Classical and Quantum Descriptions of the Channeling Effect as Mutually Complementary Approximations

Kalashnikov N.P. . Olchak A.S.

National Nuclear Research University MEPhI.
Moscow, RF

$$\Psi(\boldsymbol{\rho},z)=\exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho})=e^{im\varphi}\begin{cases}C_1 J_m(k_n\rho), & \rho<a;\\ C_2 K_m(\eta_n\rho), & \rho>a,\end{cases}$$

Classical and Quantum Descriptions of the Channeling Effect as Mutually Complementary Approximations

The Content.

1. The models of averaged planar and axial channeling potentials

***2. Approaches that h*elp to obtain analytical results**

- co-moving reference system (CMRS)

- mixed quantum – classical approaches
- interpreting the crystal lattice potential as a flow of 'photons' in CMRS
- Re-using known results from quantum and atomic physics……

3. Examples of applying simplifying analytical approaches

- calculations of the transversal motion energy levels and radiation spectra
- Estimating Intensity of radiation from channeling pelectrons
- Considering Inverse Compton scattering in crystal, resulting in conversion of the electron energy into one photon'

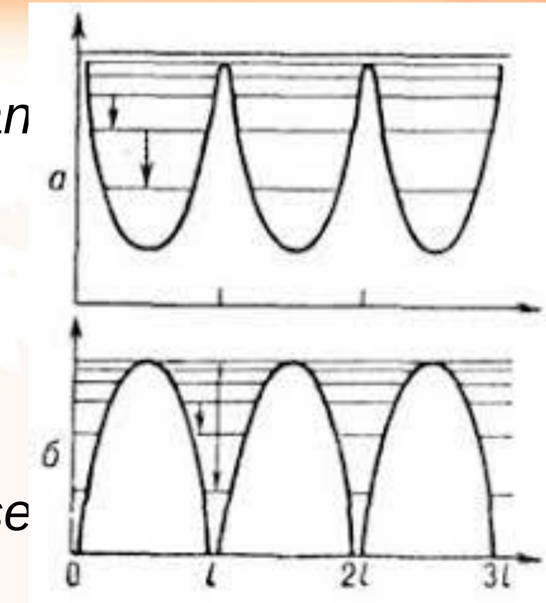
$$V(\mathbf{R}) = \sum_g V_g \exp(-i\mathbf{g}\mathbf{R}), \quad \Psi(\boldsymbol{\rho}, z) = \exp\left(\frac{ik_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

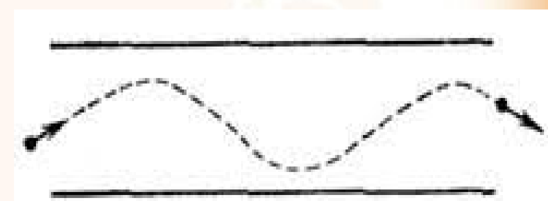
$$\Psi_{nm}(\boldsymbol{\rho}) = e^{im\varphi}\begin{cases} C_1 J_m(k_n\rho), & \rho < a; \\ C_2 K_m(\eta_n\rho), & \rho > a, \end{cases}$$

Planar averaged potential

The channeling effect occurs when a charged particle enters a crystal under small angle (less, than Lindhard's critical channeling angle) to some crystal axis or plane: $\theta < \theta_L \sim (U_0/E)^{1/2}$ *(E – the particle relativistic energy,* U_0 *- the depth/height of the averaged crystal potential)*

In Planar case the crystal potential is 1D. For positively charged particles it looks like a set of close to parabolic potential channels between densely packed planes. For negatively charged electrons channels are associated with atomic planes and the picture is inverse. The transversal motion of channeled particle in both cases is finite and limited by the potential barrier's. in most of crystals for typical densely packed directions $U_0 \sim 20\text{-}50$ *eV.*





$$V(\mathbf{R}) = \sum_g V_g \exp(-i\mathbf{g}\mathbf{R}),$$

$$\Psi(\boldsymbol{\rho}, z) = \exp\left(\frac{i k_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

