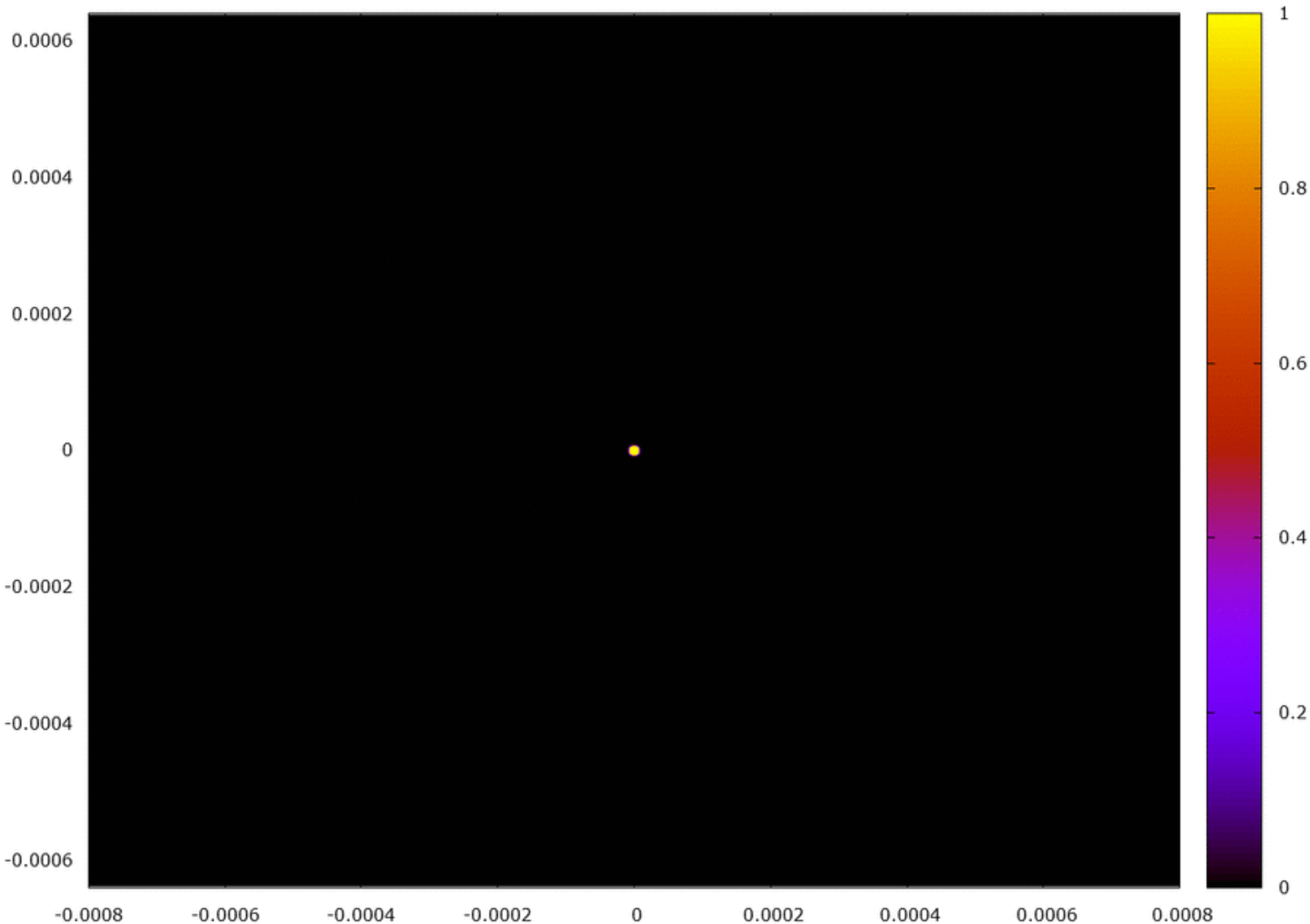
Grazie!

Classical and quantum angular distributions of 50 MeV electrons in ultrathin L=100nm Si <110> crystal

