On classical and quantum effects at scattering of ultrarelativistic electrons in ultrathin crystals

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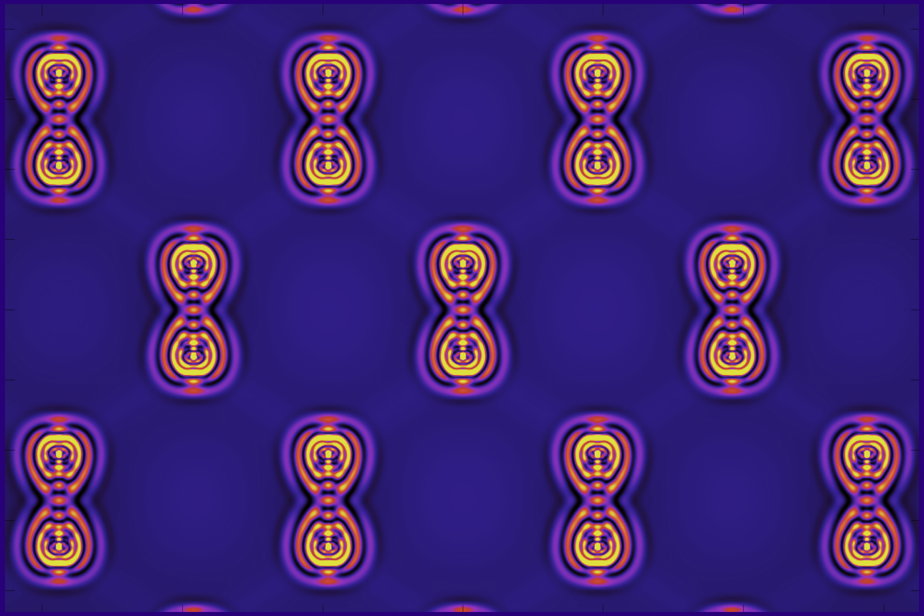
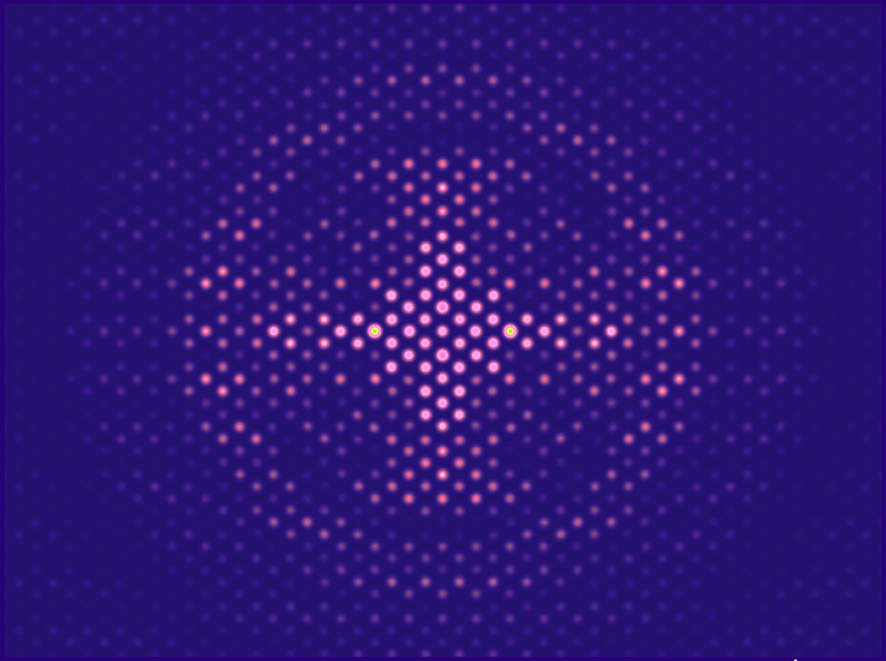


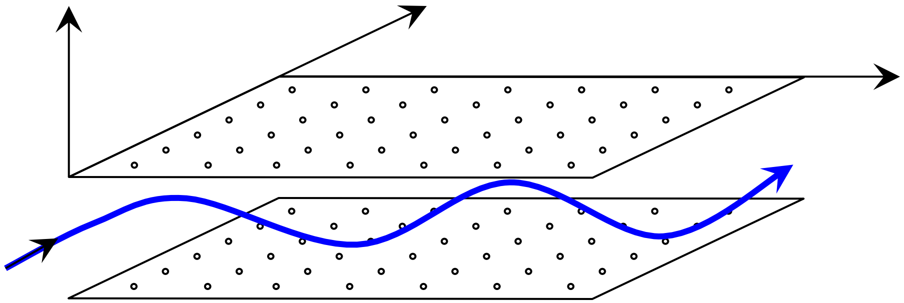


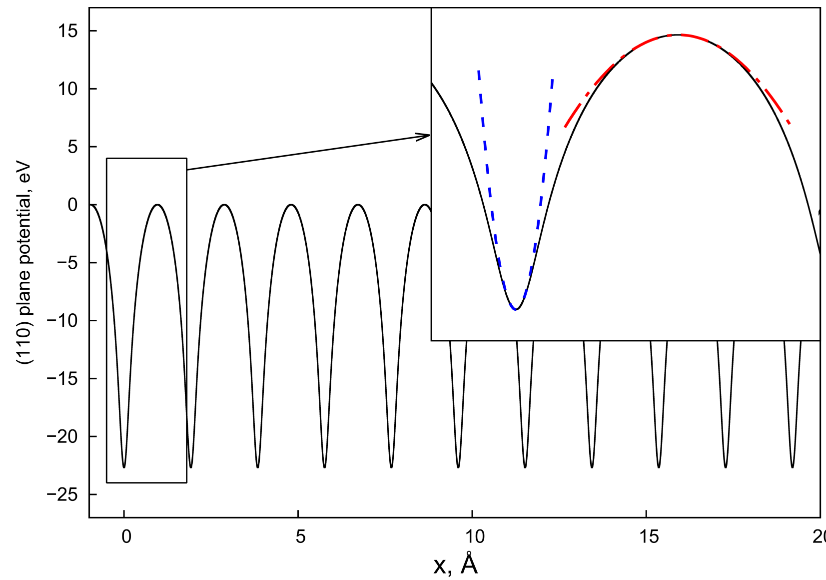
French-Ukrainian Workshop (November 6-8, 2017) LAL - Orsay, France

Continuous Planes Potential

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

$$\sim (x - x_0)^2 + U_0$$





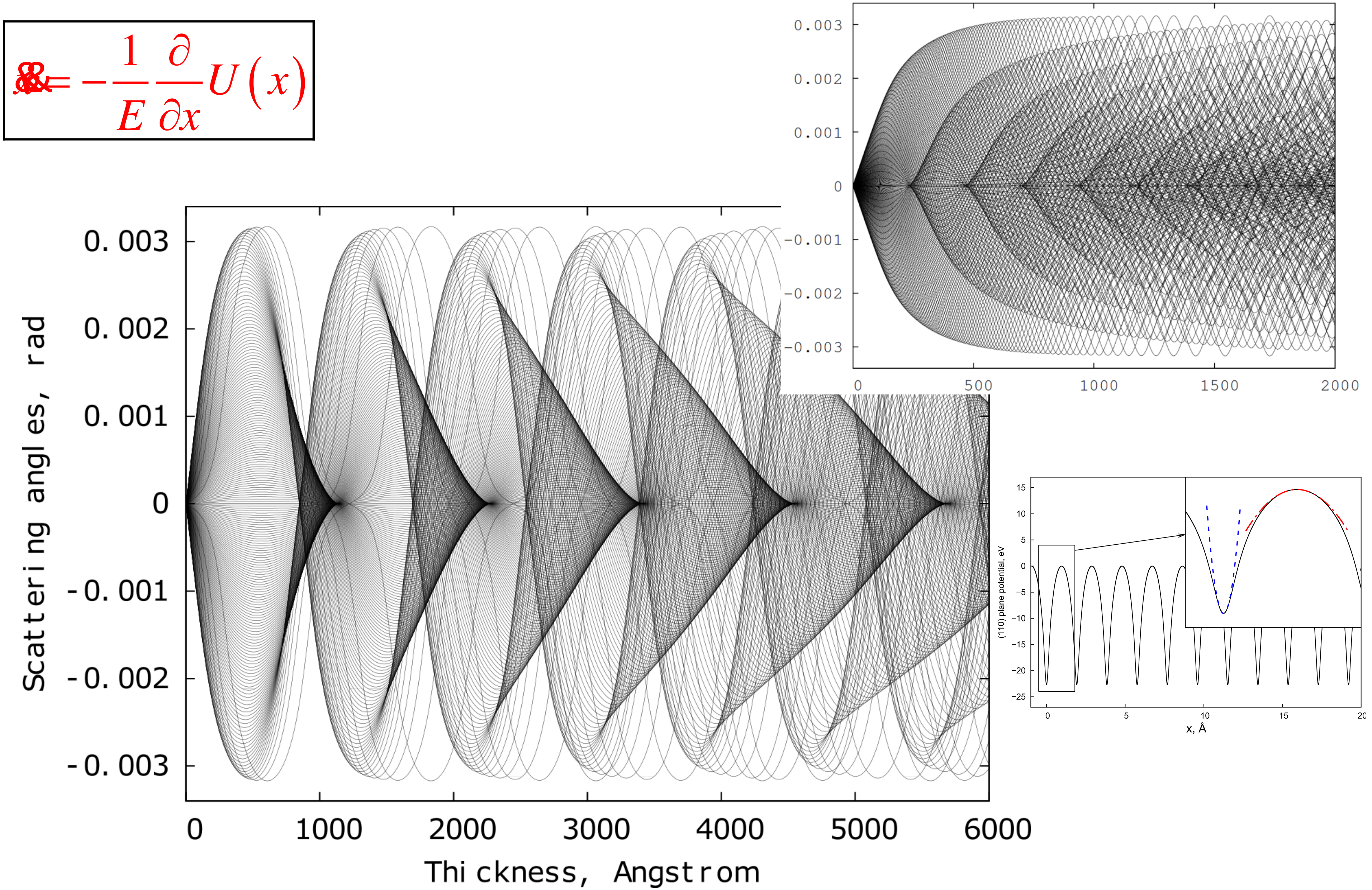
$$U_{ax}(\vec{\rho}) = \frac{1}{a_1 \overline{v}^2} \int d^2 v e^{-v^2/2\overline{v}^2} \int_{-\infty}^{\infty} dz\, u(\vec{\rho} + \vec{v}, z)$$ – string potential

v - heat oscillations of atom coordinates

$$u_m(r) = \sum_i \alpha_i \exp(-\beta_i r / R)$$ – Moliere approximation for single atoms

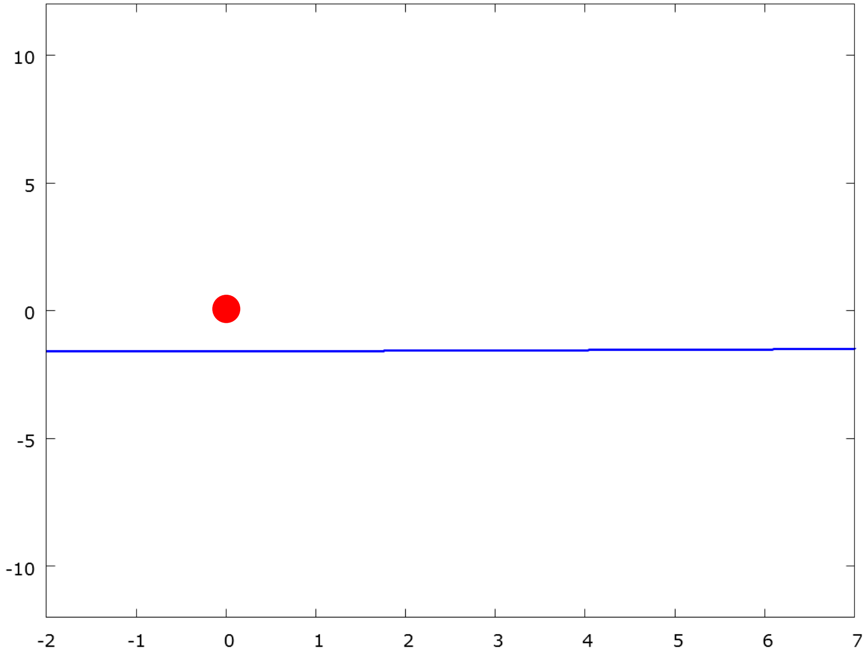
Classical scattering angles of electrons and protons in (110) planes of Si crystal as function of impact parameter and crystal thickness

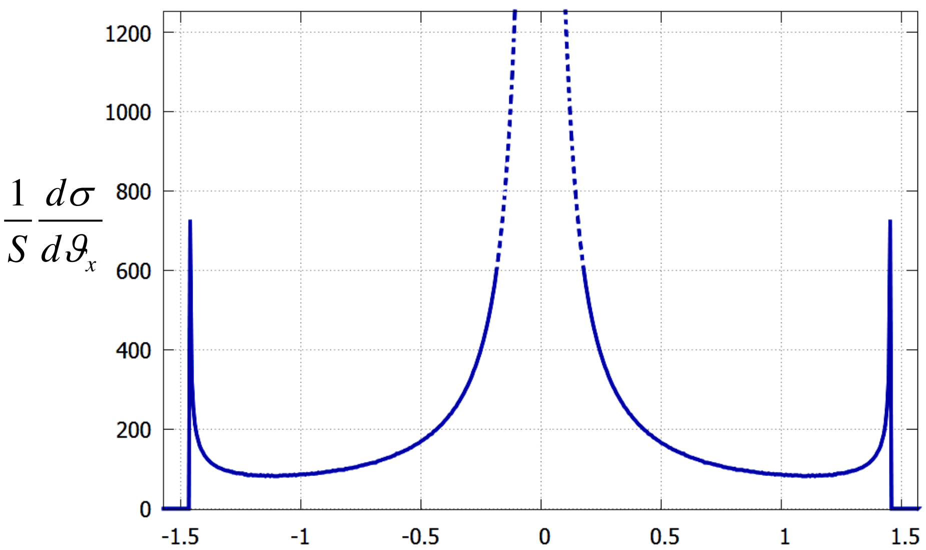
$$\ddot{x} = -\frac{1}{E}\frac{\partial}{\partial x}U(x)$$



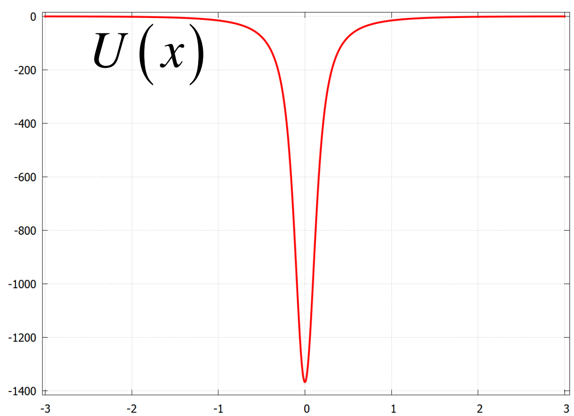
Classical rainbow on one atom

Rainbow scattering of e⁻ ’s on one atom

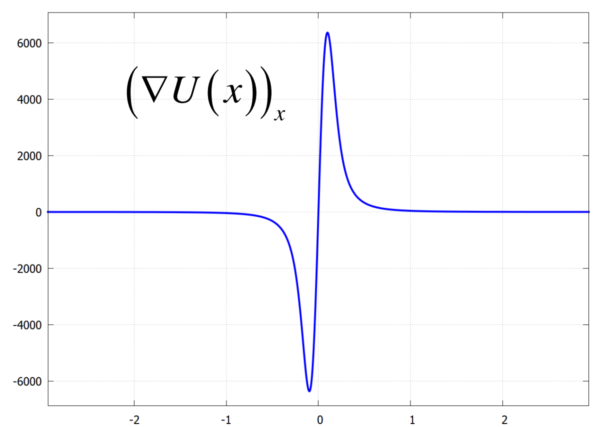




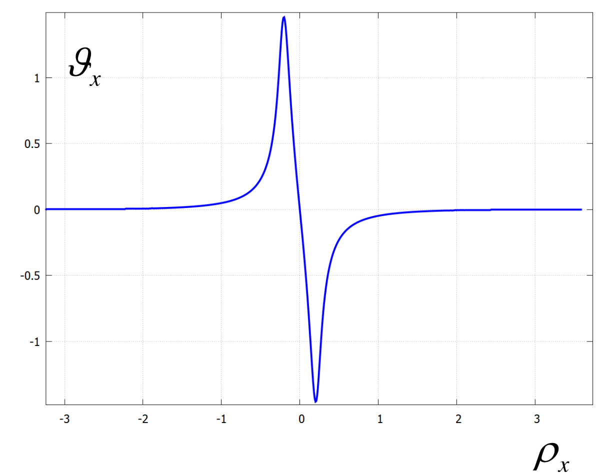
Moliere potential with heat oscillations



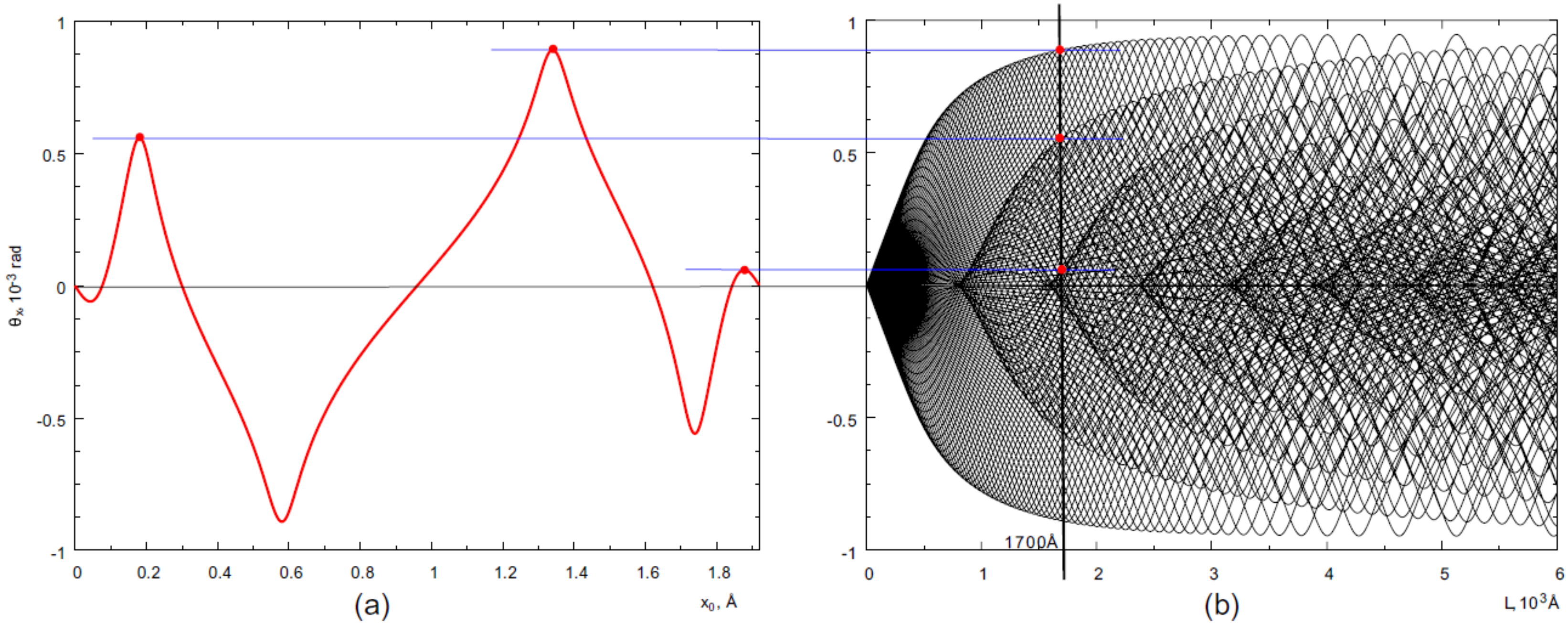
Potential gradient

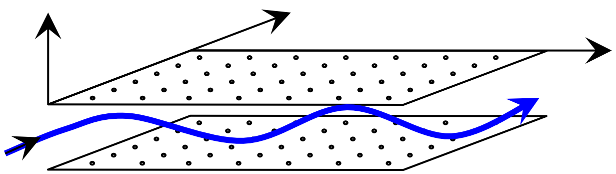


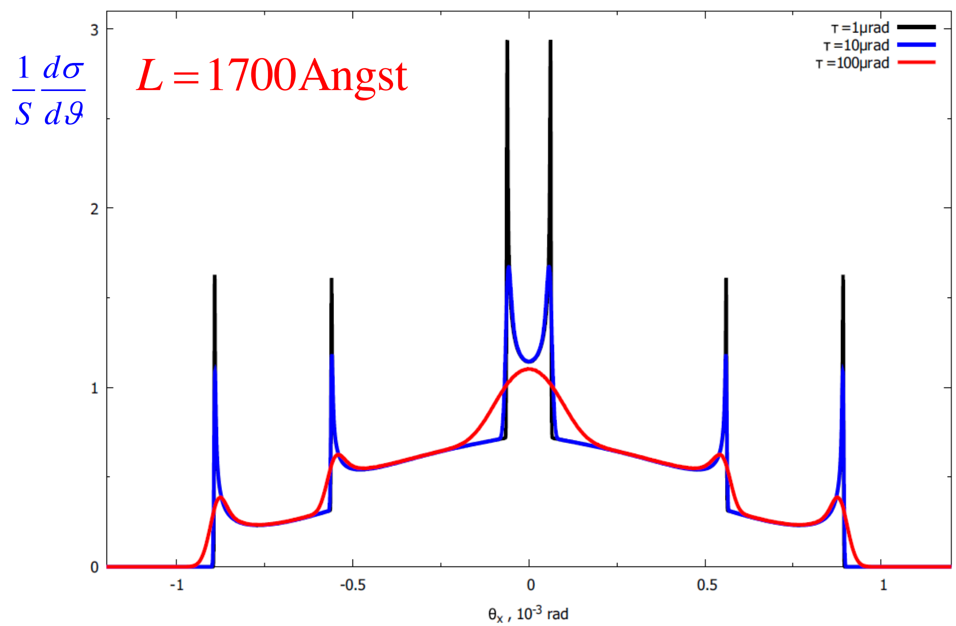
Deflection function



Deflection function and classical rainbow (e- 50MeV Si (110))