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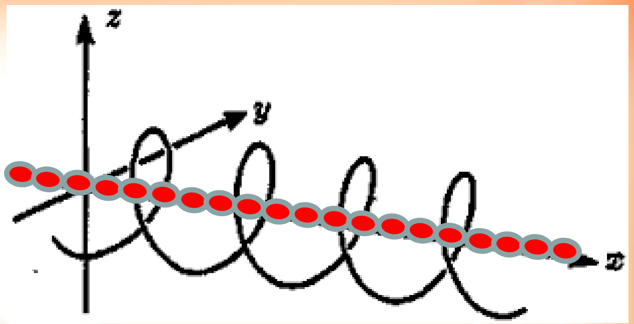
Axial averaged potentials?

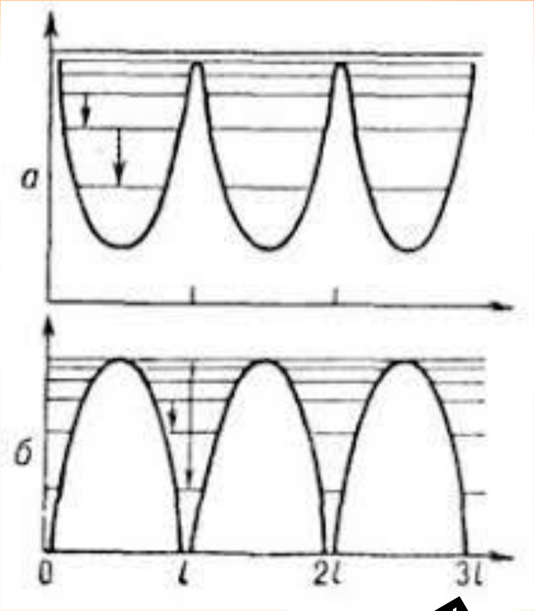


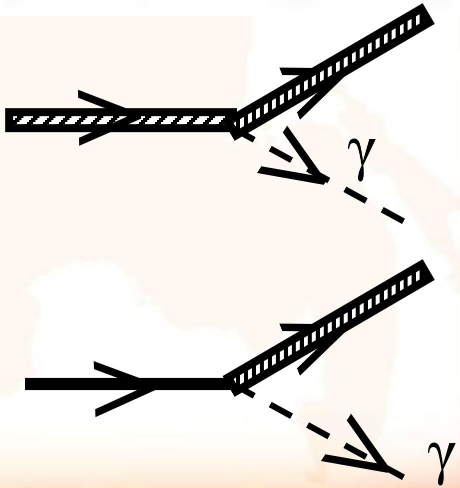
In axial case the crystal potential is 2D and the transversal motion of negatively charged electrons, orbiting around a densely packed crystal axis, is similar to the motion of electrons in atoms. The axial channeling can be considered as a realization of 2D relativistic atom with controlled variable potential parameters (E, U_0)

In literature one can find many potential models, used to describe the axial channeling motion, starting from 2D-Coulomb model $U \sim 1/\rho$ (ρ – the transversal to the channeling axis radial coordinate) to ~logarithmic potential $U = U_0 K(r)$ (K(r) – the special McDonnald's function), obtained by accurate averaging of screened Coulomb atomic potentials over channeling direction The more realistic axial potential shall not be divergent at = 0 point (with regard to thermal motion of crystal lattice ions). One of simple realistic models is a cone potential: $U = -U_0 (1- \rho/R)$, (R - the fitting parameter, close to the screening radius of crystal lattice ions) with U_0 ~ several dozen eV.

What is interesting to know about channeling motion?