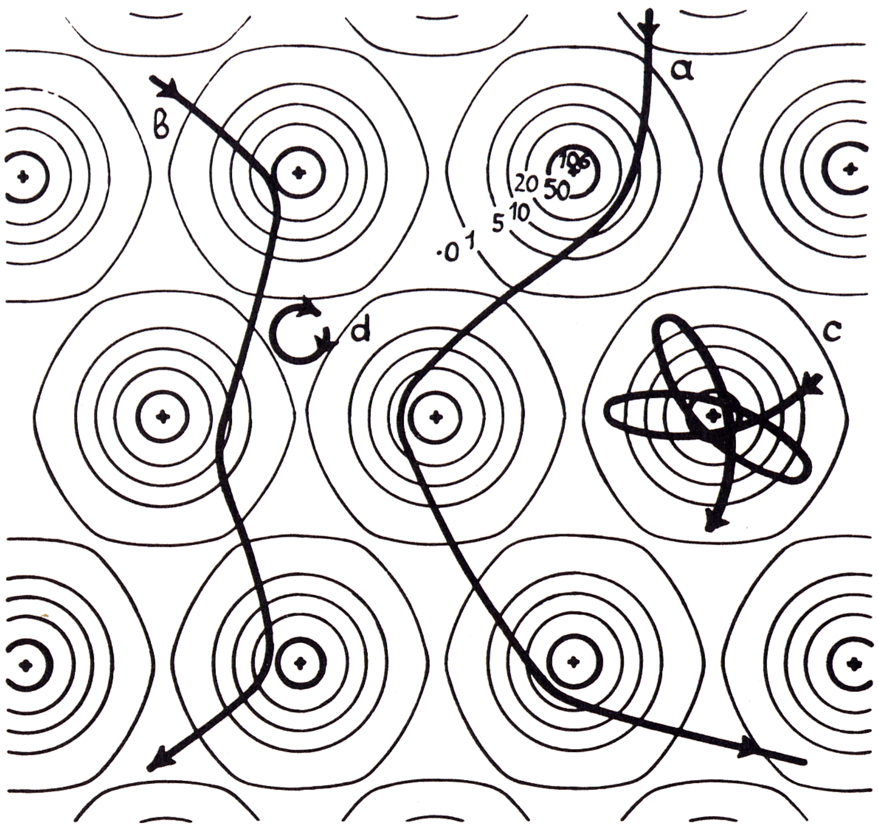




Scattering of a 140 MeV electron at (110) Si crystal axis, $\psi_i = 0$, L=0..2000Å



Particle motion in periodical field of crystal atomic strings Si <111>



Classical consideration

$$\ddot{\vec{\rho}} = -\frac{c^2}{\varepsilon}\frac{\partial}{\partial\vec{\rho}}U(\vec{\rho})$$

Quantum consideration

$$\psi = e^{i(pz-\varepsilon t)}\varphi(\vec{\rho},t)$$

$$i\hbar\partial_t\varphi = \left(-\frac{\hbar^2}{2\varepsilon}\nabla_\perp^2 + U(\vec{\rho})\right)\varphi(\vec{\rho},t)$$

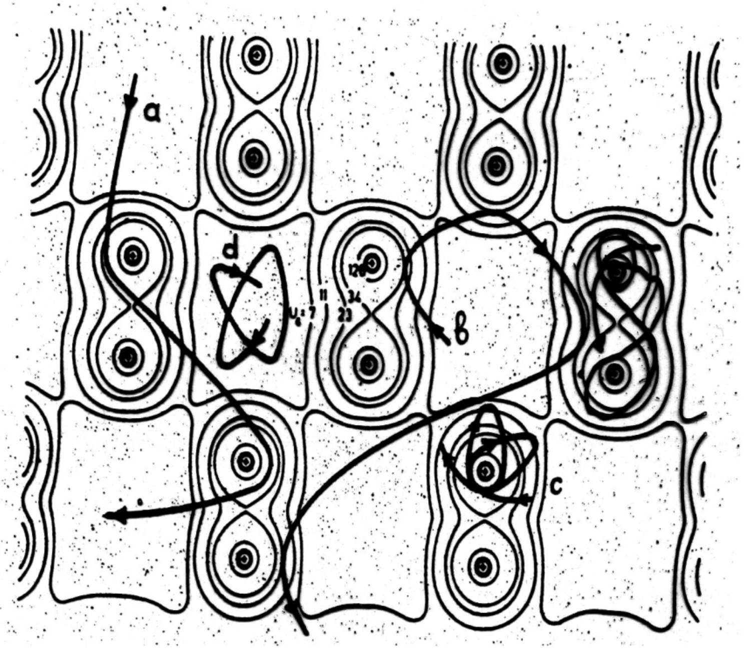
$$\boxed{n_{levels} \sim \varepsilon_{MeV}}$$

- From where appear the bound energy levels at channeling?
- How do the levels appear at dynamical chaos?