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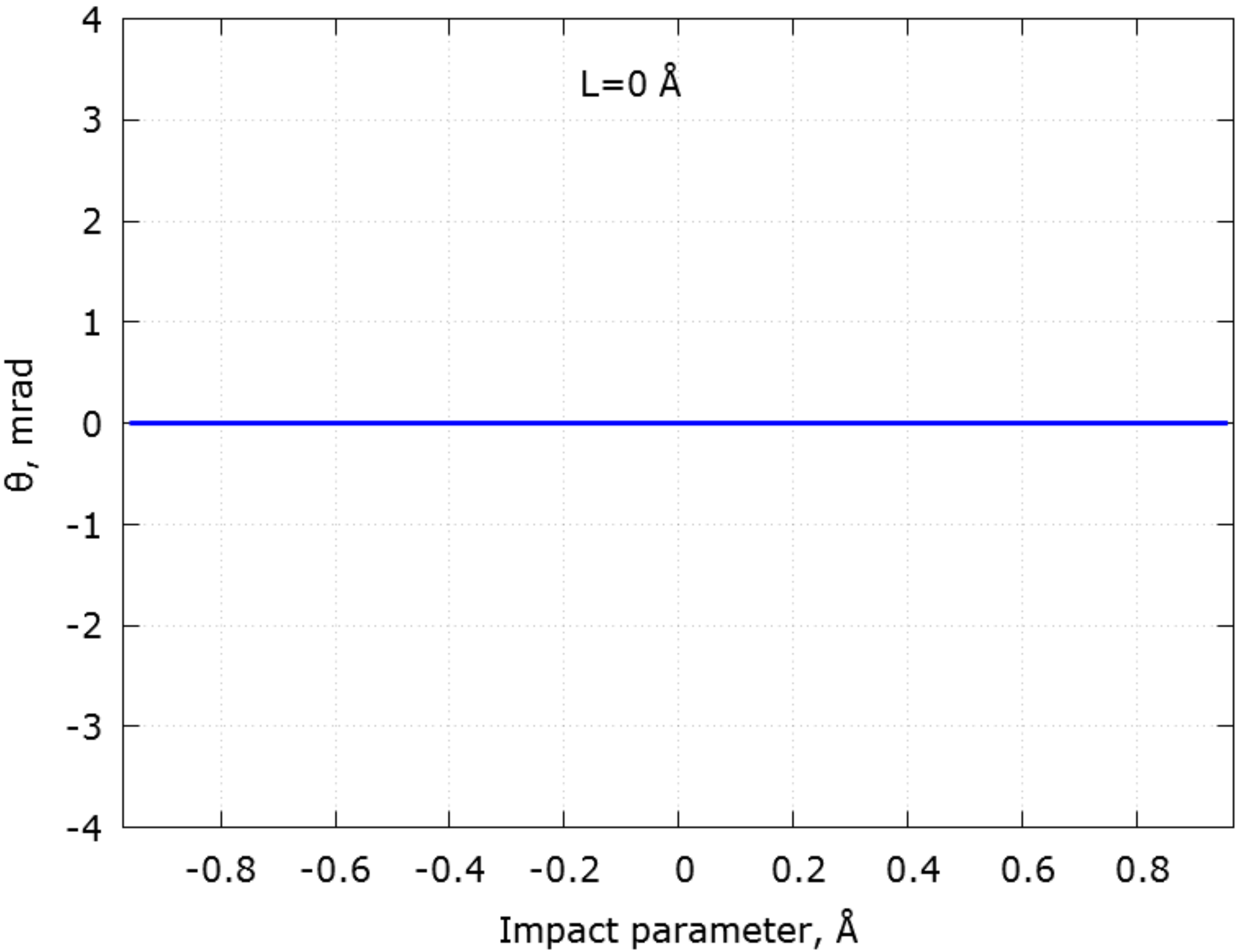
Deflection function
of 4 MeV electrons in ultrathin Si (110) crystal planes



Quantum consideration: Spectral (Operator) Method

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

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

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

- 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, J. Fleck 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. Lett. 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 Phys. Lett. B (2017) 769 (scattering)

Wave function calculation in Operator Method

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

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

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

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

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

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

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

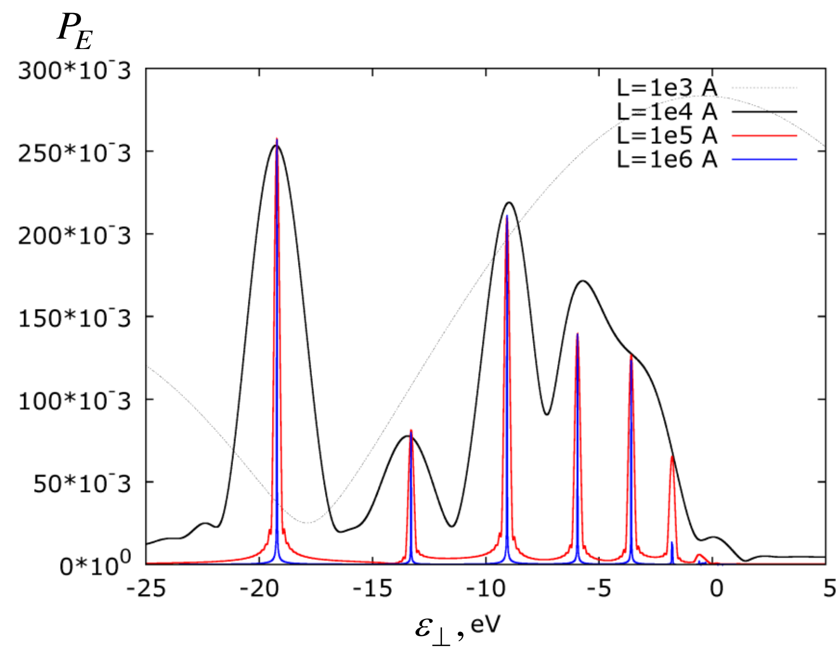
On Zassenhaus formula - D. Scholz, M. Weyrauch, J. Math. Phys. 47 (2006).

Calculation of Energy Spectrum of Channeling Radiation by the Spectral Method

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

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

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



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

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

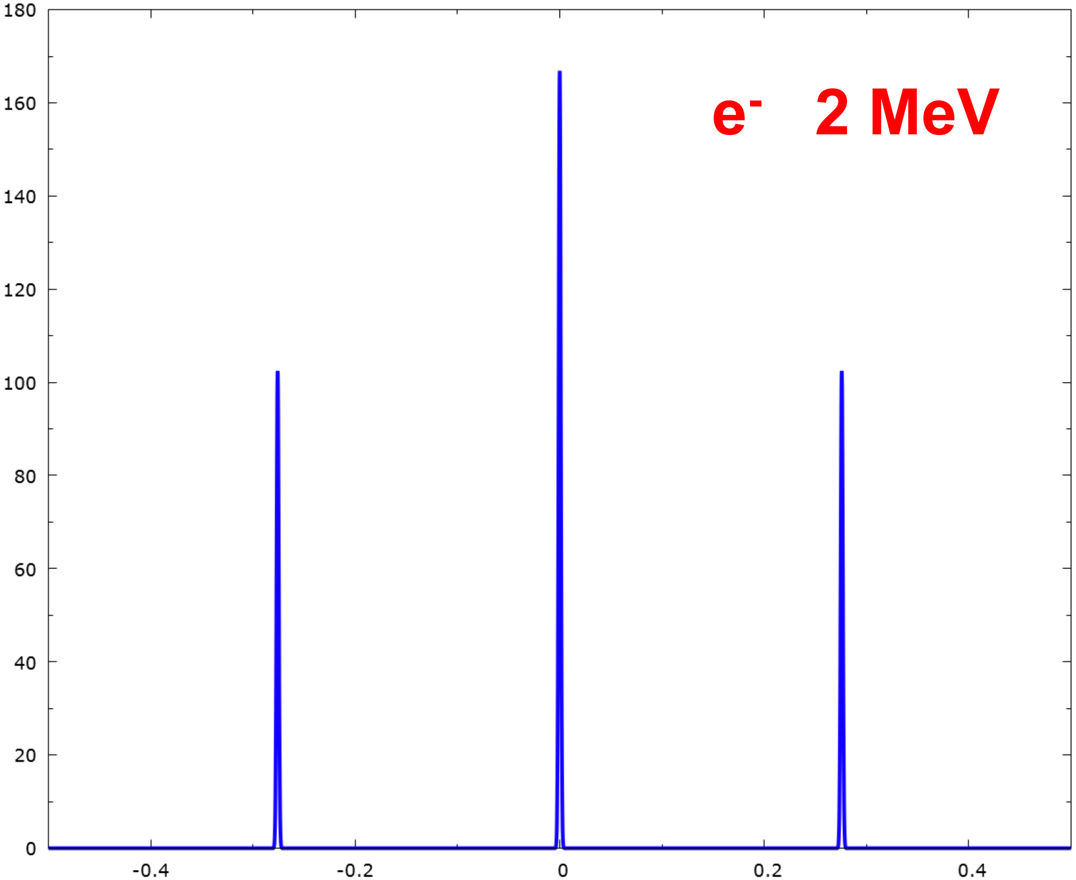
planar scattering $N_{levels} \sim \sqrt{\varepsilon[MeV]}$

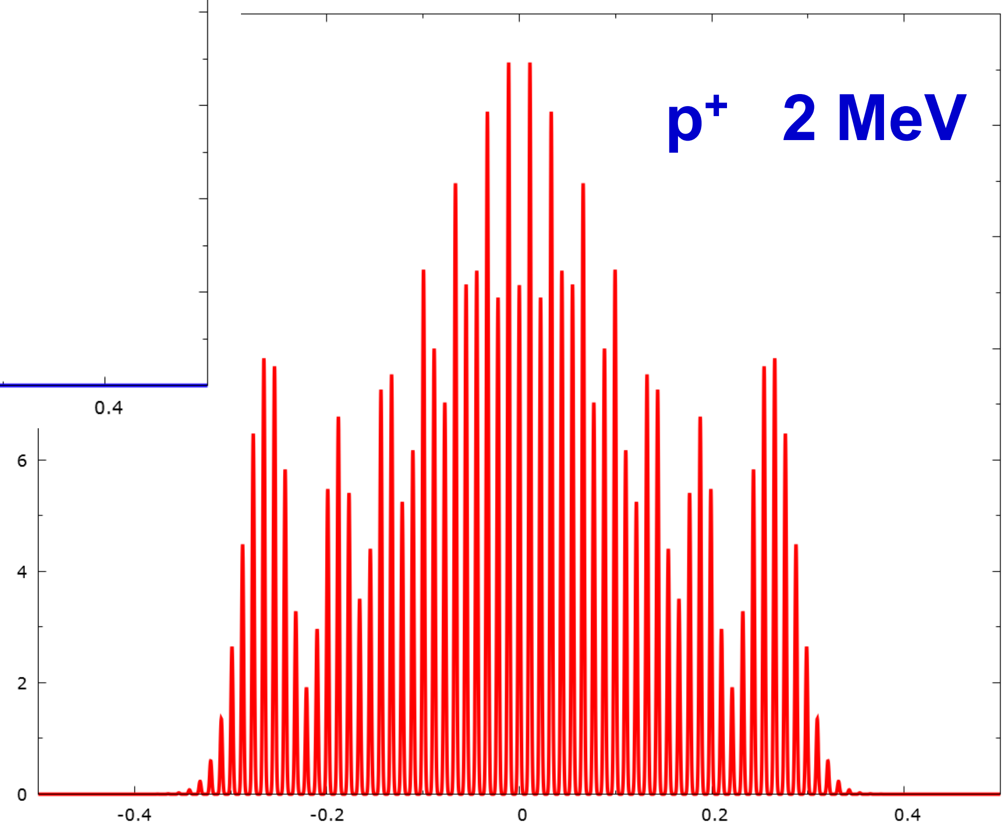
axial scattering $N_{levels} \sim \varepsilon[MeV]$

What radiation should we get at scattering by ultrathin crystal?

Possible application for study of quantum chaos

Plane wave scattering on a thin crystal (Si (110) 170Å)





$$\Delta\psi = 2\pi\hbar / d_x p_P$$

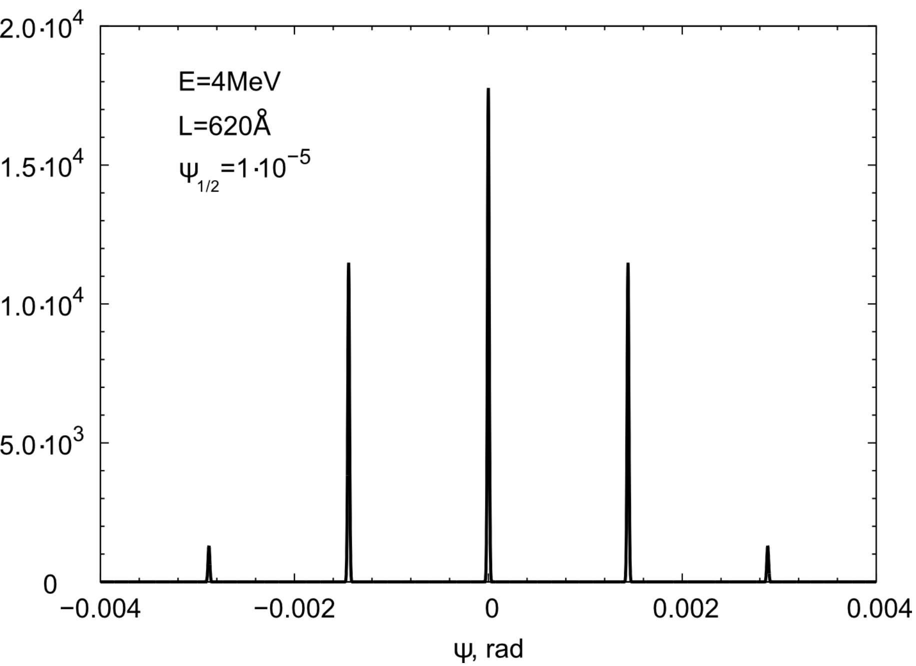
Scattering of electrons by crystal plane. Quantum case