- the transversal motion energy spectrum
- the spectrum and ***intensity*** of electromagnetic radiation,
- Conversion of electron energy into a high energy photon (*inverse Compton scattering*)
- *Other effects…*

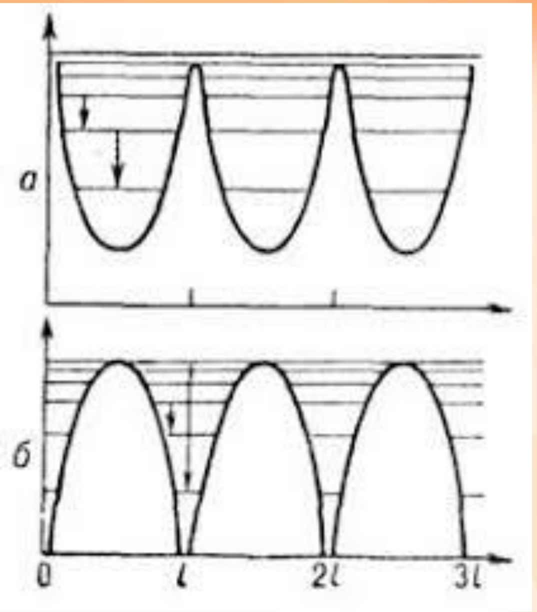




$$\Psi(\boldsymbol{\rho}, z) = \exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho}) = e^{im\varphi}\begin{cases} C_1 J_m(k_n\rho), & \rho < a; \\ C_2 K_m(\eta_n\rho), & \rho > a, \end{cases}$$

Channeling of Relativistic Electrons in Crystalls
What has to be calculated and how to do it correctly?



1. The transversal motion energy spectrum

The "correct way": to solve the relativistic Schroedinger equation (= the quadrated Dirac equation)

$$\left[-\frac{\hbar^2}{2\mu}\Delta_r + \gamma\bar{U}(\rho)\right]\Psi(r) = E\Psi(r).$$

In planar channeling the energy eigenvalues can be calculated analytically with parabolic potential: $E_n = (2U_0/E)^{1/2}(\hbar/l)(2n - 1);\ n = 1, 2, 3\ldots)$ or *with less realistic but simple Kronig-Penny (rectangular) potential* $U(x) = 0$ if $|x|<R$ and $U(x) = U_0$ if $|x|>R$. => $E_n = (2U_0/E)^{1/2}(\hbar/l)n^2$

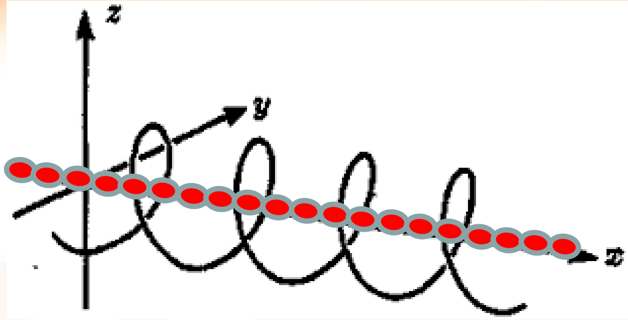
With inverse parabolic potential (realistic for electrons) and with other potential models only numerical solutions are possible

$$\Psi(\boldsymbol{\rho}, z) = \exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho}) = e^{im\varphi}\begin{cases} C_1 J_m(k_n\rho), & \rho < a; \\ C_2 K_m(\eta_n\rho), & \rho > a, \end{cases}$$

Channeling of Relativistic Electrons in Crystalls
What has to be calculated and how to do it correctly?

1. The transversal motion energy spectrum in axial channeling



$$\left[-\frac{\hbar^2}{2\mu}\Delta_r + \gamma\bar{U}(\rho)\right]\Psi(r) = E\Psi(r).$$

Analytical calculation of eigenvalues in 2D-axial case is possible with Coulomb potential/ U(ρ) ~ -1/ρ with negative eigenvalues $E_n \sim -1/n^2$ *similar to that in Hydrogen atoms , The problem is that the divergent at ρ =0 Coulomb potential is too far from being realistic for channeling case.*