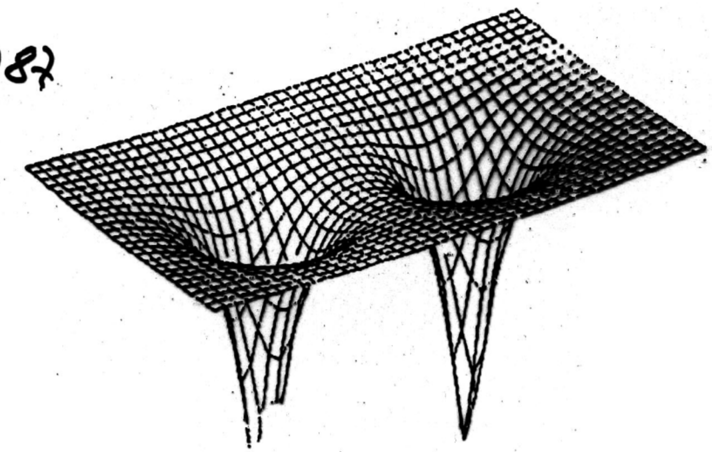
Dynamical chaos at channeling

Yu.Bolotin, V.Gonchar, V.Truten', N.Shul'ga (1986)

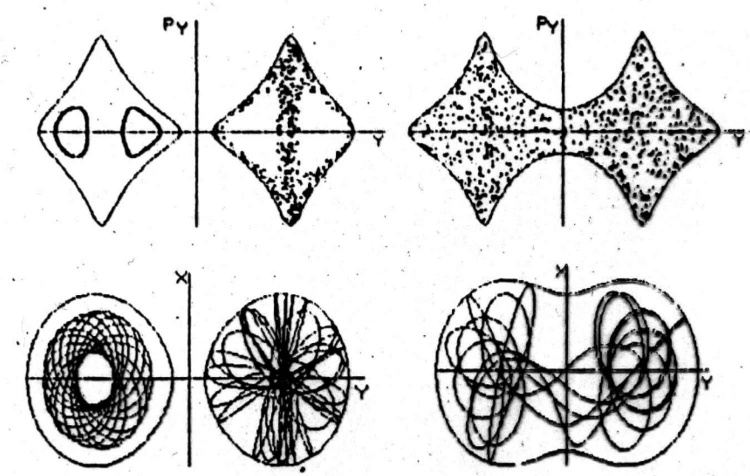
Continuous string potential Ge, <110>.



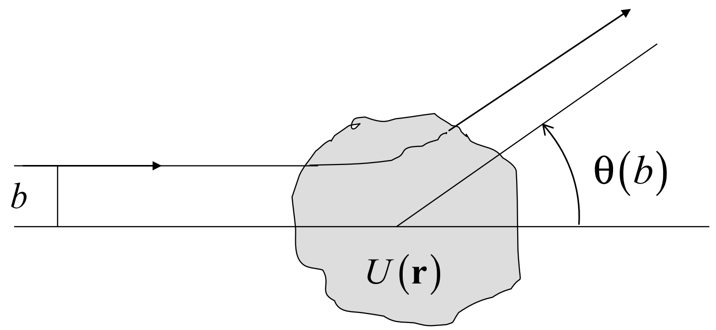
1987



Si, <110>, q~



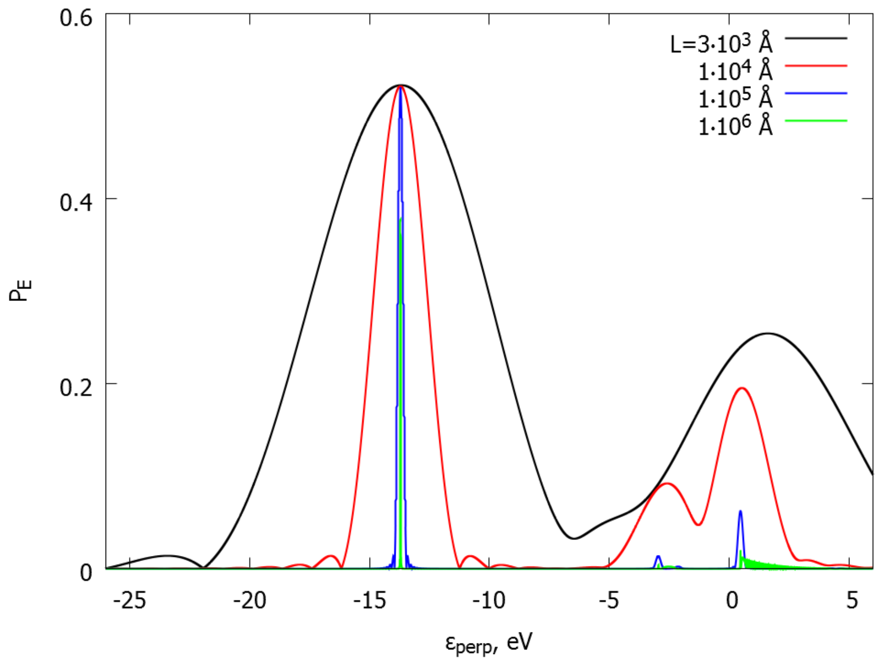
Classical theory of scattering in a compound potential



