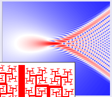
Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions

Classical patterns in the quantum rainbow channeling of high energy electrons

Marko Ćosić
`mcosic@vinca.rs`

Laboratory of Physics 010, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O.Box 522, 11001, Belgrade, Serbia

GRID2023-Distributed Computing and Grid-technologies in Science and Education, July 3-7, 2003, Dubna, Russia



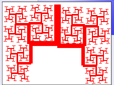
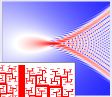


Table of Content

Introduction
- The Channeling Effect
- The Classical Caustic Pattern

The Quantum Channeling Effect
- The Numerical Implementation
- The Self-interference of Electrons
- Distributions of Channeled Electron Beam
- The Quantum Dynamics in the Phase Space

Conclusions



The Channeling Effect

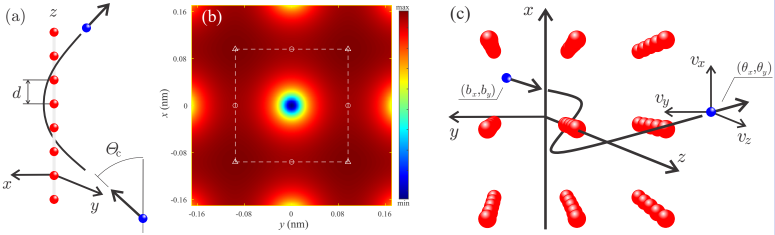


Figure 1: (a) Scattering on atomic string. (a) Axial channel potential. (c) Schematic representation of the channeling effect.

Potential of the planar chennel (220) is $V(x) = \sum_{m=-N}^{N} V_{220}^{\mathrm{th}}(x - md_{220})$

$$V_{220}^{\mathrm{th}}(x) = -\frac{7e^2 a_{\mathrm{s}}}{2\sqrt{2}\varepsilon_0 d_{220}^2} \sum_{l=1}^{3} \frac{\alpha_l}{\beta_l} e^{\frac{\beta_l^2 \sigma_{\mathrm{th}}^2}{2a_{\mathrm{s}}^2}}$$

$$\times \left\{ e^{-\beta_l \frac{|x|}{a_{\mathrm{s}}}} \operatorname{erfc}\left(\frac{\beta_l \sigma_{\mathrm{th}}}{\sqrt{2}a_{\mathrm{s}}} - \frac{|x|}{\sqrt{2}\sigma_{\mathrm{th}}}\right) + e^{\beta_l \frac{|x|}{a_{\mathrm{s}}}} \operatorname{erfc}\left(\frac{\beta_l \sigma_{\mathrm{th}}}{\sqrt{2}a_{\mathrm{s}}} + \frac{|x|}{\sqrt{2}\sigma_{\mathrm{th}}}\right) \right\}.$$

The relativistic mass, critical angle and the dynamical thickness are

$$m_{\mathrm{r}} = \gamma m_{\mathrm{e}}, \;\; \Theta_{\mathrm{c}} = \sqrt{\frac{V(d_{220}/2)}{E_k} \frac{1 + \frac{E_k}{m_{\mathrm{e}}c^2}}{1 + \frac{E_k}{2m_{\mathrm{e}}c^2}}}, \;\; \Lambda = \frac{L}{2\pi} \sqrt{\frac{\partial_x^2 V(0)}{2E_k} \frac{1 + \frac{E_k}{m_{\mathrm{e}}c^2}}{1 + \frac{E_k}{2m_{\mathrm{e}}c^2}}}.$$

Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions

The Classical Channeling of Electrons

Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions

Hamilton's equations are solved by Runge-Kutta method of 4th order

$$\frac{\mathrm{d}\theta_x}{\mathrm{d}t} = -\frac{\partial_x V(x)}{m_\mathrm{r} k_z}, \rightarrow \theta_x^{(n+1)} = \theta_x^{(n)} + \sum_s c_s F_s \left(\theta_x^{(n)}, -\frac{\partial_x V(x^{(n)})}{m_\mathrm{r} k_z} \right),$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = k_z \theta_x, \qquad \rightarrow x^{(n+1)} = x^{(n)} + \sum_s c_s F_s \left(x^{(n)}, k_z \theta_x^{(n)} \right),$$

with the initial conditions $x(0) = x^{(0)} = b$, and $\theta_x(0) = \theta_x^{(0)} = 0$.