… For simple cylindrical potential., finite at 0-point, the transcendent equation with special functions for eigenvalues can be obtained:

$$U(\rho) = \begin{cases} -V_0, & \rho < a; \\ 0, & \rho > a. \end{cases}$$

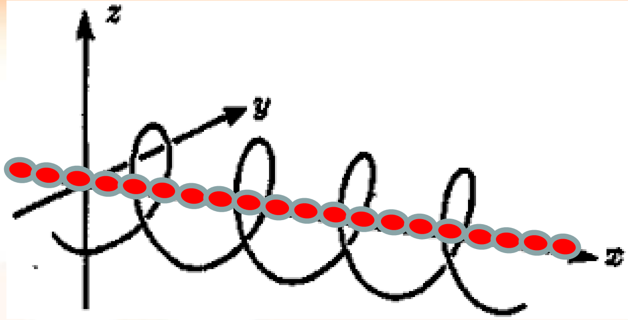
$$kJ'_m(ka)K_m(\eta a) - \eta J_m(ka)K'_m(\eta a) = 0.$$

$$k_n = \sqrt{\frac{2\mu\gamma V_0}{\hbar^2} + \frac{2\mu E_{\perp n}}{\hbar^2}}, \qquad \eta_n = \sqrt{\frac{-2\mu E_{\perp n}}{\hbar^2}},$$

$$\Psi(\boldsymbol{\rho},z)=\exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho})=e^{im\varphi}\begin{cases}C_1 J_m(k_n\rho), & \rho<a;\\ C_2 K_m(\eta_n\rho), & \rho>a,\end{cases}$$

1. Calculating wave functions of channeling states



$$\left[-\frac{\hbar^2}{2\mu}\Delta_r+\gamma\bar{U}(\rho)\right]\Psi(r)=E\Psi(r).$$

Analytical calculation of wave functions and expressing them in elementary functions is possible only for Kronig-Penny potential for planar channeling, In axial channeling even for most simple cylindrical potential Ψ-functions are special functions .

$$U(\rho)=\begin{cases}-V_0, & \rho<a;\\ 0, & \rho>a.\end{cases}$$

$$\Psi(\boldsymbol{\rho},z)=\exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho})=e^{im\varphi}\begin{cases}C_1 J_m(k_n\rho), & \rho<a;\\ C_2 K_m(\eta_n\rho), & \rho>a,\end{cases}$$

In other potentials only numerical calculations are possible..

What is important to calculate?

2. Radiation transitions matrix elements and the ***intensity*** of electromagnetic radiation from channeling electron

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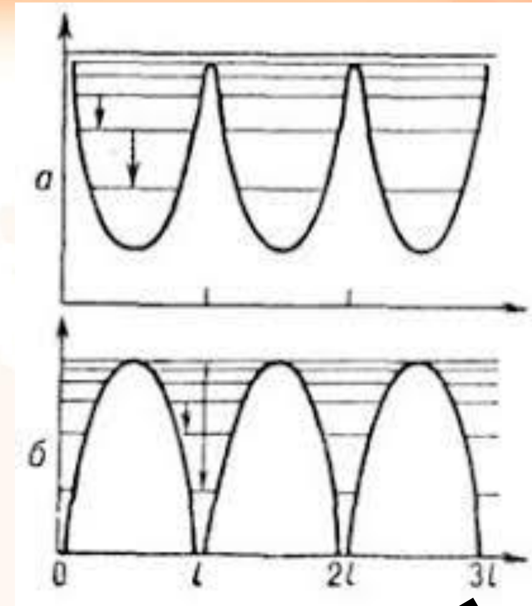
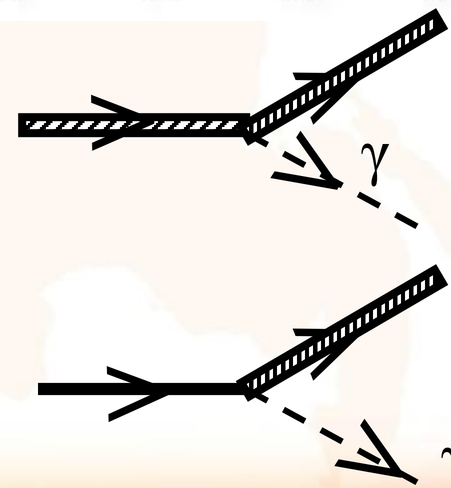
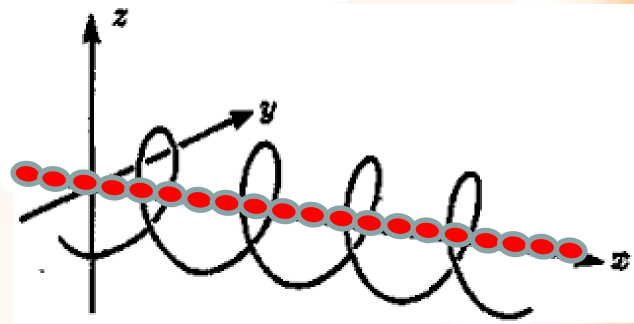
The “correct way” is to calculate the matrix elements with pre-calculated wave functions of channeling states, :what obviously can be done only numerically – means non-transparantly