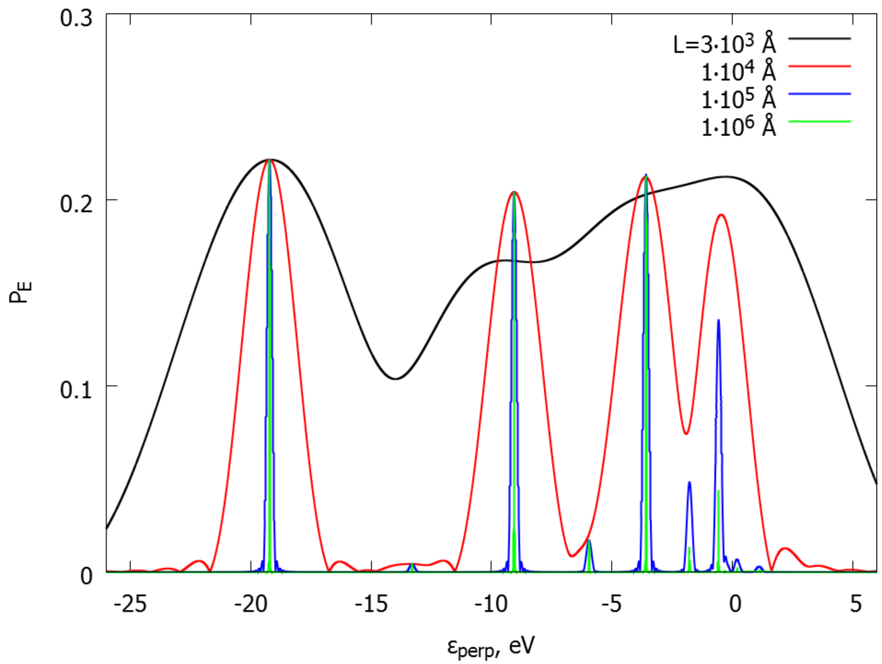
$$d\sigma_{cl} = d^2 b = \left| \frac{\partial\left(b_x, b_y\right)}{\partial\left(\vartheta_x, \vartheta_y\right)} \right| d\vartheta_x d\vartheta_y$$

$$\dot{\vec{\rho}} = -\frac{c^2}{E} \nabla U\left(\vec{\rho}\right)$$

Bound states levels for 4 MeV and 50 MeV electrons at different thicknesses in (110) Si crystal



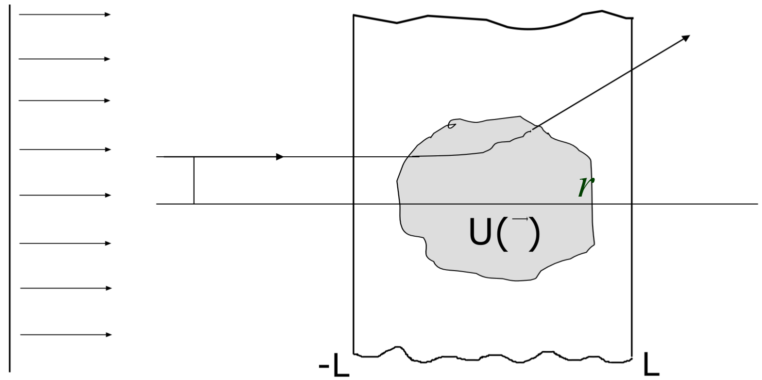
$E_{kin} = 4MeV$



$E_{kin} = 50MeV$

Gauss Theorem in the Theory of Scattering

N. Bondarenco, N. Shul'ga Phys.Lett. B 427 (1998) 114.



$$\psi = e^{i\vec{p}\vec{r}}\varphi(\vec{r})$$

$$a(\vartheta) = -\frac{1}{4\pi}\int_V d^3r\, e^{-i\vec{p}'\vec{r}}\,\overline{u'}\gamma_0 U(\vec{r})\psi(\vec{r}) =$$

$$= -\frac{i}{4\pi}\oint d\vec{S}\,\overline{u'}\vec{\gamma}\psi(\vec{r})\,e^{-i\vec{p}'\vec{r}} =$$