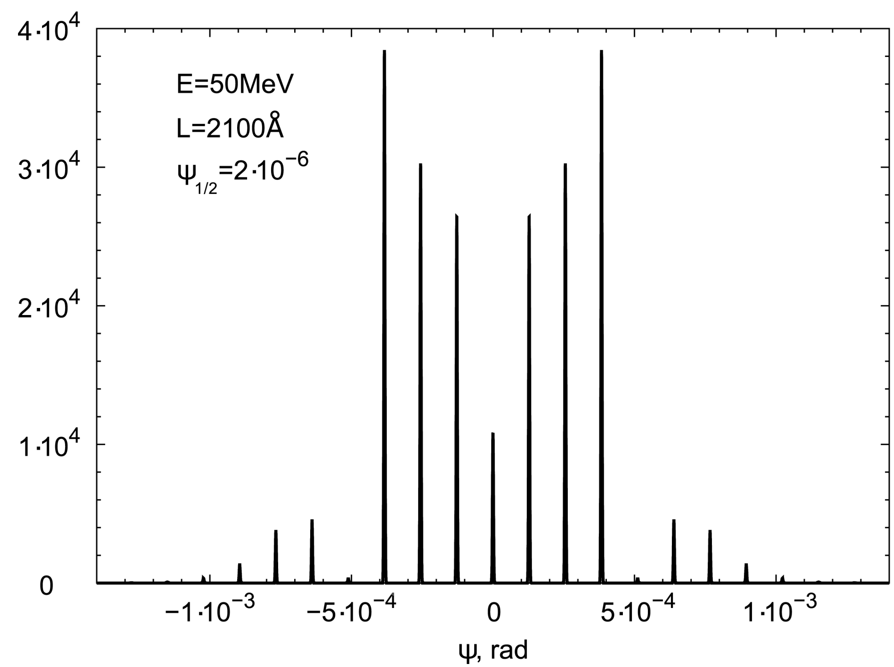
Electrons are considered as plane waves

$$\psi_n = \frac{2\pi\hbar n}{d_x}\frac{1}{p_{\parallel}}$$

Expansion over reciprocal lattice vectors

d_x – lattice period

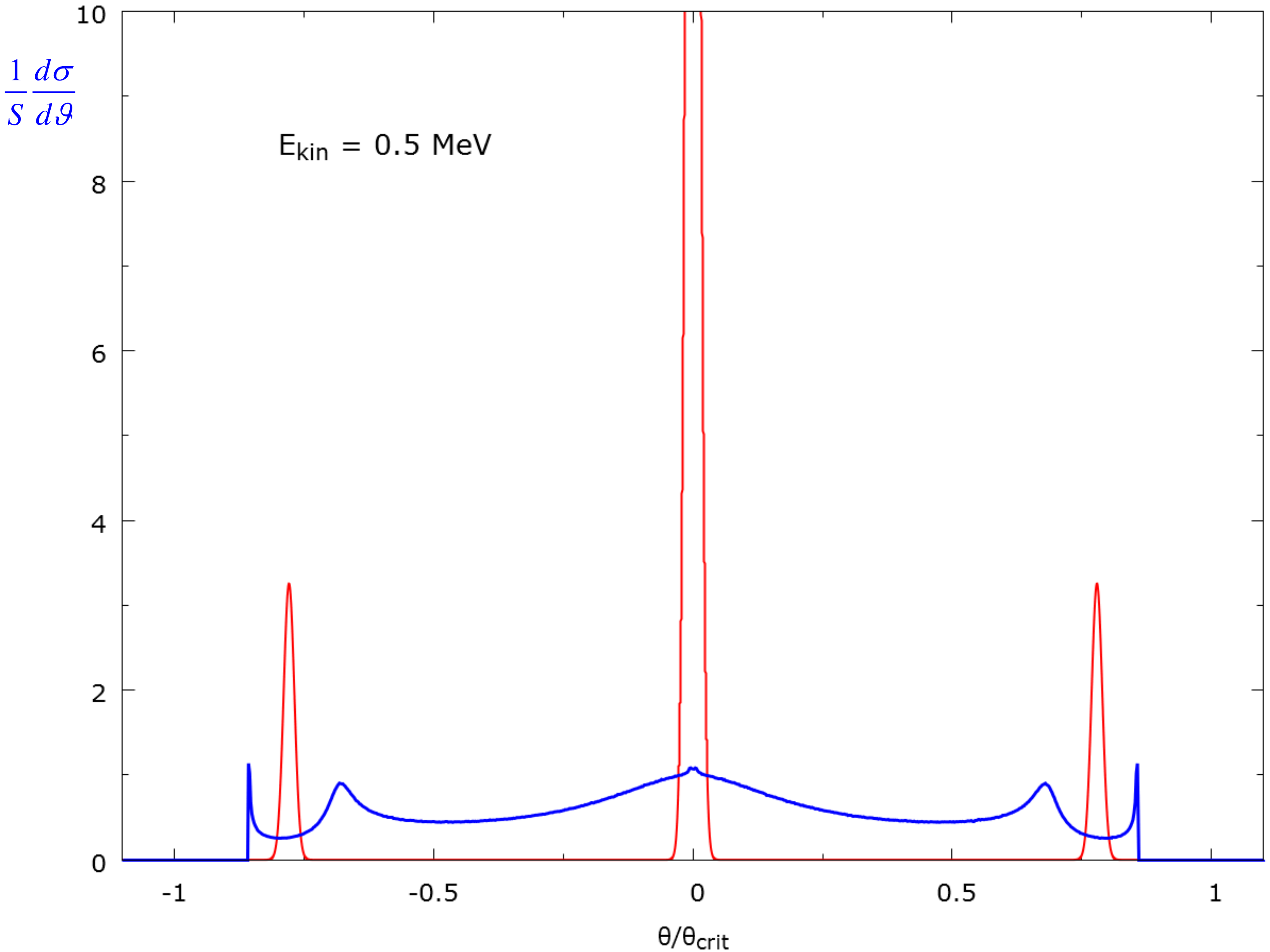




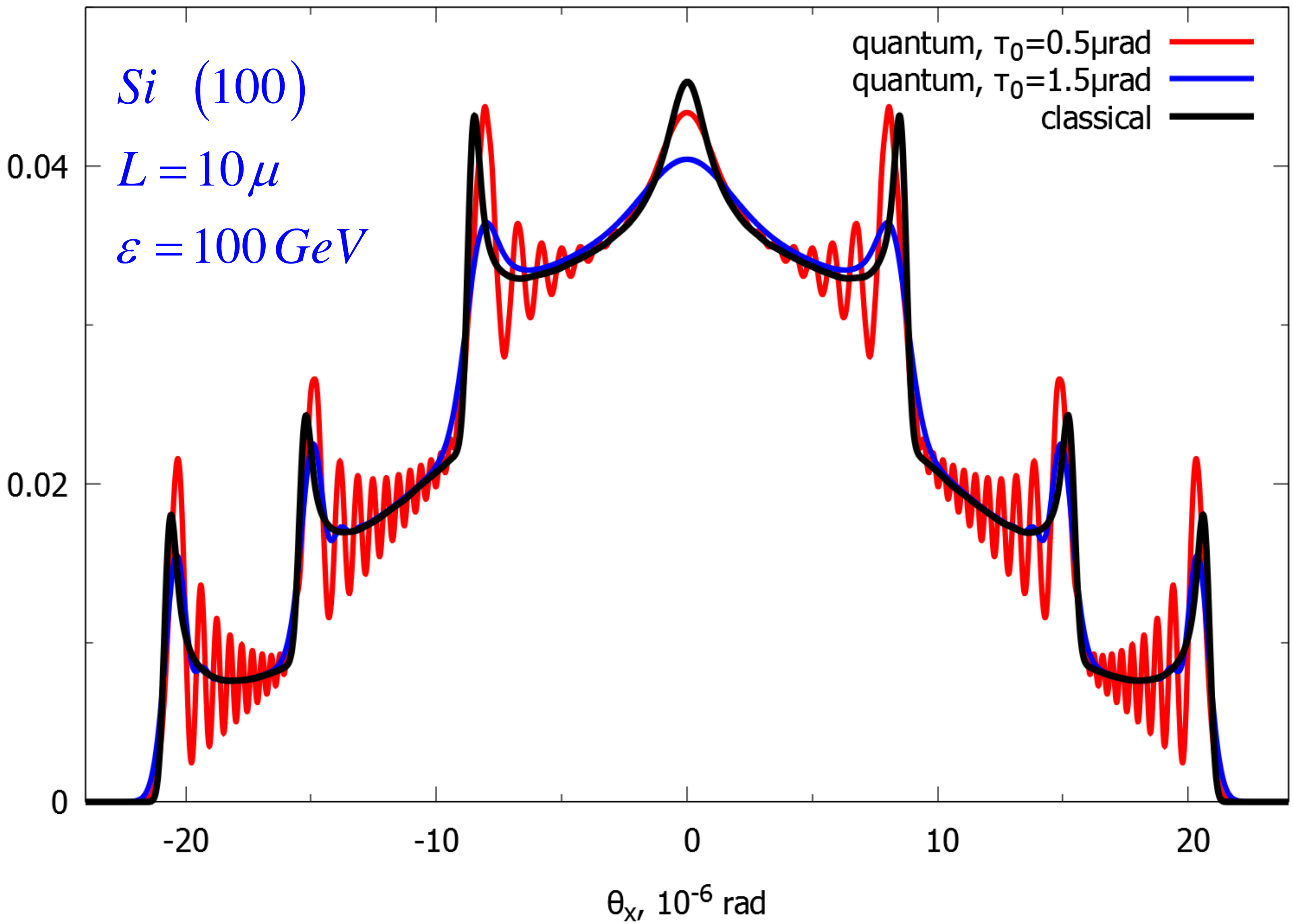
Convolution over different incidence angles corresponding to different electrons of a beam with divergence σ_{beam}

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

Planar scattering of positrons in a thin Si crystal: changing energy



Rainbow scattering in the field of ultrathin Si (110) crystal planes



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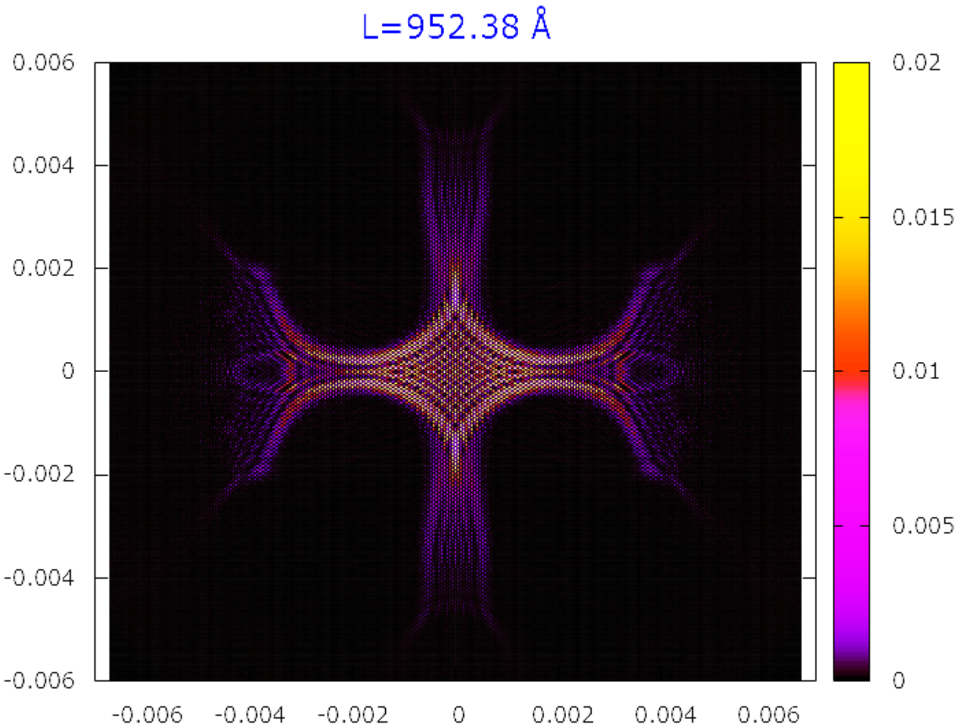
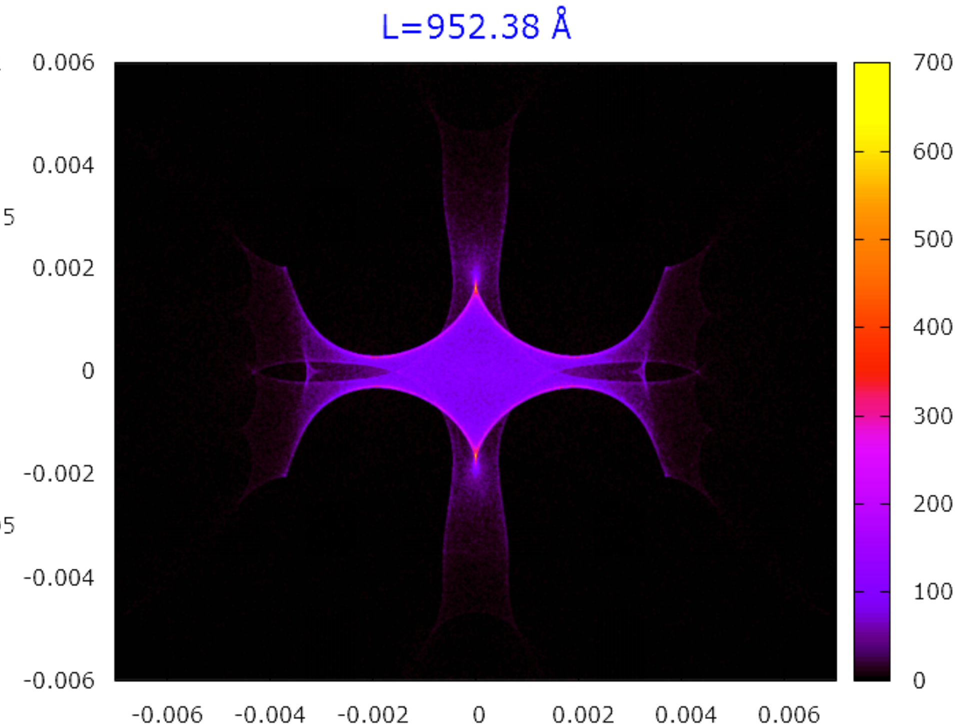
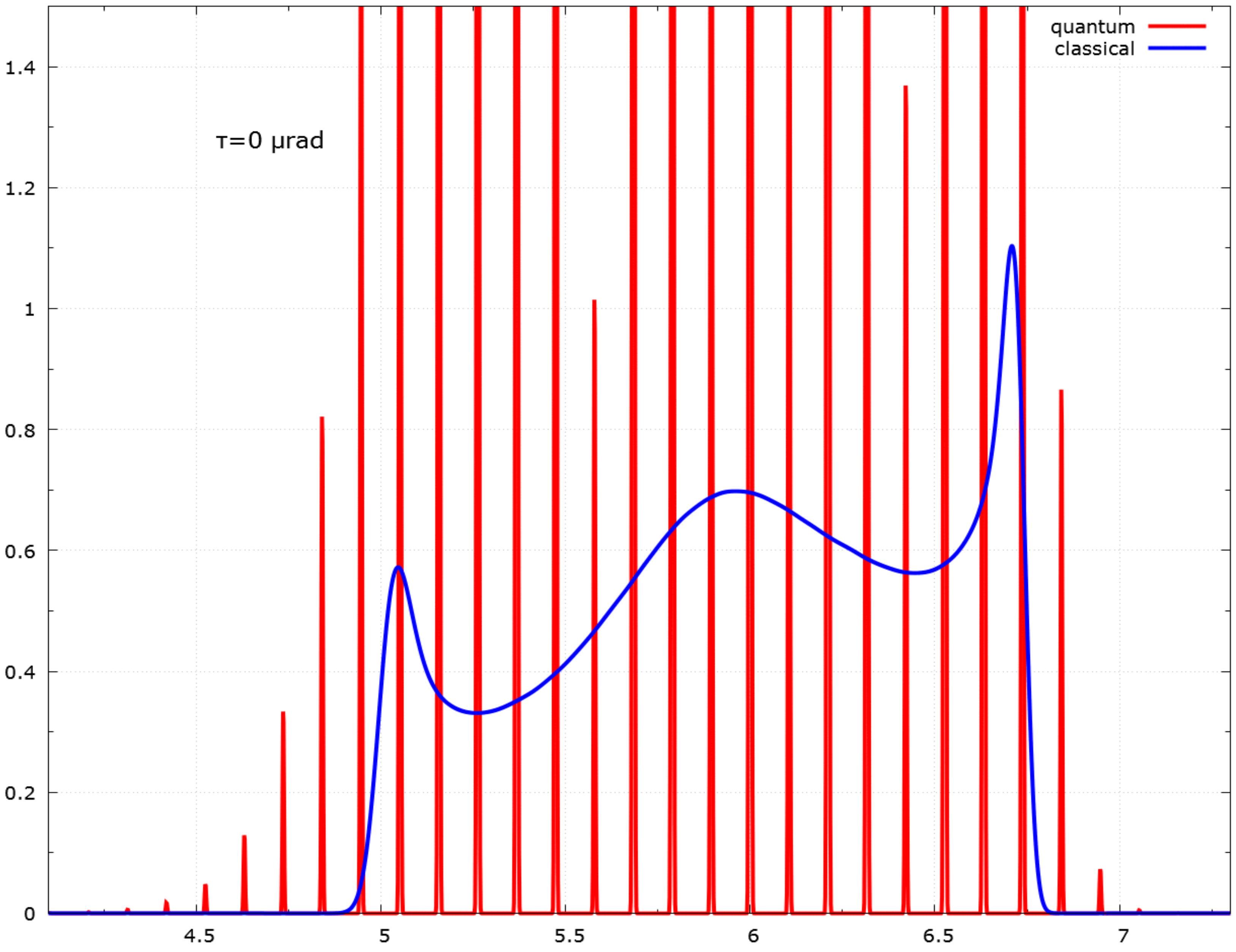
Scattering of protons on a thin crystal (Si <110> 952Å)
Axial case. Quantum results VS classical



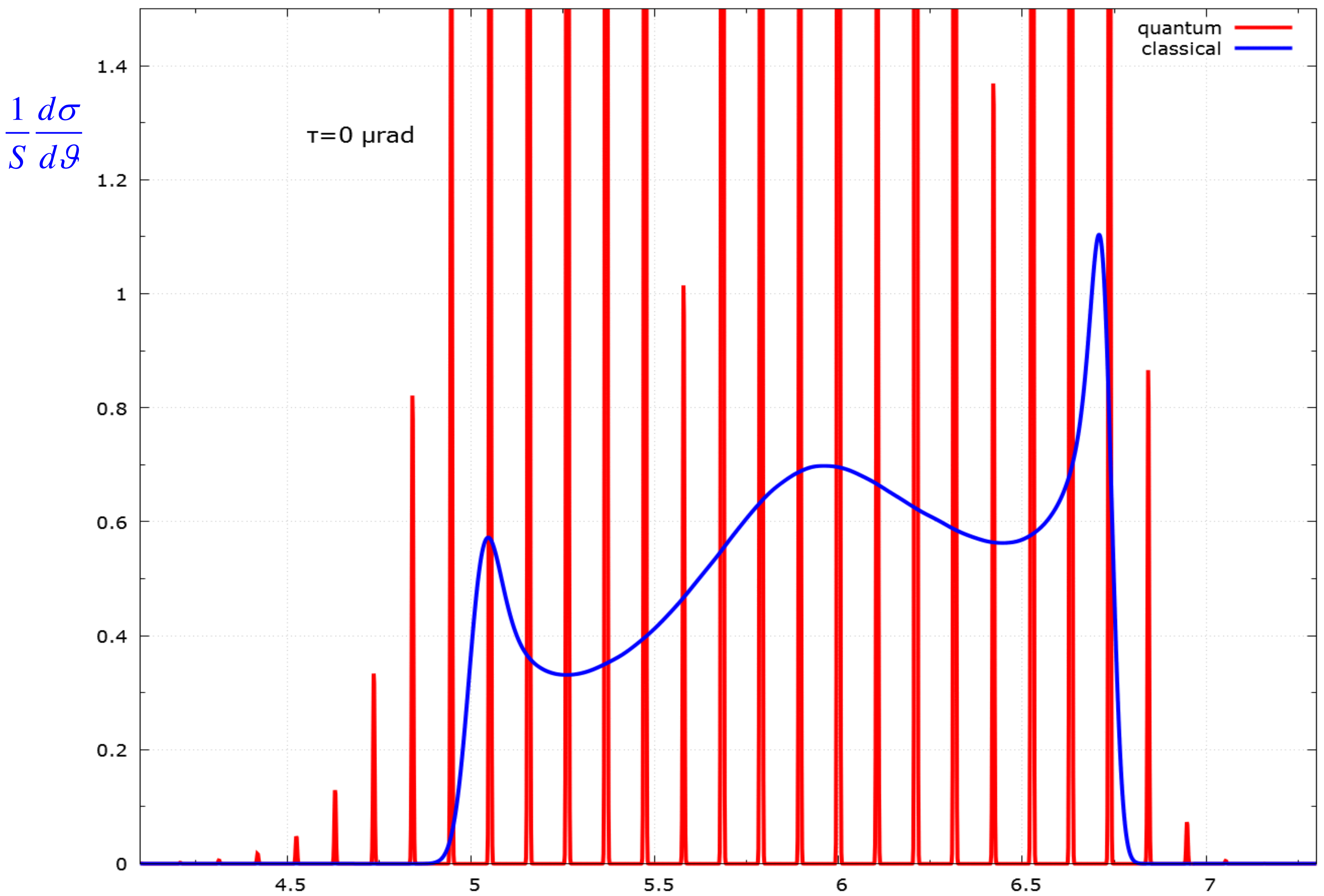


Dependence on beam divergence

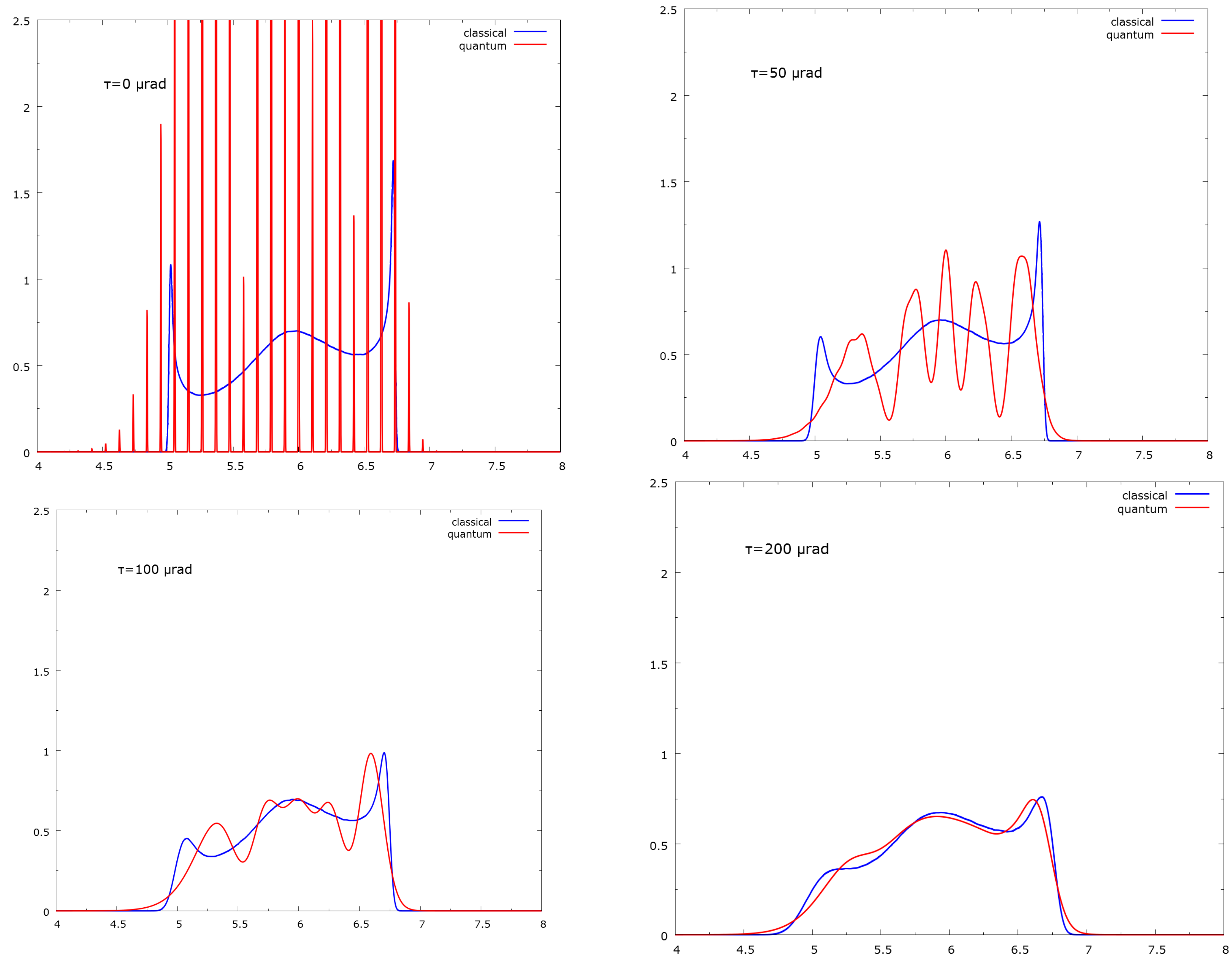
$$\frac{1}{S}\frac{d\sigma}{d\vartheta}$$