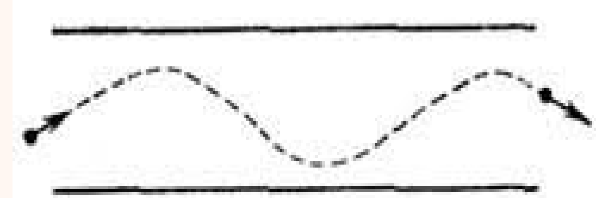
What is important to calculate?

1. ***"Co-moving reference system" (CMRS)*** – the reference system, *moving along the channeling direction with the speed, equal to the longitudinal component of the particle speed.*



In CMRS the motion od channeling particle is either 2-D (axial case) or 1-D (planar case).

Due to Doppler effect te averaged potential and the transversal energy eigenvalues in CMRS are multiplied by the Lorenz-factor $\gamma = E/mc^2$ *:*



$U_{CMRS} = EU_0/mc^2 \qquad E_{n\,CMRSc} = Ee_n/mc^2$

If $U_{CMRS} < EU_0/mc^2 \Rightarrow E < (mc^2)^2/U_0$ ~ several GeV the transversal motion of channeling particle is thus giving the way to apply corresponding simplifying approximations

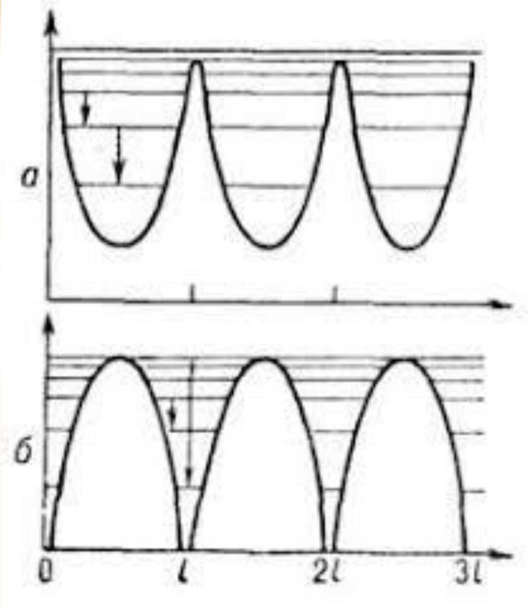
Channeling of Relativistic Electrons in Crystals
Approaches that produce results without numerical calculations

In ***CMRS) it is possible to apply simplifying approximations:***

In ***planar 1D case***: the ***Bohr–Sommerfeld quantization rule*** (BSR), defining the eigenvalues of transversal energy

$\int(2E(E_n-U(x))^{1/2}dx = hcn/2$ (n = 1, 2, 3,

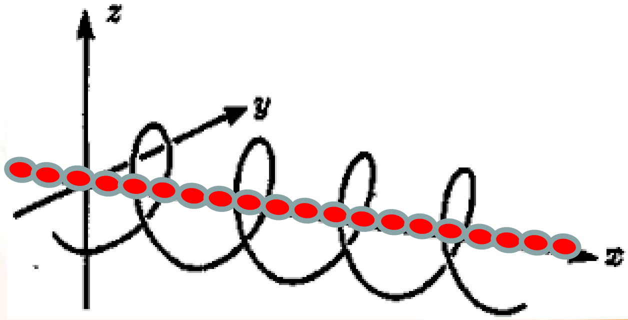
The integration is done between the two stop-points of finite transversal motion. For parabolic and rectangular (Kronig-Penny) potentials it gives the same results as the accurate calculation with Schroedinger equation. We may expect not worse match with other potentials also.