$$\vec{q} = \vec{p} - \vec{p}'$$

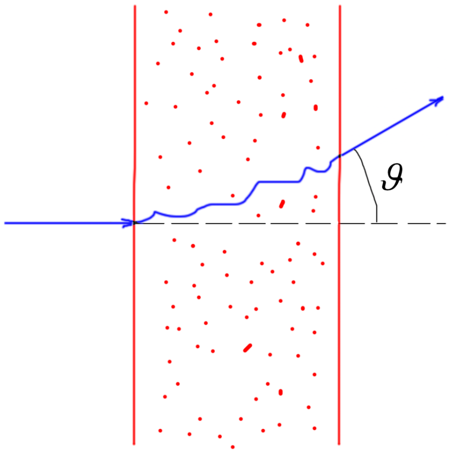
$$= -\frac{ip}{2\pi}\oint d^2\rho\, e^{i\vec{q}\vec{r}}\left(\varphi(\vec{r}) - 1\right)\Big|_{z=-L}^{z=L}$$

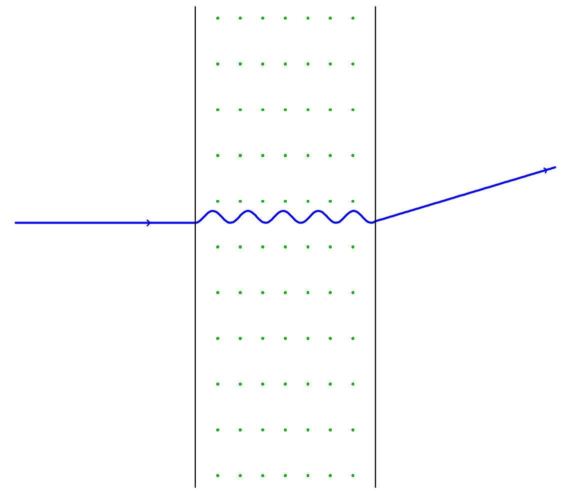
$$\frac{d\sigma_q}{do} = \left|a(\vartheta)\right|^2$$

Classical and Quantum effects at Channeling in Ultrathin Crystals

- Transitional region from ultrathin to thin crystals
- Scattering (rainbow, bound states levels, interference, coherence, …)
- How do quantum levels appear at regular motion and dynamical chaos?

Scattering in amorphous and crystalline media



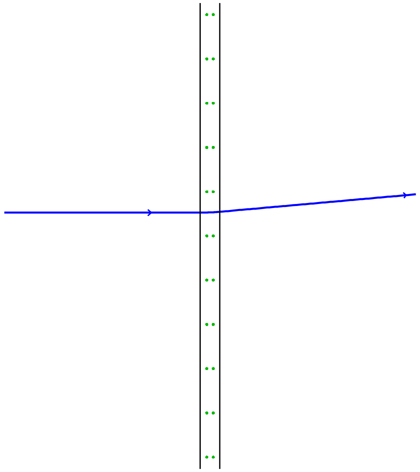


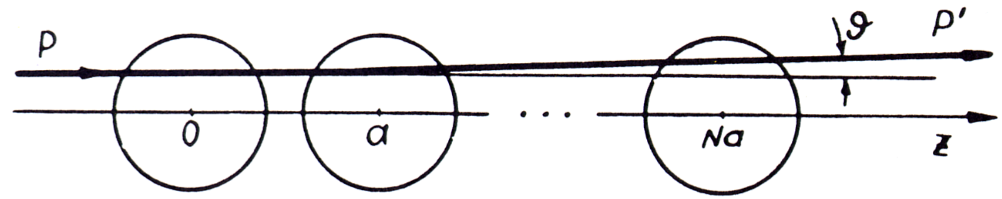
channeling (planar, axial)
above barrier motion

$$\frac{d}{dt} f\left(\vec{\vartheta},t\right)=n\int d\sigma(\vec{\chi})\left[f\left(\vec{\vartheta}-\vec{\chi},t\right)-f\left(\vec{\vartheta},t\right)\right]$$

$$f_{B-M}\left(\vec{\vartheta},t\right)=\int\frac{d^2\xi}{4\pi^2}\exp\left\{i\vec{\xi}\vec{\vartheta}-nt\int d\sigma\left(\chi\right)\left[1-e^{i\vec{\xi}\vec{\chi}}\right]\right\}$$

Scattering by atomic string





$$a^{(N)}(q_\perp) = \frac{ip}{\hbar}\int_0^\infty \rho\, d\rho\, J_0(q_\perp \rho/\hbar)\left\{1 - \exp\left[\frac{i}{\hbar}\left(\chi_0^{(N)} + \chi_1^{(N)} + \ldots\right)\right]\right\}$$