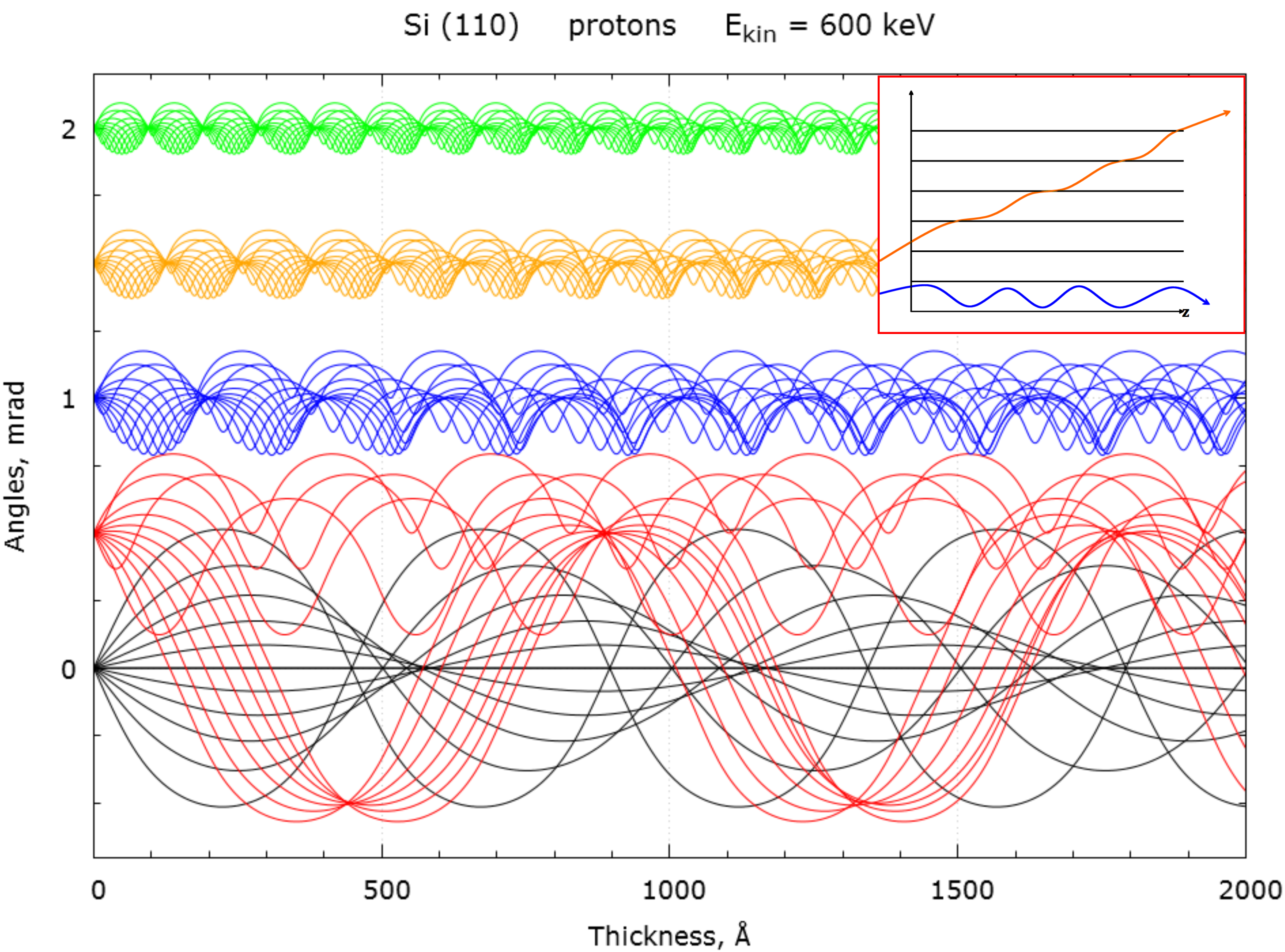


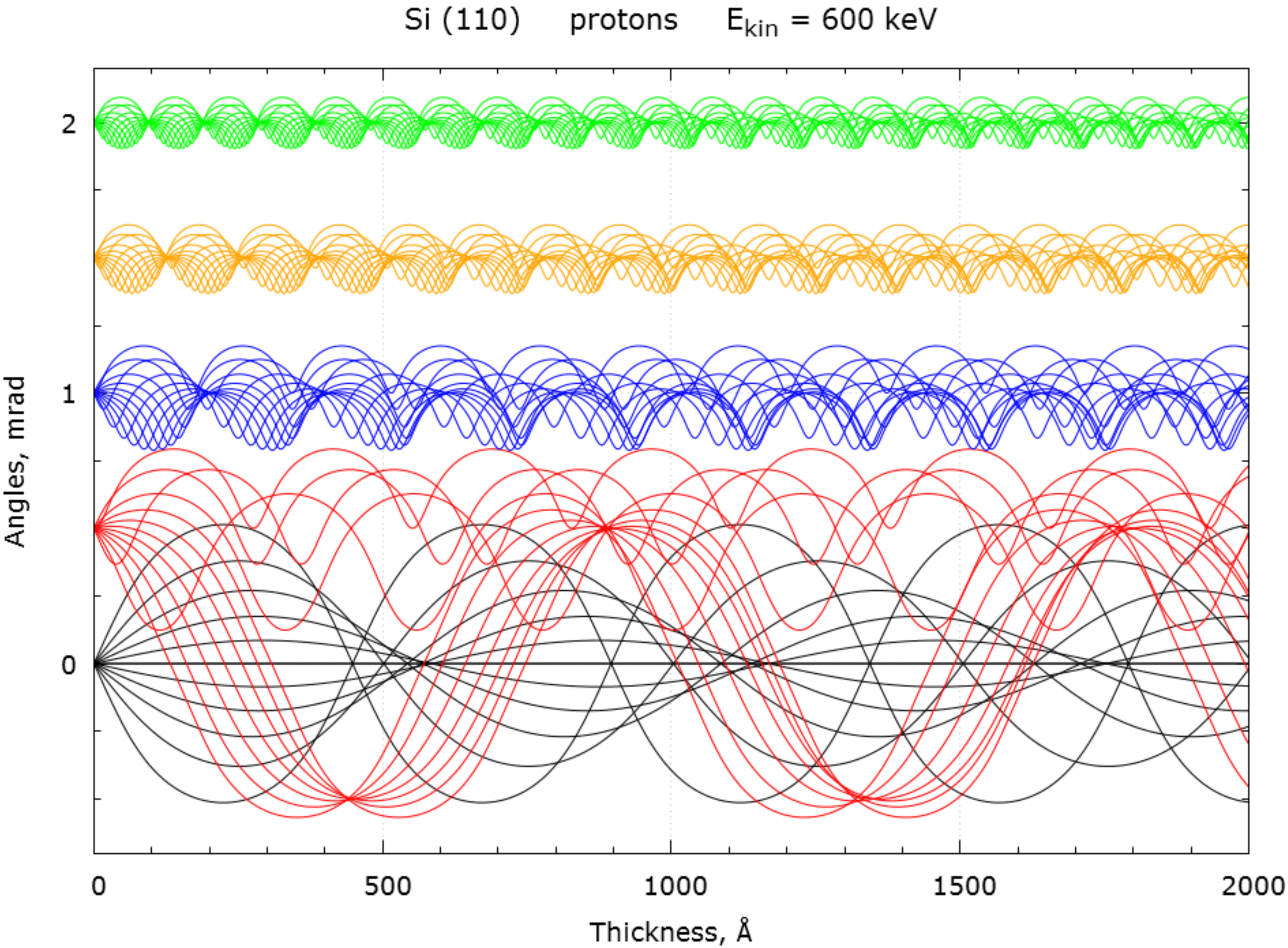
Dependence on beam divergence



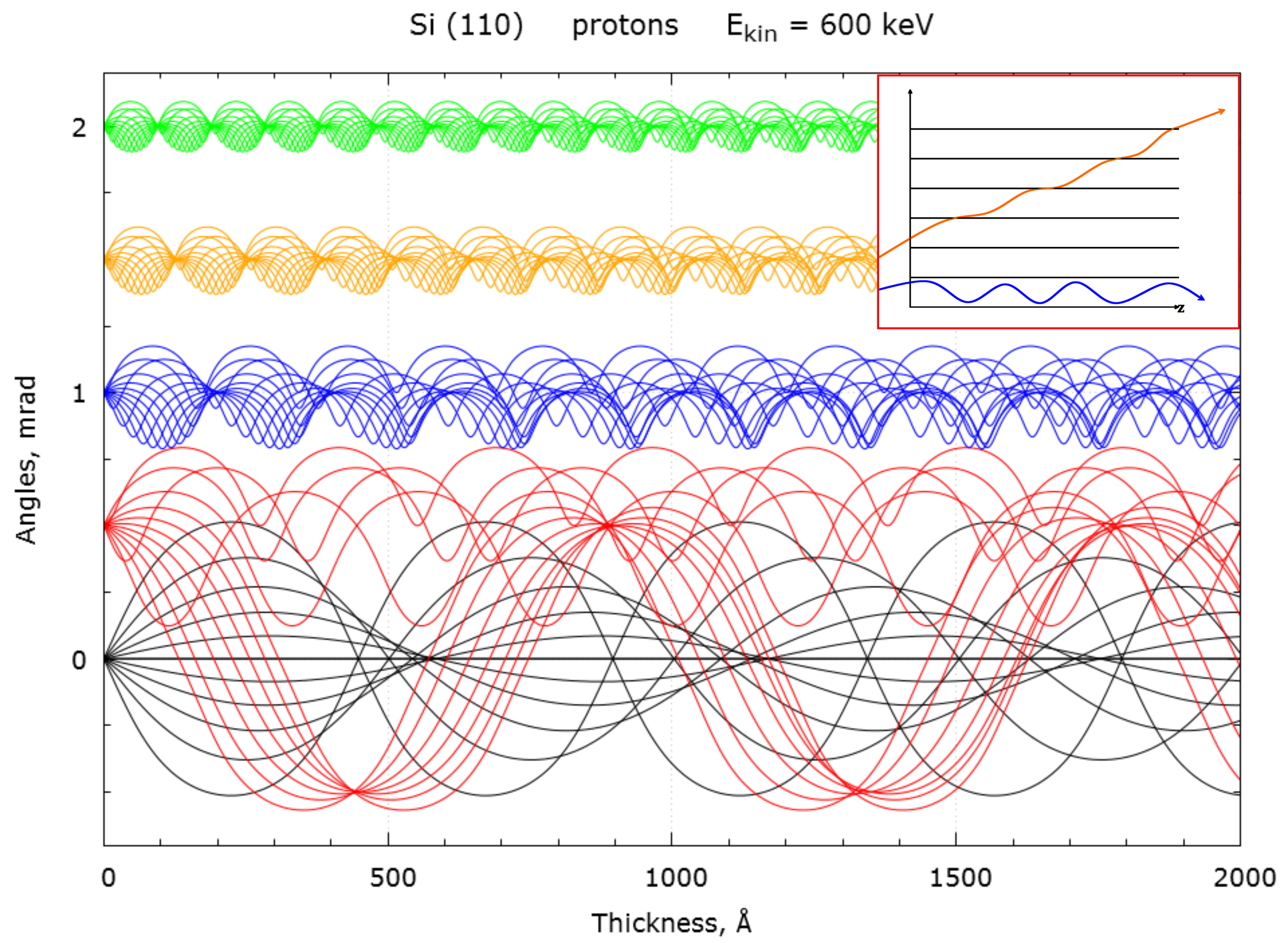
Dependence on beam divergence



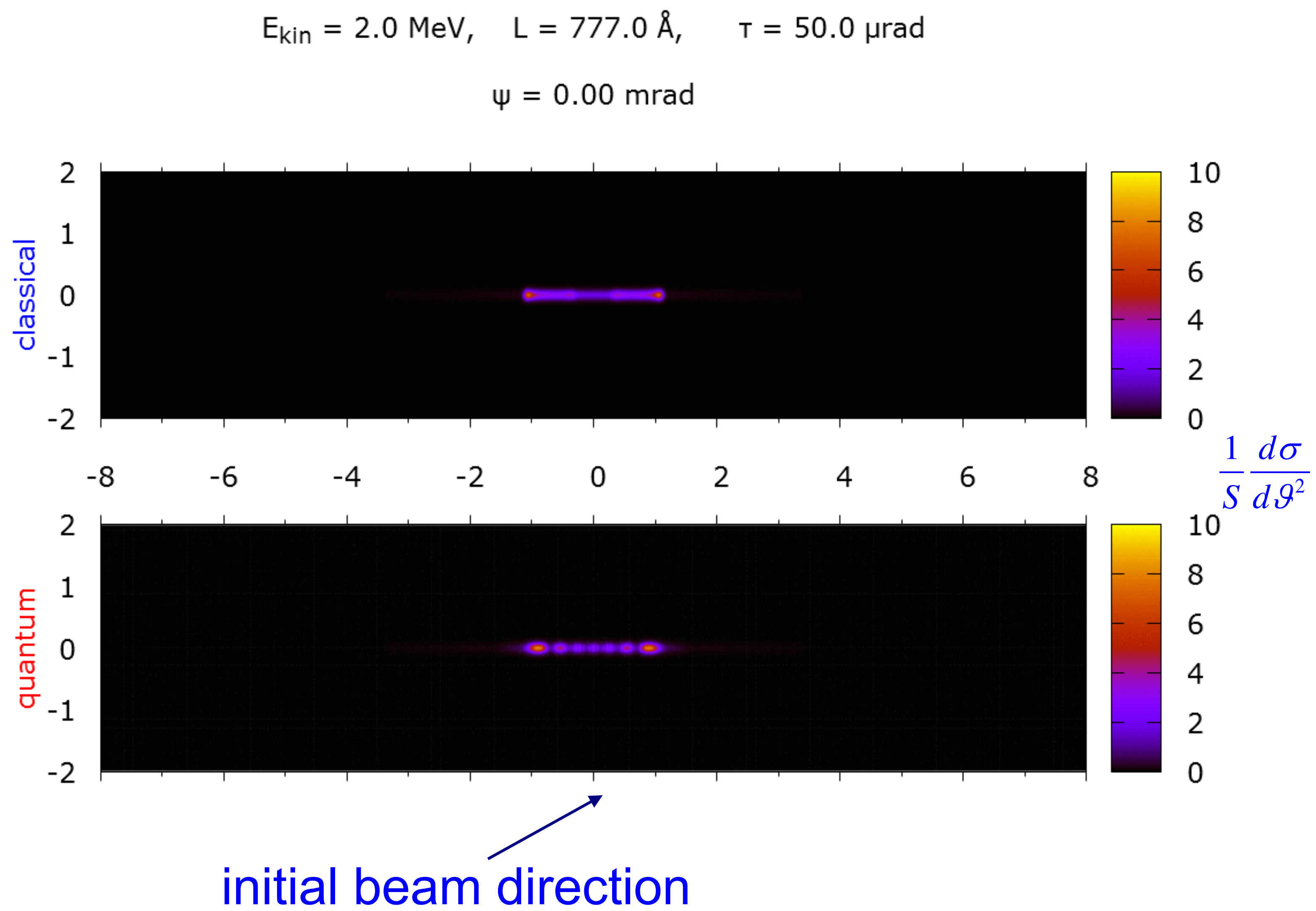

Si (110) protons E_{kin} = 600 keV
Angles, mrad
Thickness, Å
0
1
2
0
500
1000
1500
2000
z

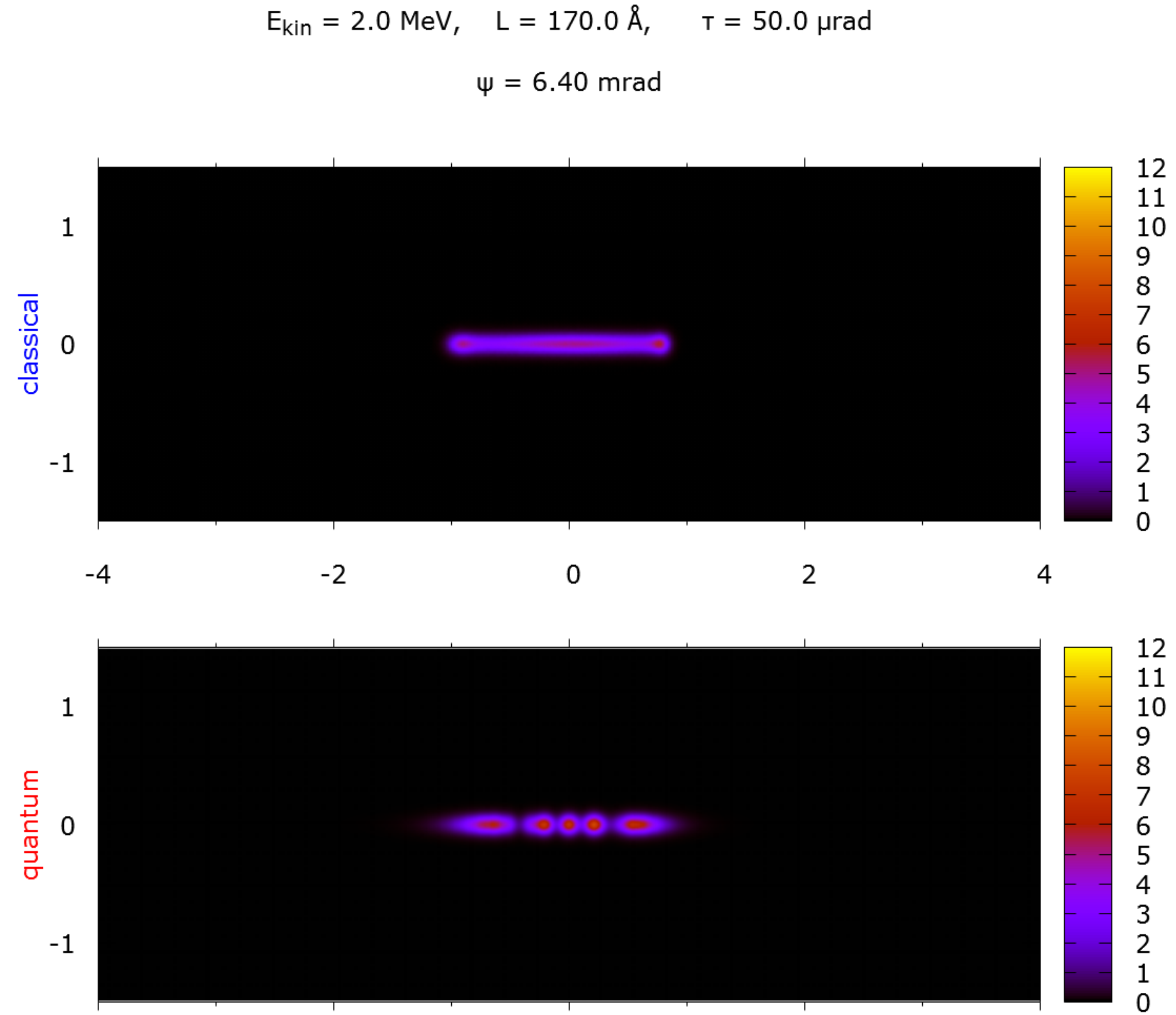


Si (110) protons E_{kin} = 600 keV
2
1
0
Angles, mrad
0
500
1000
1500
2000
Thickness, Å