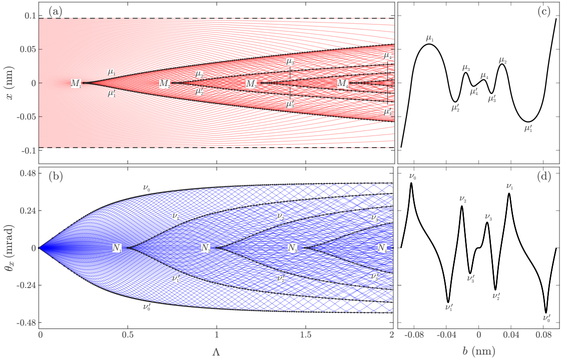
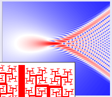


Figure 2: (a), (b) Spatial and angular trajectories of 255-MeV electron beam in planar channels (220) of Si crystal. The black dotted lines show corresponding caustics. (c), (d) The corresponding transmission functions.



The Quantum Channeling of Electrons

Channeling of quantum particles is governed by the Schrödinger equation

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m_{\rm r}}\partial_x^2\psi(x,t) + V(x)\psi(x,t).$$

Propagator $\hat{U}(t) = \exp[-i\hat{H}t/\hbar]$ is expanded in the basis of the Chebyshev polynomials T_n

$$\psi(t) = \hat{U}(t)\psi_0 \approx e^{-\frac{i}{\hbar}\bar{E}t}\sum_{n=0}^{N} a_n(\alpha)T_n\left(-\frac{i}{\hbar}\hat{\mathcal{H}}\right)\psi_0,$$

$$a_n(\alpha) = (2-\delta_{n0})i^n J_n(\alpha), \quad \alpha = \frac{\Delta E t}{2\hbar}, \quad \hat{\mathcal{H}} = \frac{2}{\Delta E}(\hat{H}-\bar{E}).$$

where $\Delta E = E_M - E_m$, $\bar{E} = (E_M + E_m)/2$. At the boundaries of computational domain absorptive potential is used

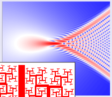
$$V_{\rm abs}(x) = \begin{cases} i\frac{V_0}{\cosh^2[\alpha(|x|-x_{\max})]}, & |x| \geq x_{\max}, \\ 0, & |x| < x_{\max}. \end{cases}$$

Main iteration of the method becomes

$$\psi_n = 2\hat{\mathcal{H}}\psi_{n-1} - \psi_{n-2}, \rightarrow \psi_n = e^{-\gamma}\left(2\hat{\mathcal{H}}\psi_{n-1} - e^{-\gamma}\psi_{n-2}\right),$$

where $\gamma(x) = -iV_{\rm abs}(x)$.

Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions



Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions

The Electron's Self-Interference

The initial electron state is represented by a Gaussian wave packet

$$\psi_b(x) = \sqrt{\mathcal{N}\left(b, \frac{1}{2k_z\Omega}\right)}.$$

Electron state in the angular representation is given by the integral

$$\varphi_b(\theta_x) = \sqrt{\frac{k_z}{2\pi}} \int \psi_b(x) e^{-ik_z\theta_x x}\, \mathrm{d}x, \quad \varphi_b \sim \mathrm{FFTW}\left[\psi_b\right].$$

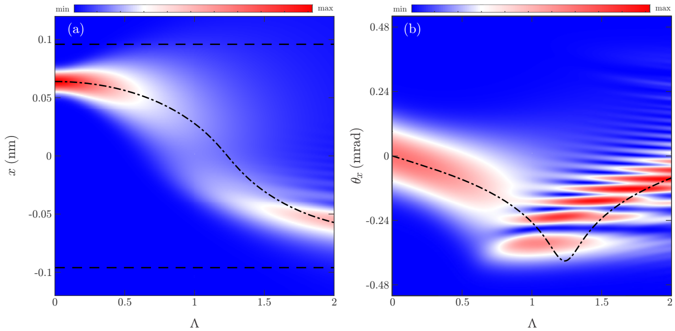


Figure 3: Evolution of the 255-MeV quantum state having $b = d_{220}/3$ in the (a) spatial and (b) angular representations. The dashed lines show boundaries of (220) channels. The dot-dashed lines show the corresponding classical trajectories.

The Probability Densities of Electron Beam

The probability densities of ensemble of noninteracting particles

$$\rho_x(x) = \frac{1}{d_{220}} \int\limits_{-d_{220}/2}^{d_{220}/2} |\psi_b(x)|^2 \, \mathrm{d}b, \quad \rho_{\theta_x}(\theta_x) = \frac{1}{d_{220}} \int\limits_{-d_{220}/2}^{d_{220}/2} |\varphi_b(x)|^2 \, \mathrm{d}b.$$