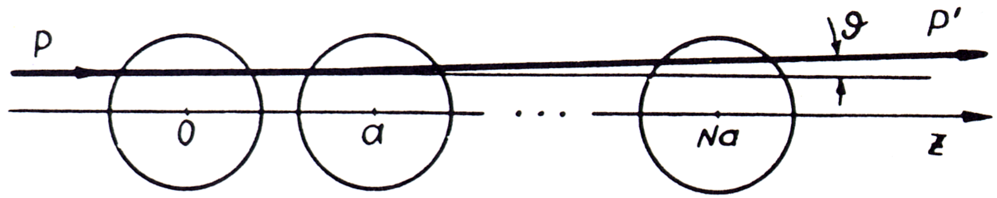
$$\chi_0^{(N)} = N\chi_0, \qquad \chi_1^{(N)} = \frac{N^3 a}{12p}\left(\frac{\partial}{\partial\rho}\chi_0\right)^2, \qquad \chi_0 = -\frac{1}{v}\int_{-\infty}^{\infty} dz\, u(\rho, z)$$

Classical description

$$\alpha_{eff}^{(N)} = \frac{\chi_0^{(N)}}{\hbar} = N\frac{Ze^2}{\hbar c} >> 1$$

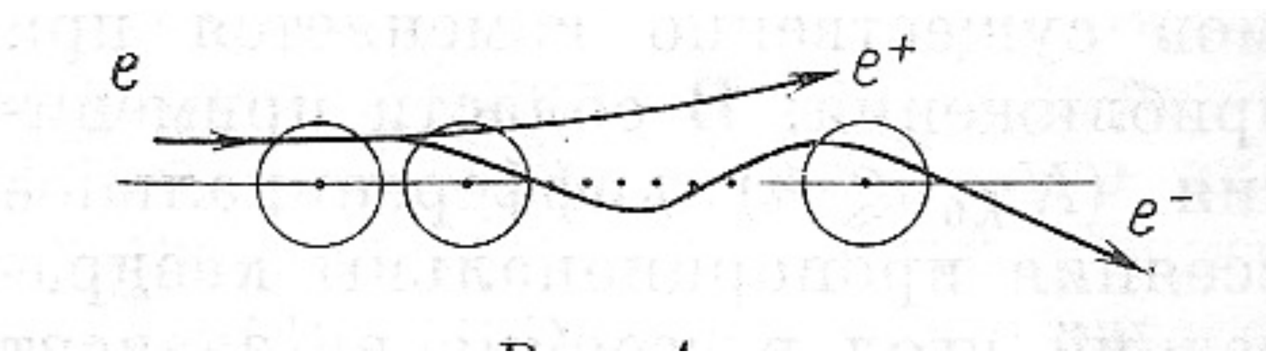
Scattering by atomic string

$$\chi_0^{(N)} >> \chi_1^{(N)} \qquad \frac{N^2 aZe^2}{p\,R^2} << 1$$

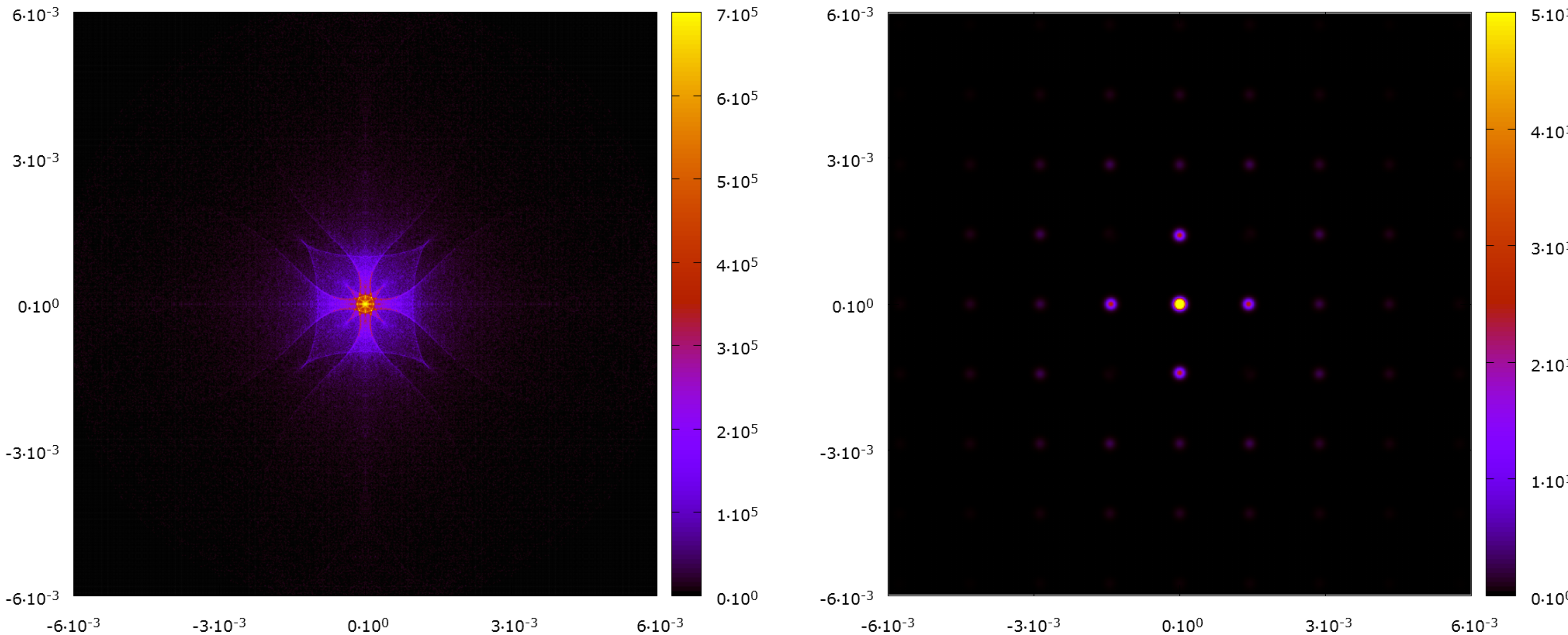


Channeling

$$\chi_0^{(N)} \sim \chi_1^{(N)}, \qquad \frac{N^2 aZe^2}{p\,R^2} \sim 1$$



Classical and quantum angular distributions of 4 MeV electrons in ultrathin L=354nm Si <100> crystal