Si (110) protons E_{kin} = 600 keV
Angles, mrad
Thickness, Å
0
1
2
0
500
1000
1500
2000
z

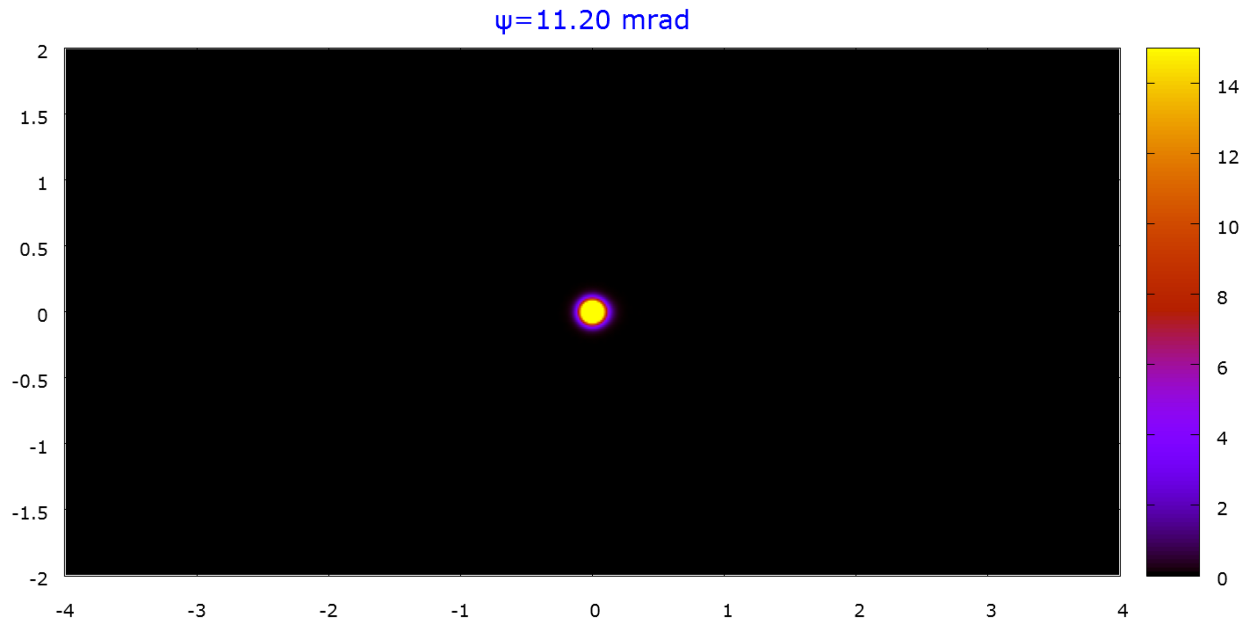
Planar scattering of 2 MeV protons in a 777A Si (110) crystal: changing angular tilt



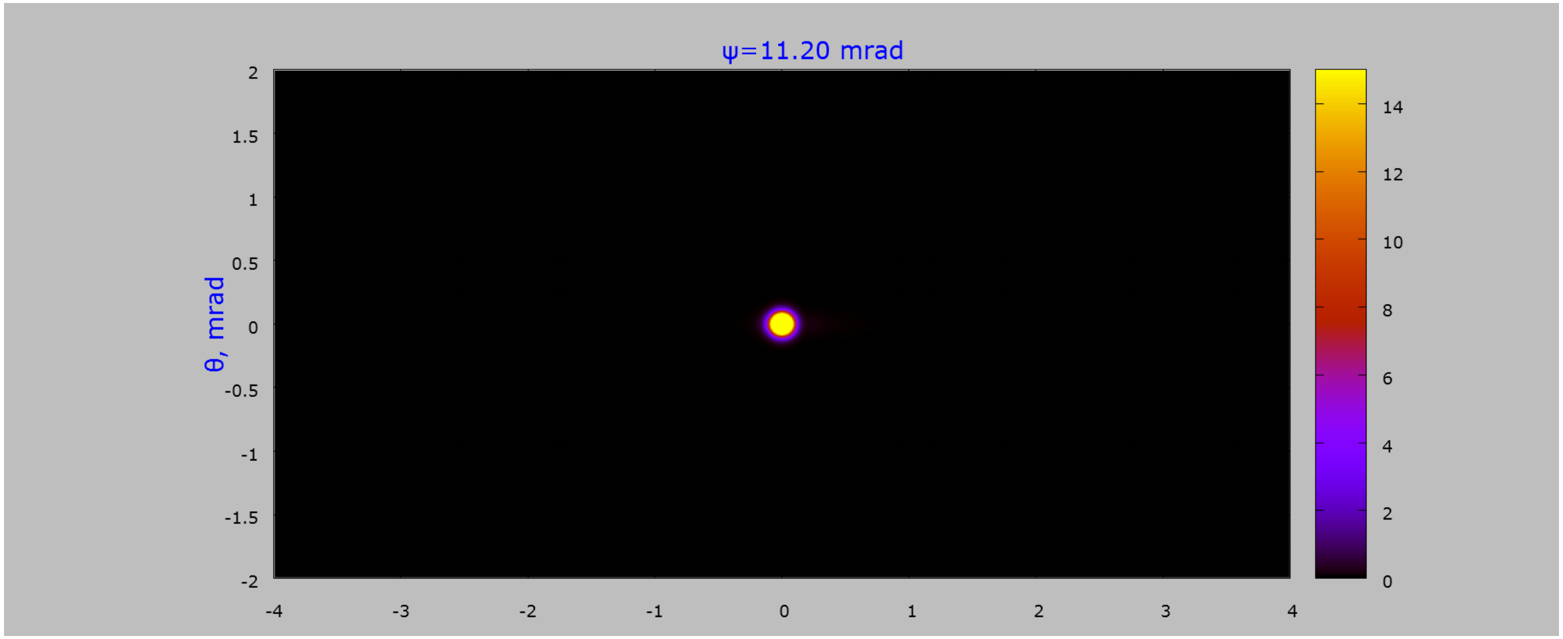


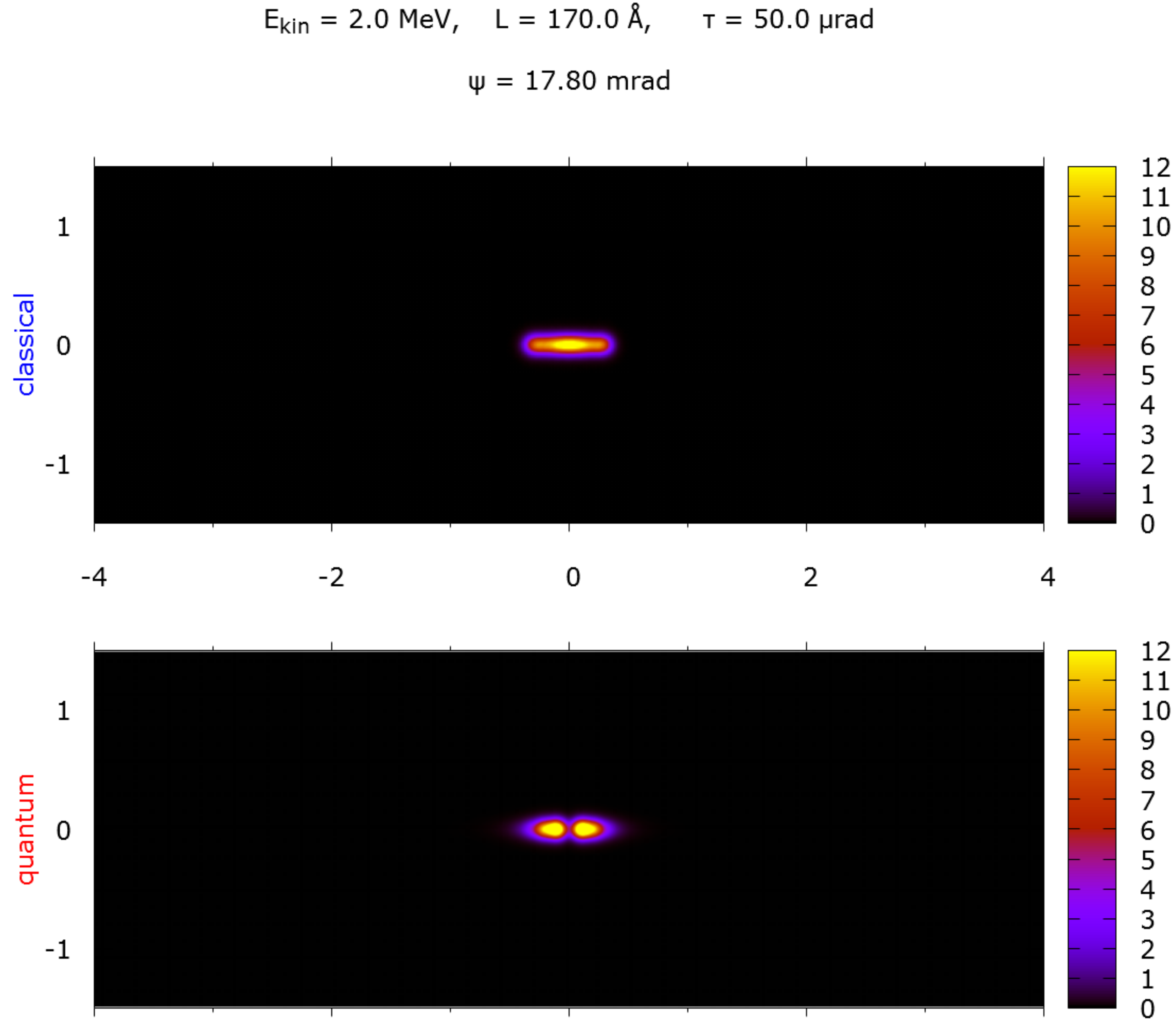
E_{kin} = 2.0 MeV, L = 170.0 Å, τ = 50.0 μrad
ψ = 6.40 mrad
classical
quantum
-4
-2
0
2
4
1
0
-1
0
1
2
3
4
5
6
7
8
9
10
11
12

classical

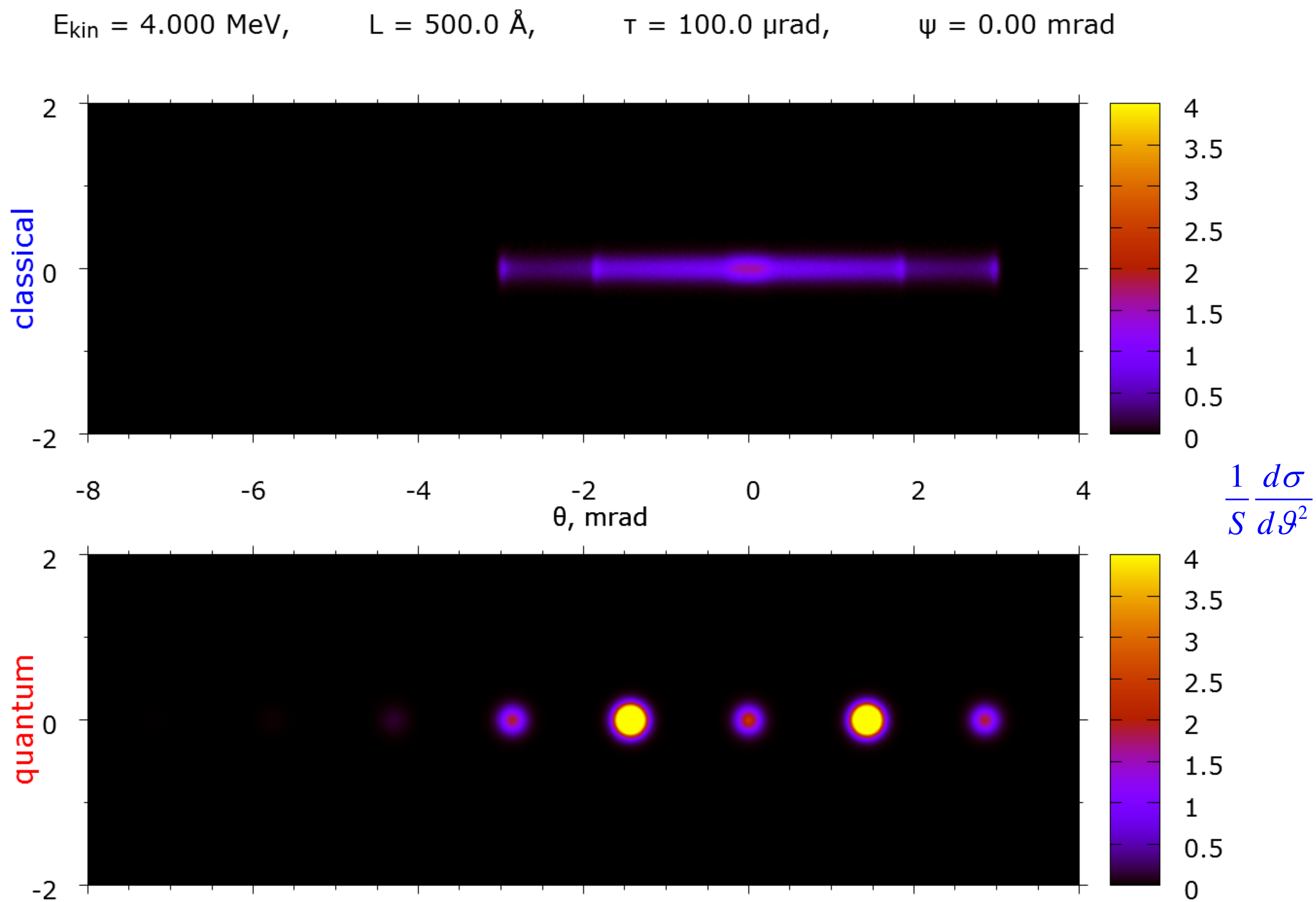


quantum

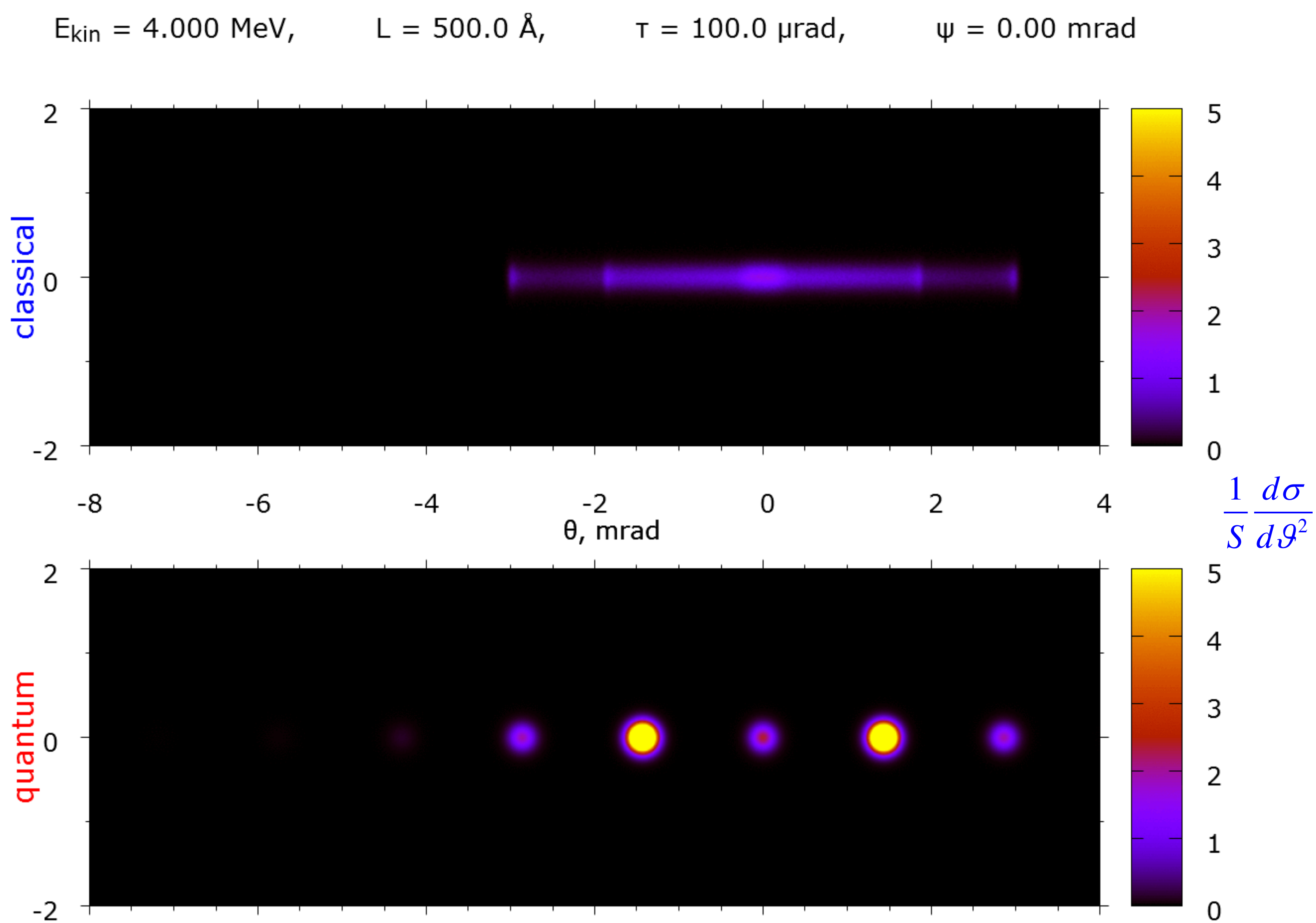




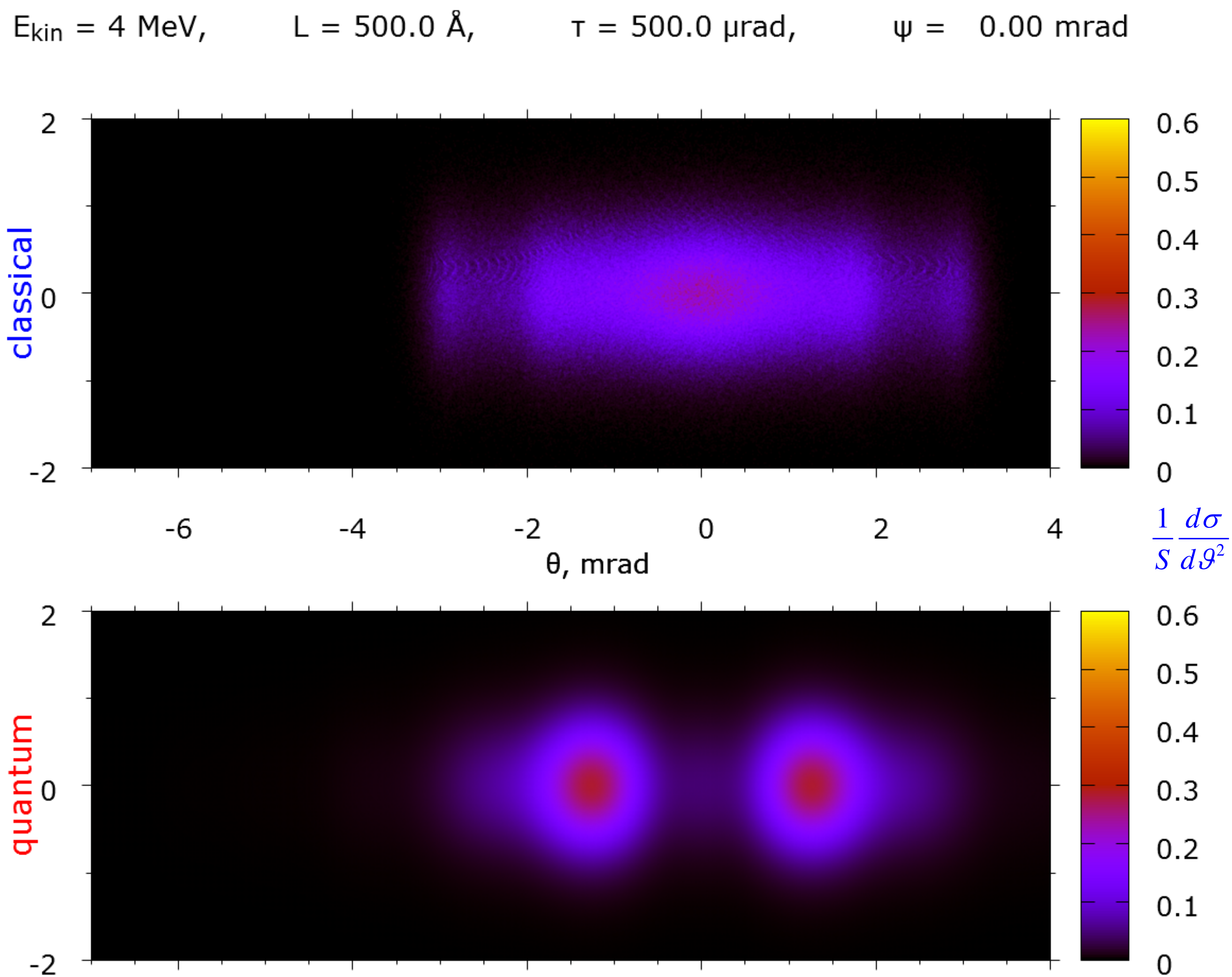
E_{kin} = 2.0 MeV, L = 170.0 Å, τ = 50.0 μrad
ψ = 17.80 mrad
classical
quantum
1
0
-1
-4
-2
0
2
4
12
11
10
9
8
7
6
5
4
3
2
1
0