reflects a classical caustic pattern

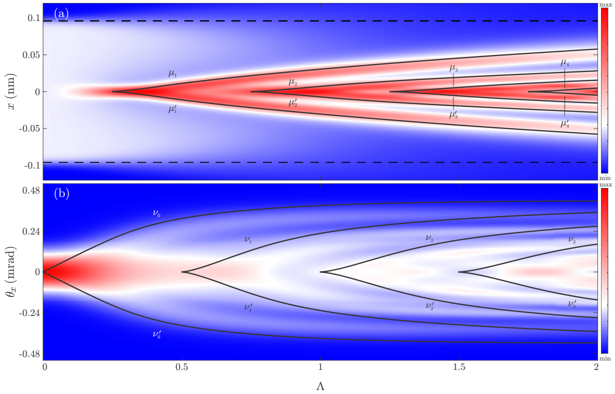


Figure 4: The probability density of the 255-MeV electron beam for $\Omega = 0.25\Theta_c$ in (a) spatial and (b) angular representations. Full and dashed lines show classical caustics and boundaries of (220) channels, respectively.

The Probability Densities of Electron Beam

or canonical diffraction patterns, depending on the value of the angular divergence of the electron beam Ω.

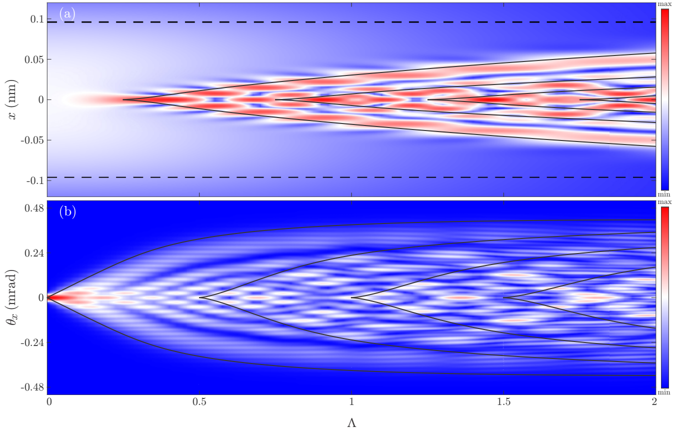


Figure 5: The probability density of the 255-MeV electron beam for $\Omega = 0.03\Theta_c$ in (a) spatial and (b) angular representations. Full and dashed lines show classical caustics and boundaries of (220) channels, respectively.

Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions

Channeling in the Phase Space

Wigner function in the (x, θ_x) phase space is defined by the following integral

$$W(x,\theta_x) = \frac{k_z}{2\pi}\int \psi_b^\dagger\left(x-\frac{\xi}{2}\right)\psi_b\left(x+\frac{\xi}{2}\right)e^{-ik_z\theta_x\xi}\,\mathrm{d}\xi,$$

$$W \sim \mathrm{CZT}\left[\psi_b^\dagger\psi_b, -k_z\Theta_c, k_z\Theta_c\right].$$

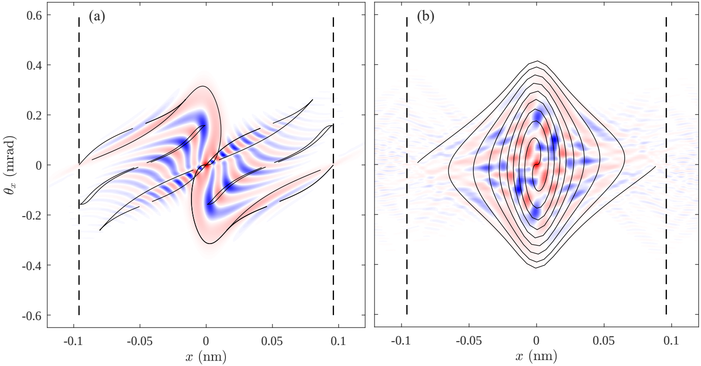


Figure 6: Wigner function for (a) $\Lambda = 0.5$ and (b) $\Lambda = 5$.The thin lines show the corresponding semiclassical catastrophic manifold. Dashed lines indicate boundaries of the planar channels (220).

Conslusions

- The classical dynamics electrons can be efficiently simulated using Runge-Kutta method of the 4th order.
- Distributions of the channeled beam can obtained by easily parallelized Monte-Carlo simulation.
- The quantum dynamics can be obtained accurately using Chebyshev method of global propagation.
- Efficiency of the calculation can be increased by the Task parallelism where the master thread executes the Chebyshev iteration, while slaves accumulate results to get time evolution of the quantum state.
- The dynamics in the phase space can be obtained efficiently if Wigner transform is implemented using CZT transform.
- The results show that quantum-classical transition can emerge on the level of the ensemble without the need for wave packets to transform into mass points.

Pafnuty Chebyshev (4. May 1821 - 26. December 1894).

Introduction
The channeling effect
The classical caustics
Quantum channeling
The numerical simulation
The self-interference
Distributions of electrons
The phase space dynamics
Conclusions