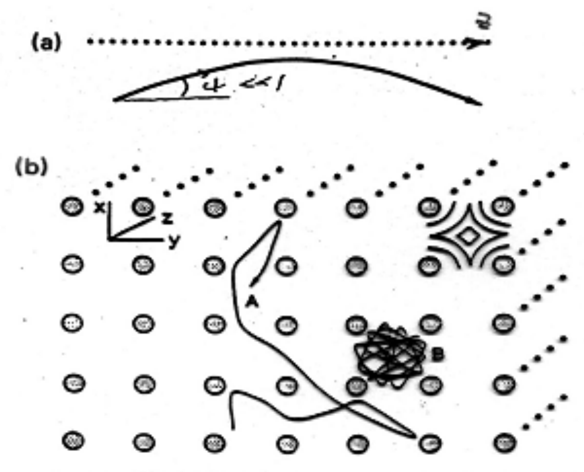
$$\text{for}\, \varepsilon = 4MeV, \quad Si\langle 100 \rangle$$

$$\theta_c \approx 6 \cdot 10^{-3} \qquad \Delta\vartheta_g \cong \frac{2\pi}{pd} \approx 1.45 \cdot 10^{-3}$$

Axial Channeling and Above-Barrier Motion (continuous string potential)

$$\frac{d\mathbf{p}}{dt} = -\nabla U(\mathbf{r})$$

$$U(\mathbf{r}) \to U(x,y) = \frac{1}{L}\int_0^L dz \sum_n u(\mathbf{r}-\mathbf{r}_n)$$



$$\frac{d\mathbf{p}}{dt} = -\nabla U(x,y) \qquad \to \qquad \begin{cases} p_z = const >> p_\perp \\ \ddot{\vec{\rho}} = -\dfrac{1}{\varepsilon}\nabla U_\perp(x,y) \end{cases}$$