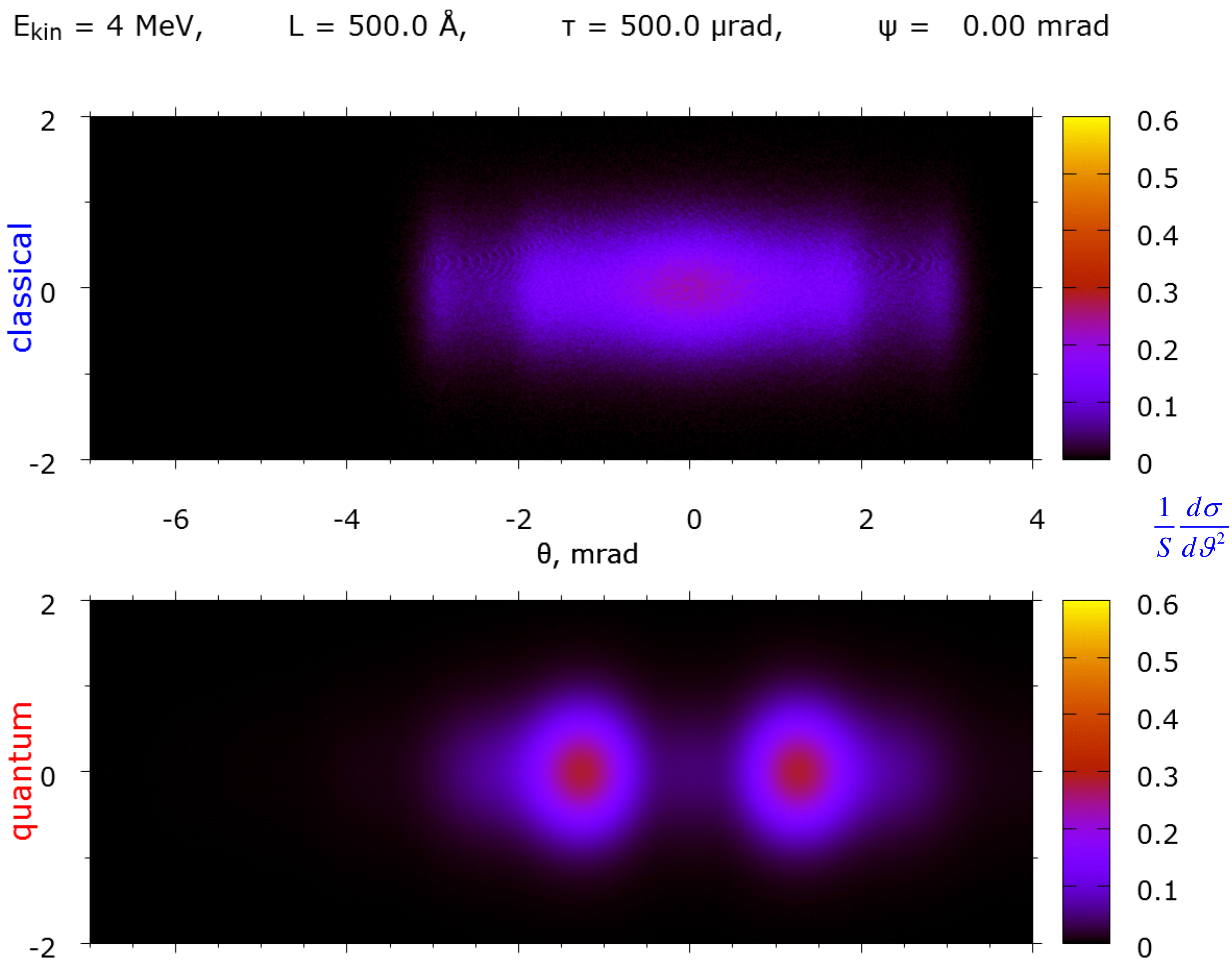
E_{kin} = 4.000 MeV,
L = 500.0 Å,
τ = 100.0 μrad,
ψ = 0.00 mrad
classical
quantum
θ, mrad
-8
-6
-4
-2
0
2
4
0
0.5
1
1.5
2
2.5
3
3.5
4
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$



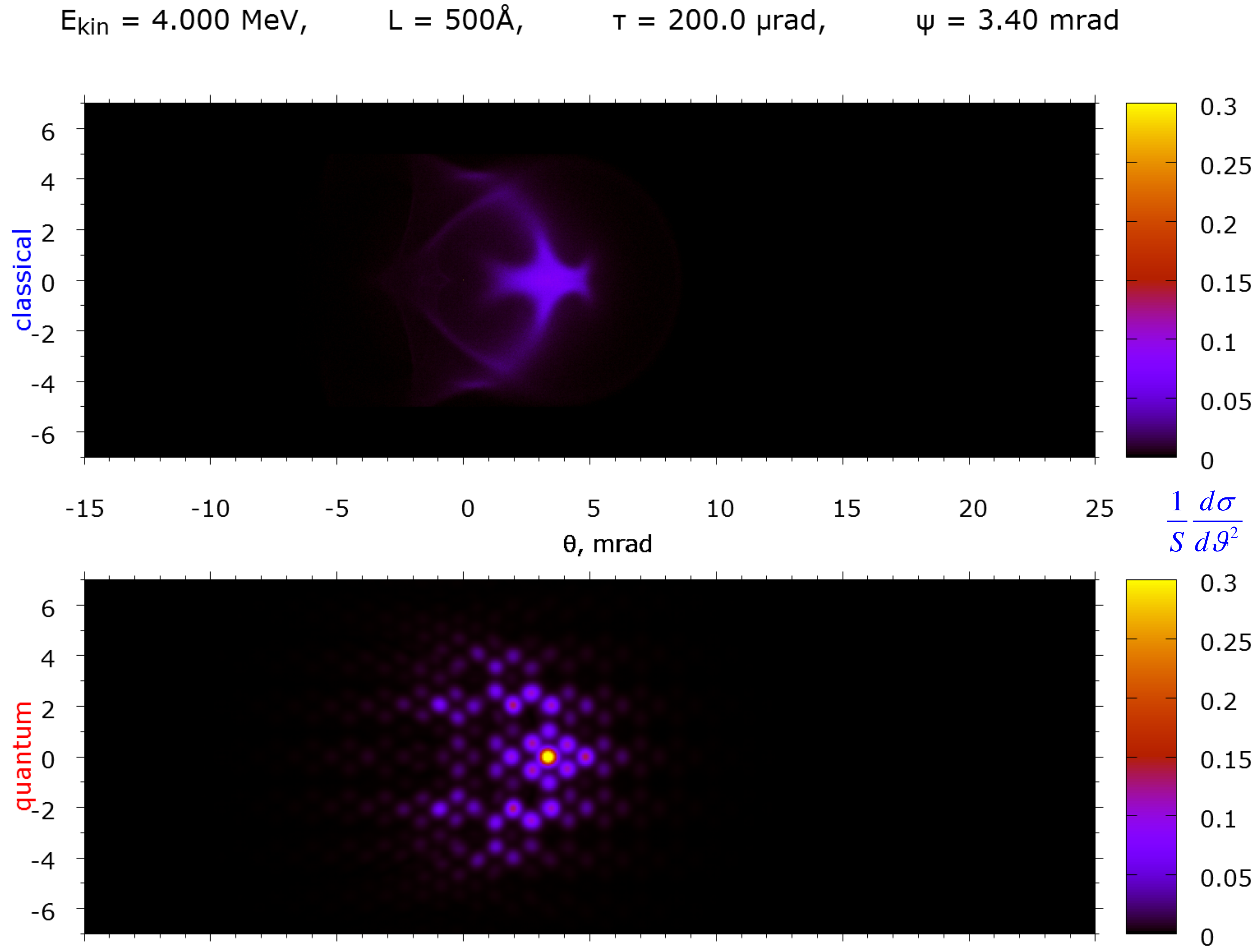
E_kin = 4.000 MeV,
L = 500.0 Å,
τ = 100.0 μrad,
ψ = 0.00 mrad
classical
quantum
θ, mrad
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$



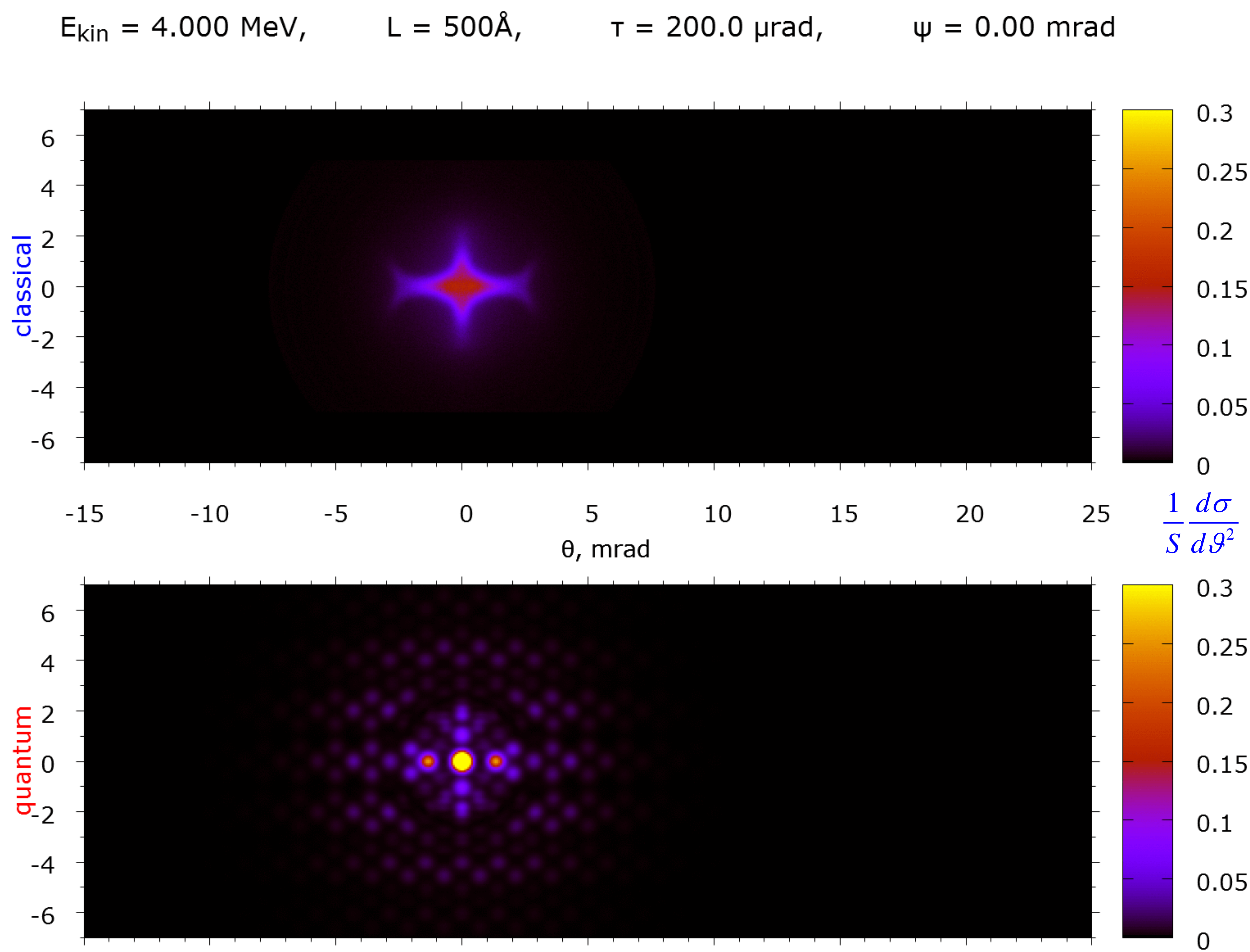
E_{kin} = 4 MeV, L = 500.0 Å, τ = 500.0 μrad, ψ = 0.00 mrad
classical
quantum
θ, mrad
-6
-4
-2
0
2
4
0
0.1
0.2
0.3
0.4
0.5
0.6
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$



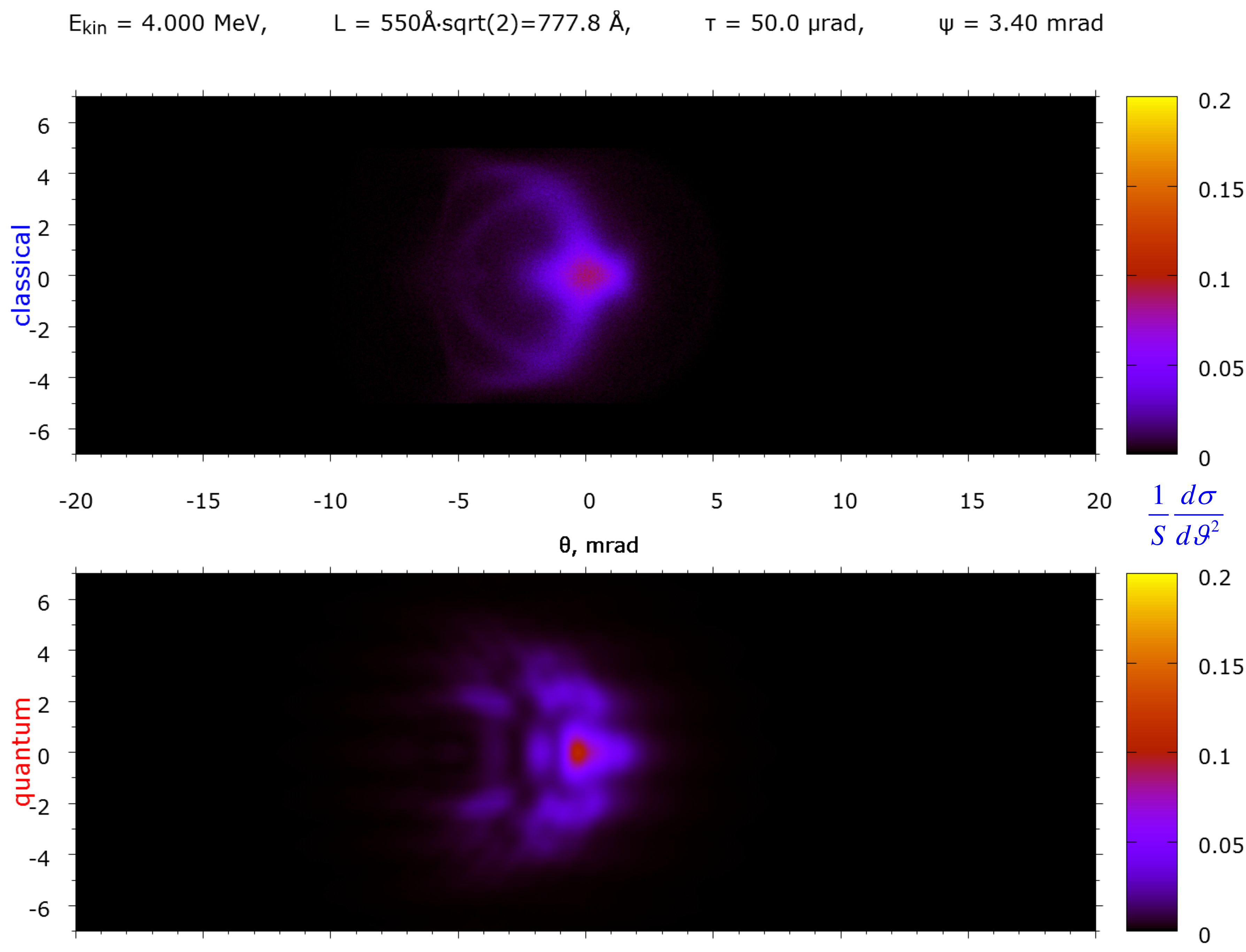
E_{kin} = 4 MeV, L = 500.0 Å, τ = 500.0 μrad, ψ = 0.00 mrad
classical
quantum
θ, mrad
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$
-6 -4 -2 0 2 4
2 0 -2
0 0.1 0.2 0.3 0.4 0.5 0.6



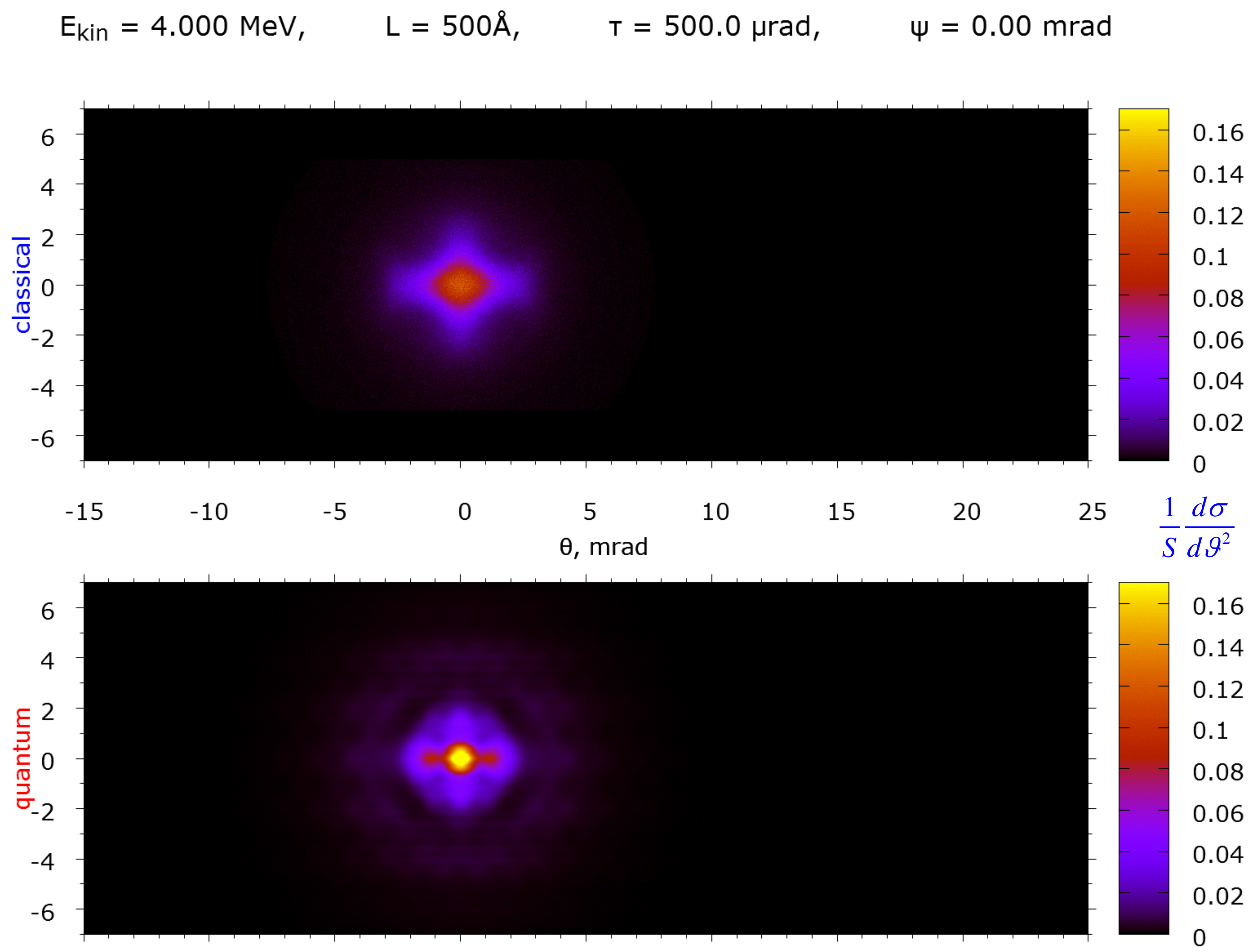
E_kin = 4.000 MeV, L = 500Å, τ = 200.0 μrad, ψ = 3.40 mrad
classical
quantum
θ, mrad
-15 -10 -5 0 5 10 15 20 25
6 4 2 0 -2 -4 -6
0.3 0.25 0.2 0.15 0.1 0.05 0
1/S dσ/dϑ²



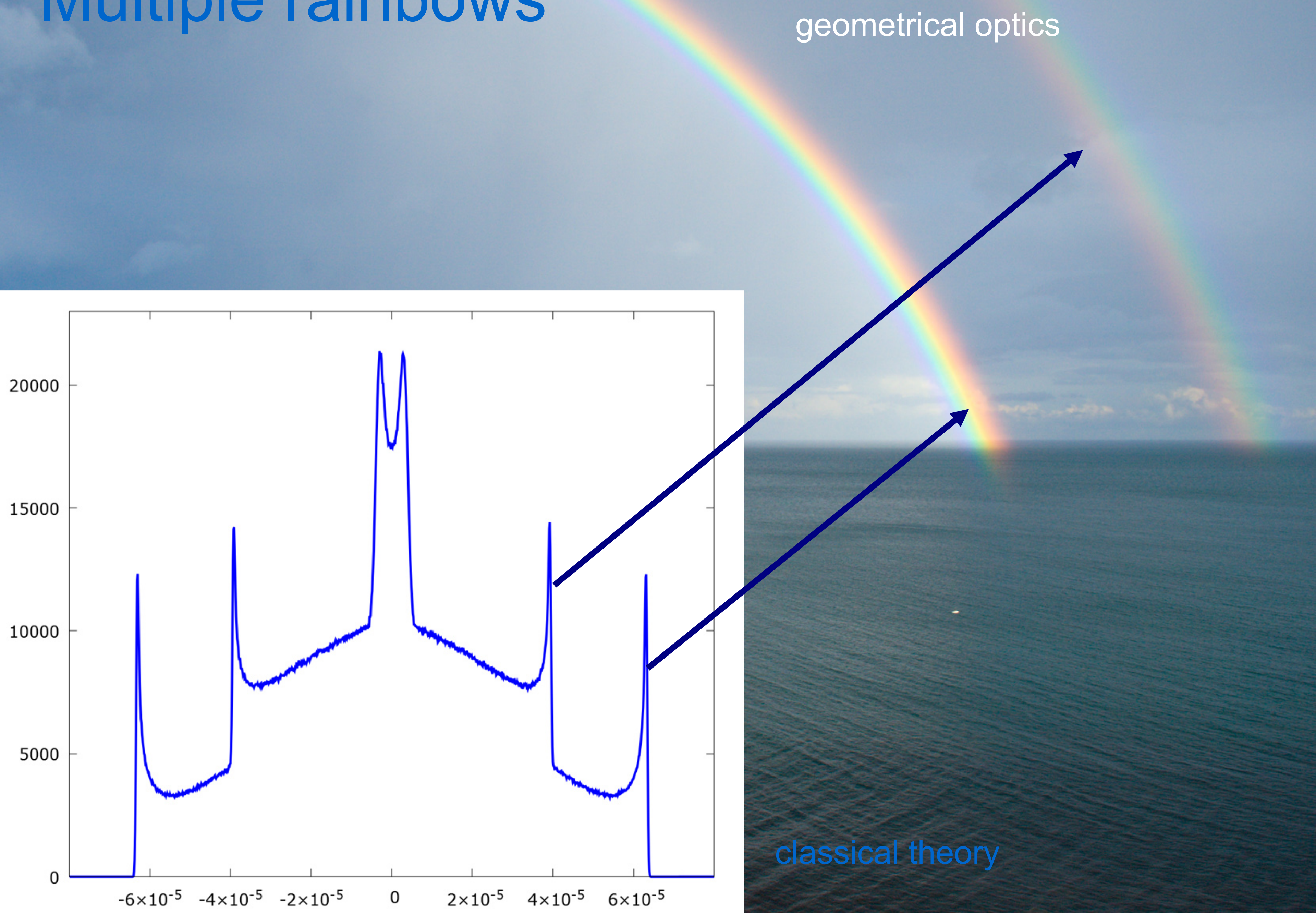
E_kin = 4.000 MeV, L = 500Å, τ = 200.0 μrad, ψ = 0.00 mrad
classical
quantum
θ, mrad
-15
-10
-5
0
5
10
15
20
25
6
4
2
0
-2
-4
-6
0.3
0.25
0.2
0.15
0.1
0.05
0
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$



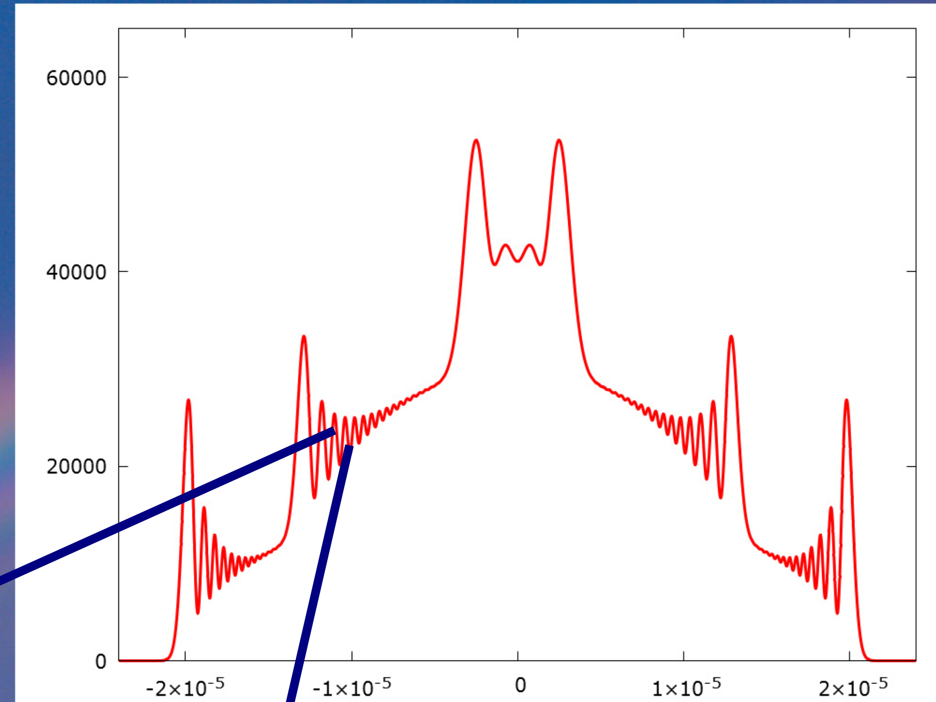
E_{kin} = 4.000 MeV, L = 550Å·sqrt(2)=777.8 Å, τ = 50.0 μrad, ψ = 3.40 mrad
classical
quantum
θ, mrad
-20
-15
-10
-5
0
5
10
15
20
6
4
2
0
-2
-4
-6
0.2
0.15
0.1
0.05
0
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$


E$_{kin}$ = 4.000 MeV, L = 500Å, τ = 500.0 μrad, ψ = 0.00 mrad
classical
quantum
θ, mrad
$\frac{1}{S}\frac{d\sigma}{d\vartheta^2}$
-15 -10 -5 0 5 10 15 20 25
6 4 2 0 -2 -4 -6
0.16 0.14 0.12 0.1 0.08 0.06 0.04 0.02 0

Multiple rainbows



Supernumerary rainbows



wave optics

Summary

Quantum effects can be observed even at scattering of particles as heavy as protons

• Beam diveregence has important impact onto the result of scattering

•Planar orientation is preferable VS axial one for observing quantum effects for heavy particles

Quantum effects reveal themselves depending on the beam angular tilt respect to the plane

Quantum nature has influence onto rainbow scattering

Possibility of experimental observation

Summary

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• Beam diveregence has important impact onto the result of scattering

•Planar orientation is preferable VS axial one for observing quantum effects for heavy particles

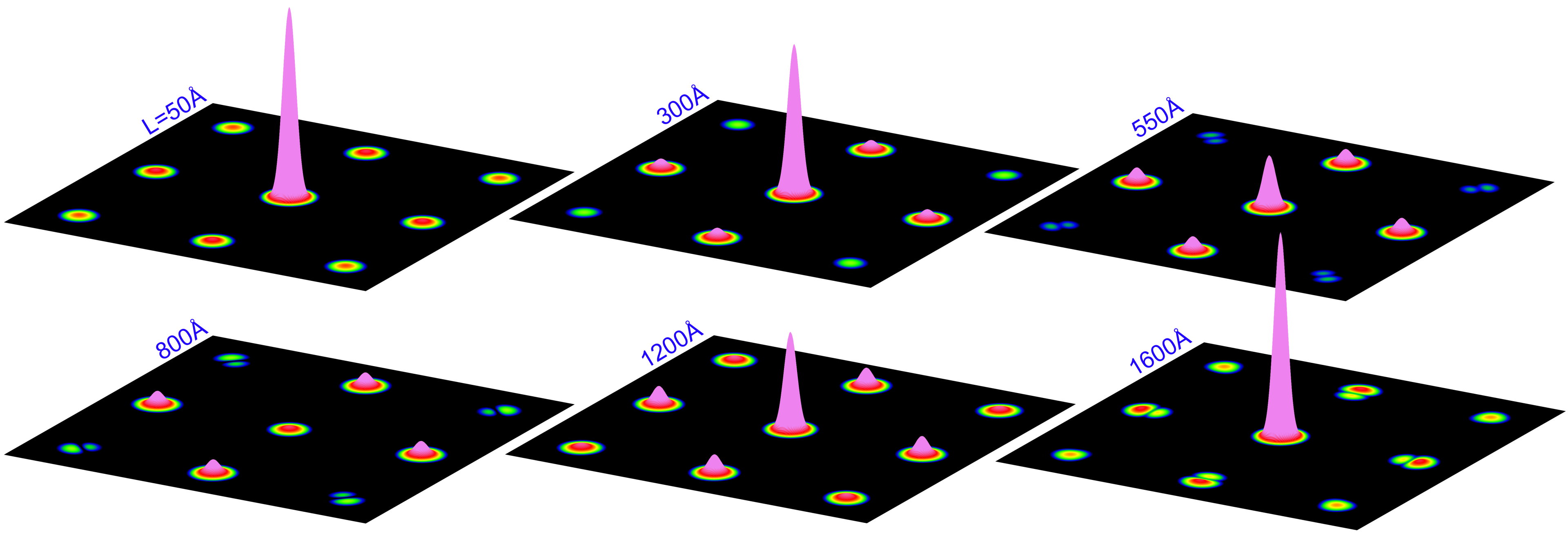
Quantum effects reveal themselves depending on the beam angular tilt respect to the plane

Quantum nature has influence onto rainbow scattering

Possibility of experimental observation

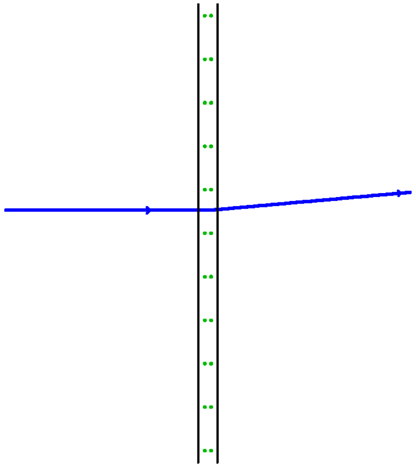
Merci! Дякую!

Quantum angular distributions of electrons in ultrathin Si <100> crystal

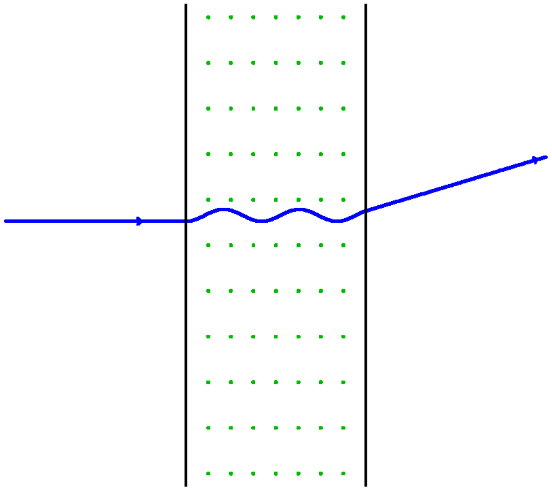


electrons 5MeV Si <100> 50-1600Å

Ultrathin, Thin and Thick Crystals



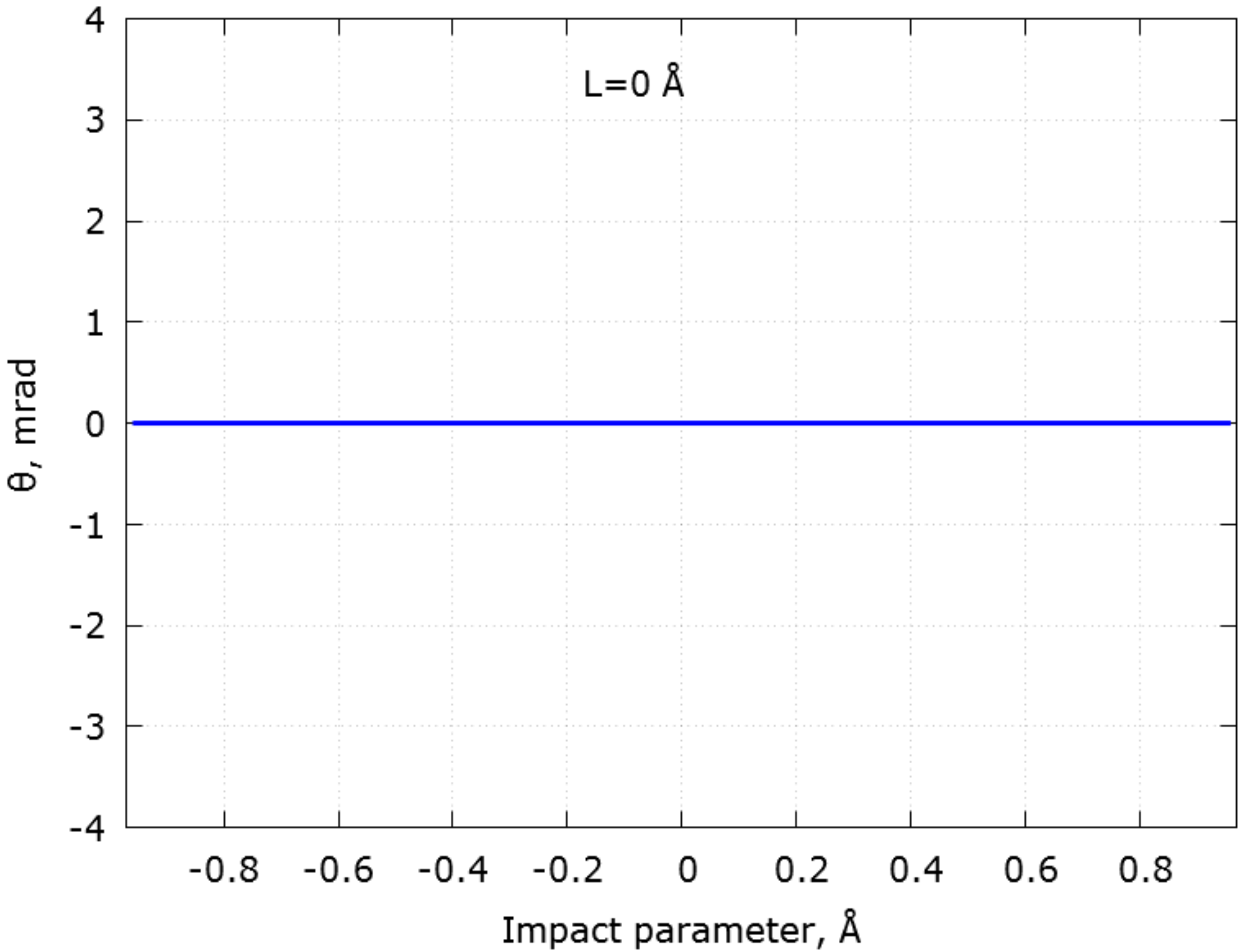
~~Channeling~~



Channeling

V. Guidi et al. Phys. Rev. Lett. (2012)
M. Mothapothula et al. NIM B283 (2012) 29

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

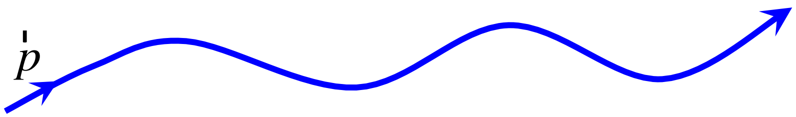


Phenomenon of Planar Channeling

J.Lindhard (1965)

$$p_z = const \approx p$$

$$p_y = const \approx 0$$



$$\boxed{\ddot{x} = -\frac{1}{E}\frac{\partial}{\partial x}U(x)}$$

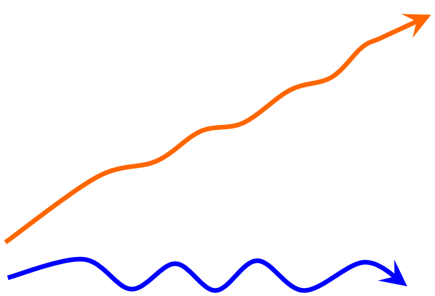
$$\boxed{E_\perp = \frac{E\dot{x}^2}{2} + U(x)}$$