Exteriment: 2MeV protons scattering in L=55nm Si

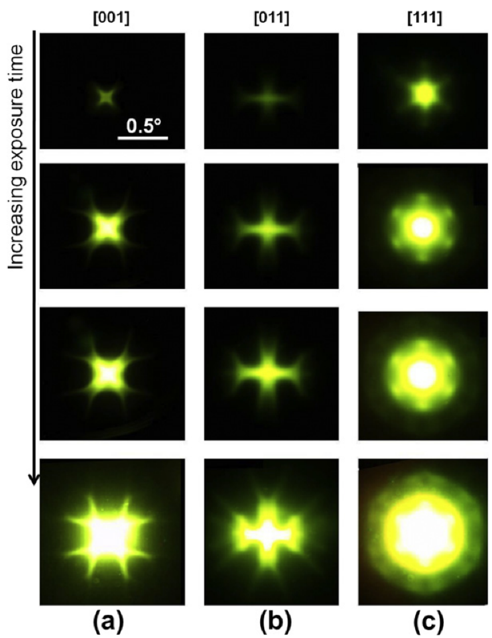
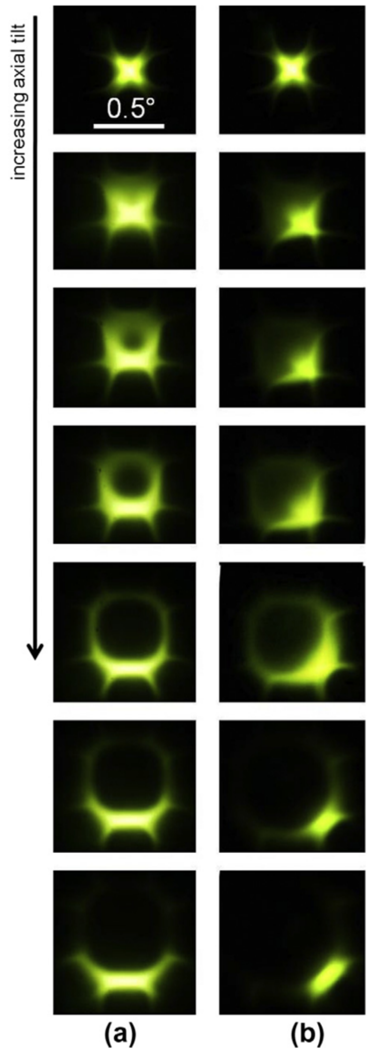


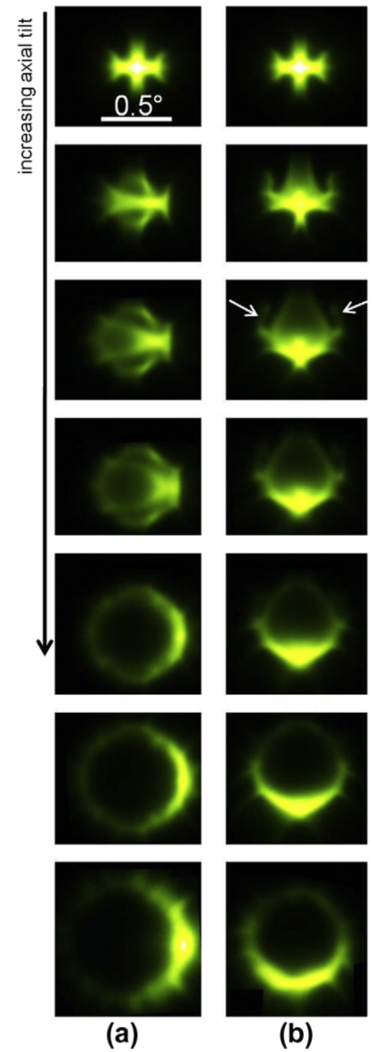
Fig. 2. Experimental channeling patterns for 2 MeV protons from a 55 nm [001] Si membrane at alignment with the (a) [001], (b) [011] and (c) [111] axes. Downwards direction shows the effect of increasing camera exposure.

$$\psi = 0$$

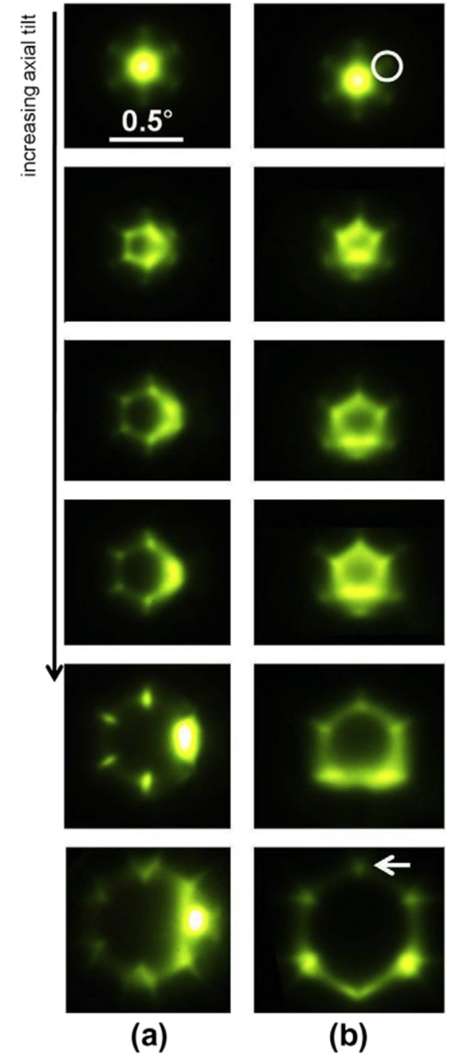
different expositions



$\langle 100 \rangle$



$\langle 110 \rangle$



$\langle 111 \rangle$

$$\psi_c > \psi > 0$$

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