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

Quantum consideration

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

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



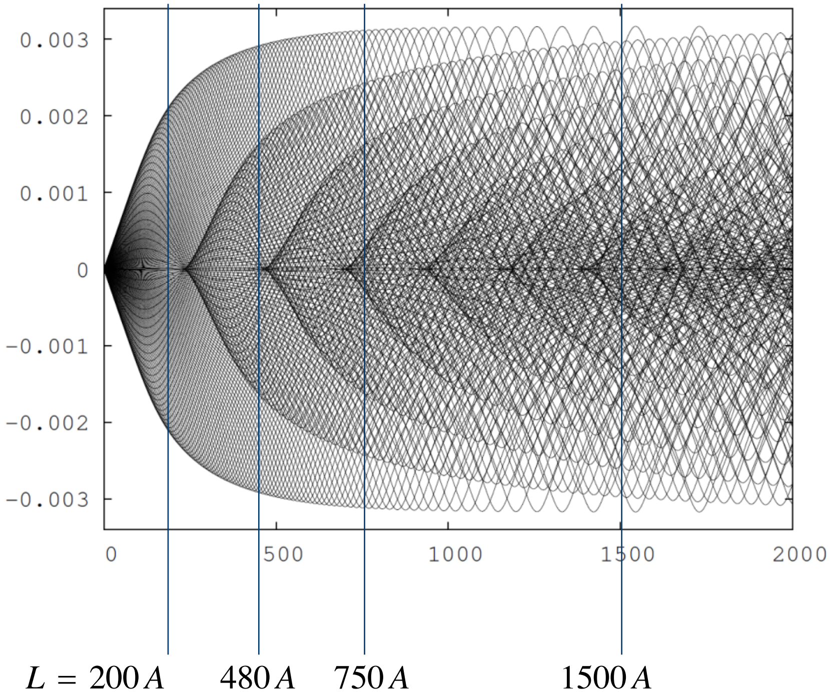
$E_{\perp p} > U_{\max}$

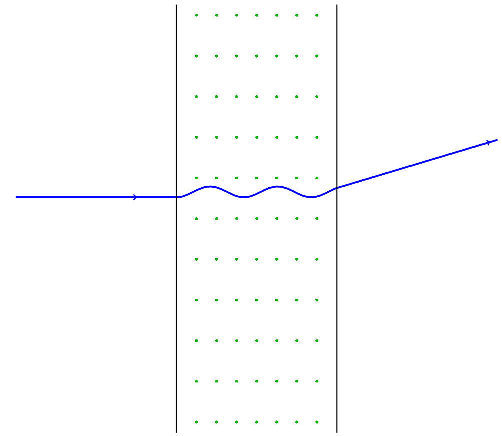
$E_{\perp p} < U_{\max}$

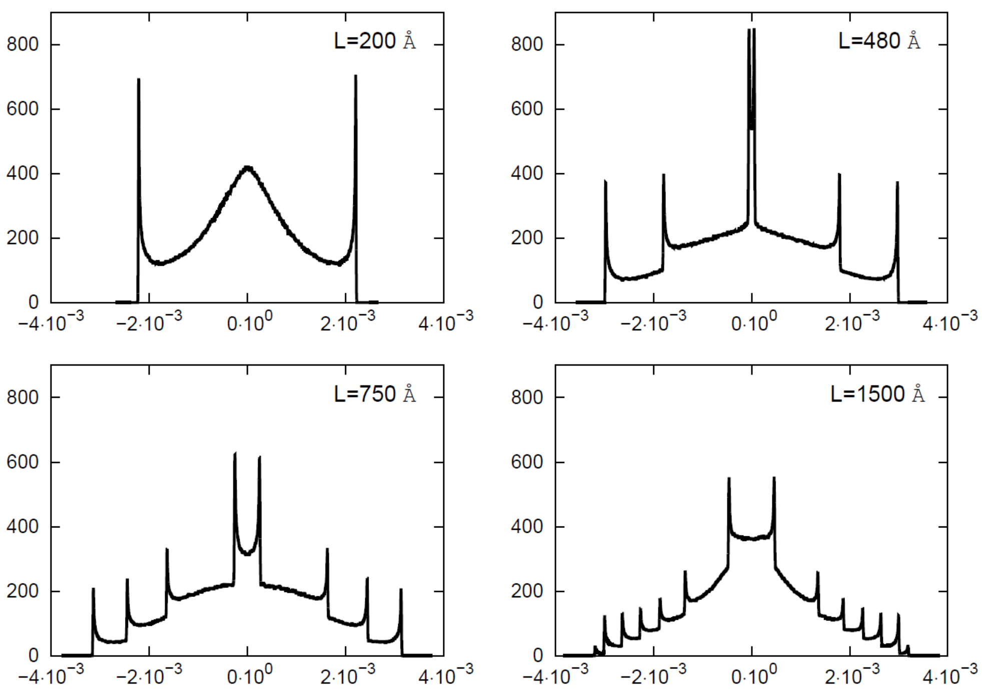
$$\boxed{n_{levels} \sim \sqrt{E_{MeV}}}$$

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

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





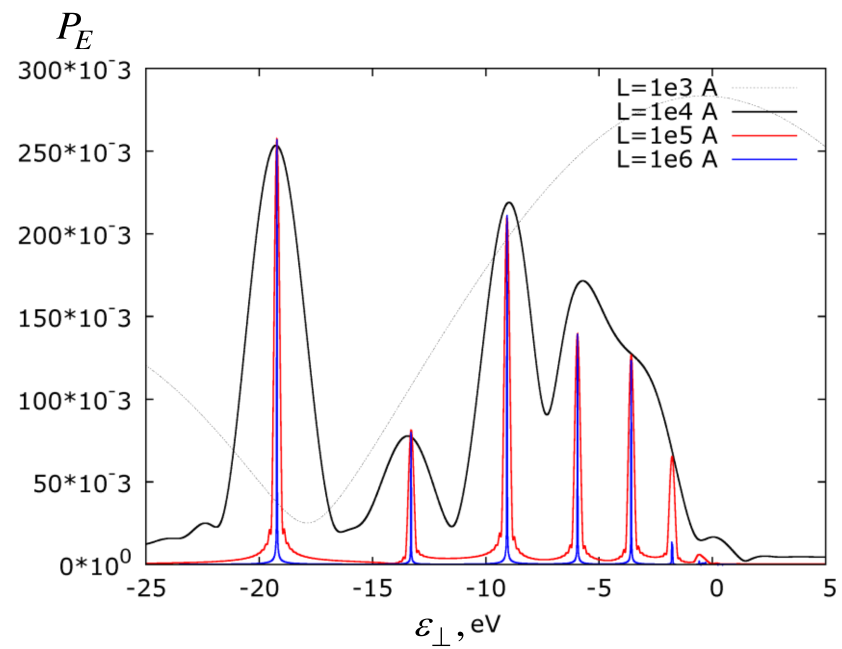


Calculation of Energy Spectrum of Channeling Radiation by the Spectral Method

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

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

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



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

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

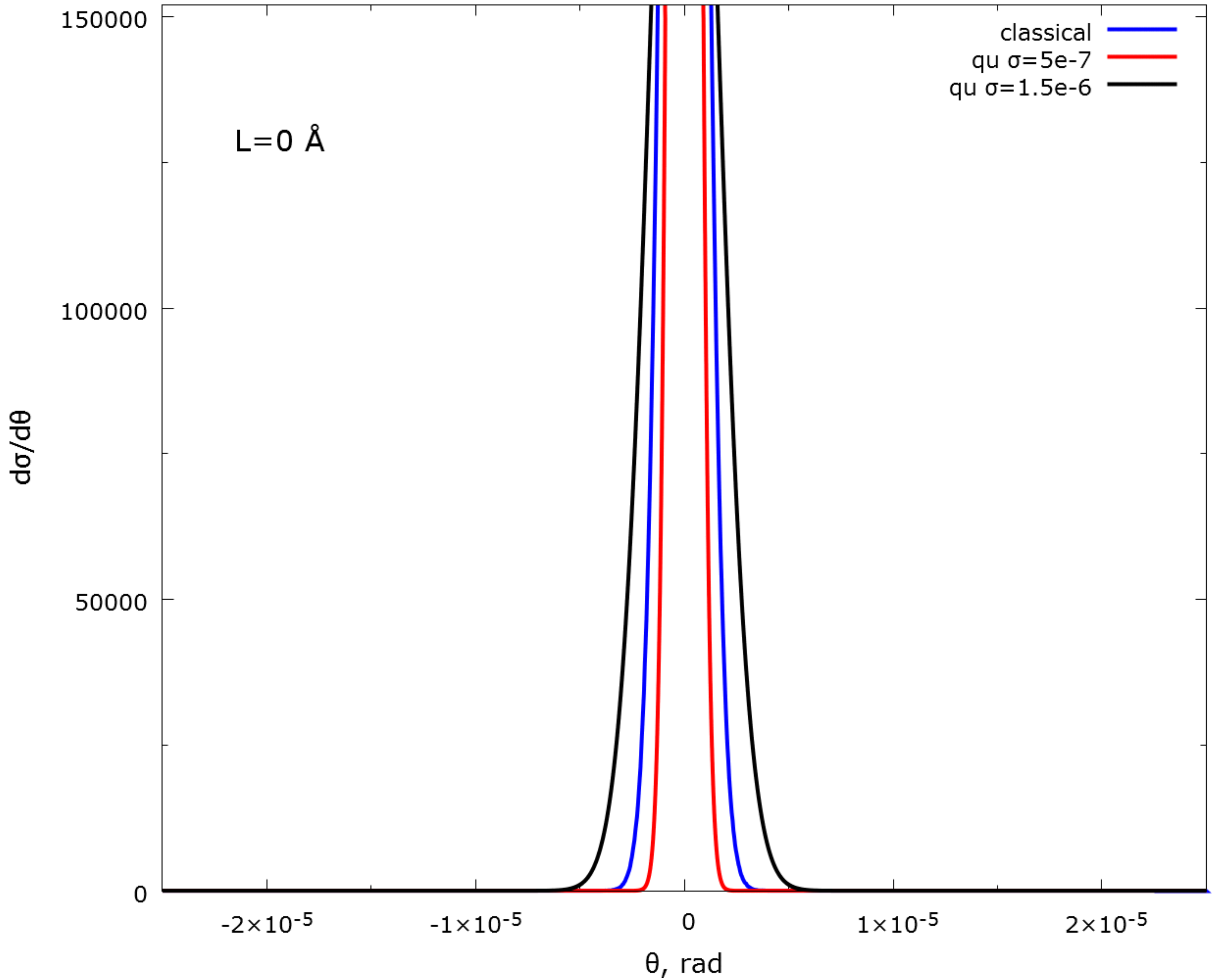
planar scattering $N_{levels} \sim \sqrt{\varepsilon[MeV]}$

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

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

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

Nous ne pouvons pas afficher cette image pour l'instant.



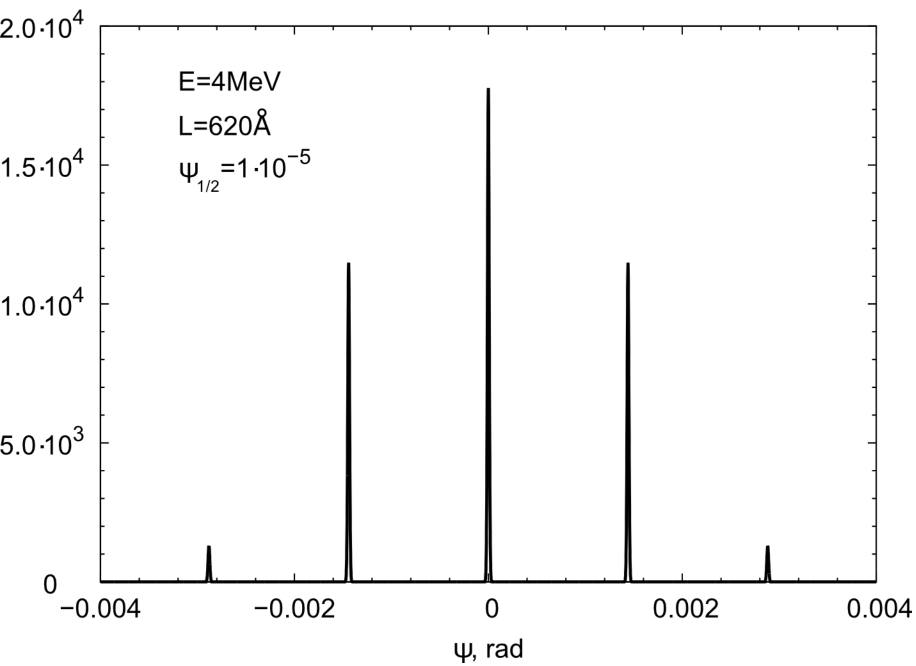
100 GeV electrons

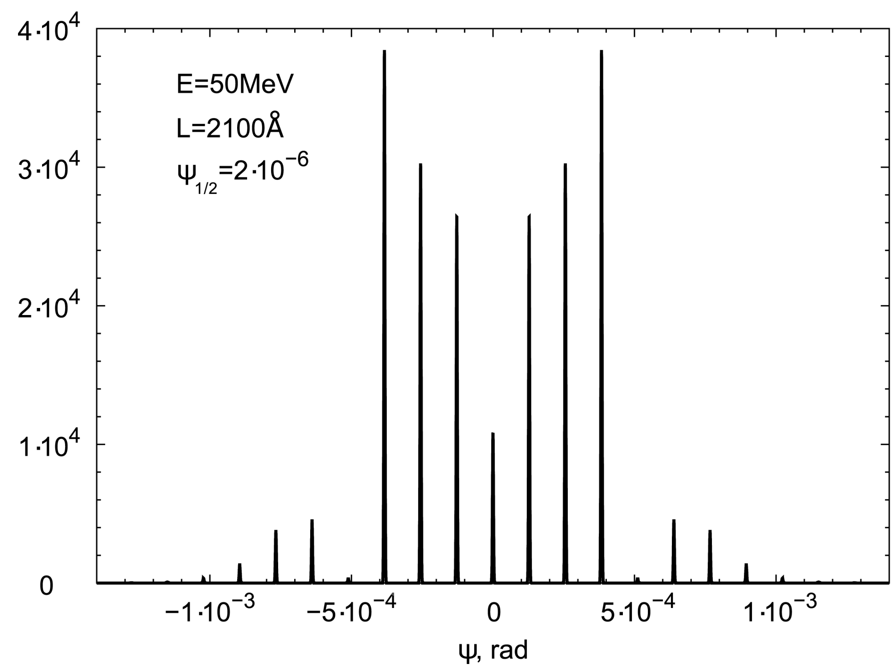
Scattering of electrons by crystal plane. Quantum case

Expansion over reciprocal lattice vectors

d_x –

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





σ_{beam}

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

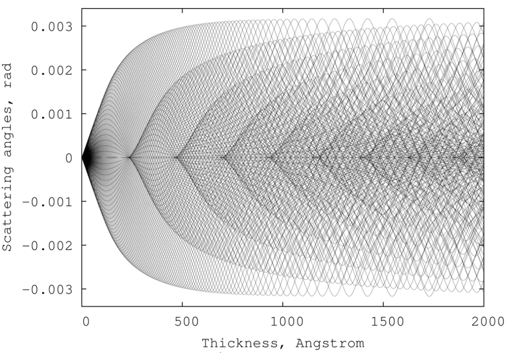
Classical and quantum angular distributions of 4 MeV electrons in ultrathin Si crystal

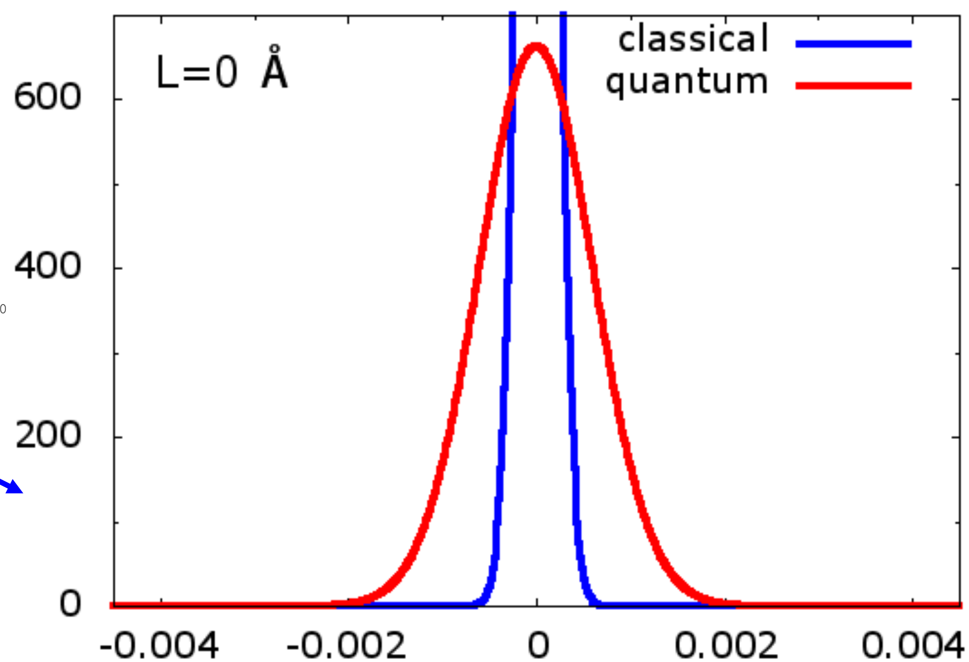
$$d\sigma_{cl} = d^2 b = \left| \frac{\partial(b_x, b_y)}{\partial(\vartheta_x, \vartheta_y)} \right| d\vartheta_x d\vartheta_y$$

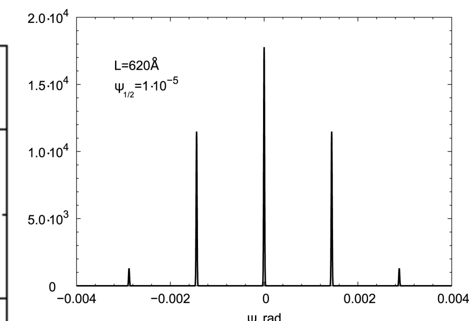
$$\ddot{\vec{\rho}} = -\frac{c^2}{E} \nabla U(\vec{\rho})$$

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

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



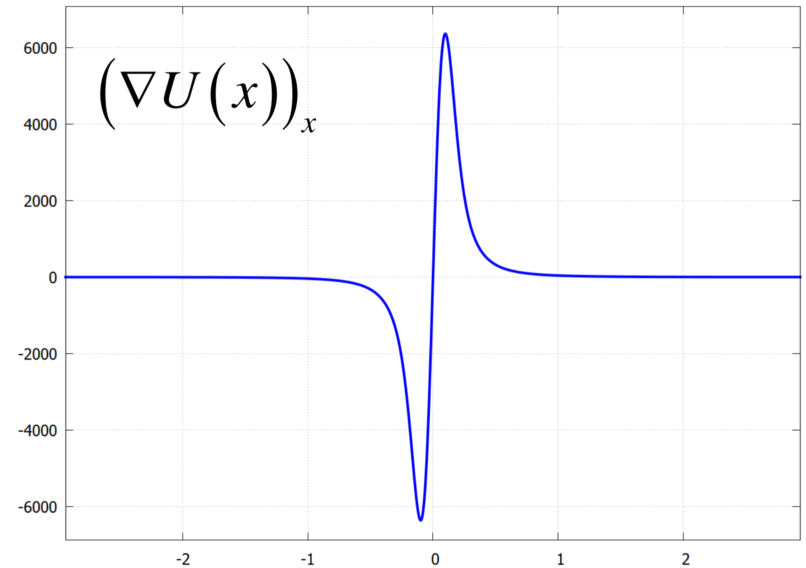




S.Shulga, N.Shul'ga, R.Chehab, S. Barsuk, I. Chaikovska NIMB 402 (2017) 16

Classical rainbow on one atom

Once, at a party in Copenhagen, Dirac suggested a theory according to which the face of a woman looks best at a certain optimum distance. He argued that at d=∞ it is impossible to see the face, and at d=0 it looks deformed because of <...> hence there must be a distance between these two values at which the face looks best (it is unknown whether Dirac's argument is valid only for women)...



H.Kragh. Dirac: A Scientific Biography 1990,
Физики продолжают шутить 1968