For any potential model the total number of channeling states may be estimated as $N \sim= \int(2E|^{1/2}U(x)|^{1/2}dx/hc \sim (2EU_0)^{1/2}l//hc$, Here l - the effective width and U_0 - the effective depth of the potential channel / Estimation is valid for practically any realistiv potential model.

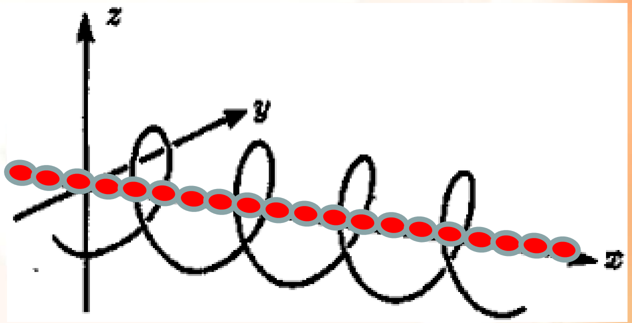
*In **CMRS) it is possible to apply simplifying approximations:***

The eigenvalues of transversal energy for orbiting 2D-motion in ***axial case***: can be defined by the **Bohr quantization rule (BQR)**: the orbital momentum of electron $L_n = \hbar n$ *(n = 1, 2, 3,*



In orbital motion parameters in Bohr's approach are calculated in classical mechanics frameworks. In atomic physics the Bohr approach gives correct values for the H-atom energy levels. We may expect not worse match with other potential models in axial channeling.

In ***CMRS) it is possible to apply simplifying approximations:***

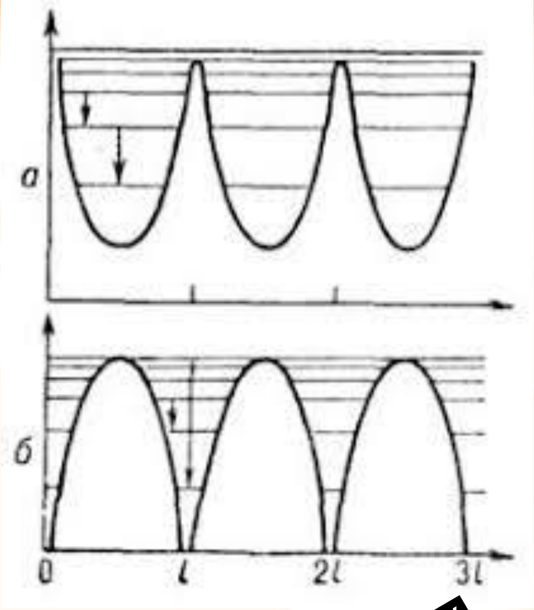


The eigenvalues of transversal energy for orbiting 2D-motion in ***axial case***: can be defined by the Bohr quantization rule (BQR): the orbital momentum of electron equals the multiple of Plank constant; $L_n = \hbar n$ *(n = 1, 2, 3,*

For any potential model the total maximal number $n_{max} = N$ corresponds to the maximal possible orbital momentum with radius of orbit close to maximum r ~ R. It is easy to demonstrate that N is defined by the expression, similar to that for the planar channeling: $N \sim (2EU_0)^{1/2} R\ hc$, practically independent on the particular potential model.

Channeling of Relativistic Electrons in Crystalls
Examples of analyses

2. The spectrum and ***intensity*** of electromagnetic radiation)



The spectrum of radiation is defined by the spectrum of quantum states of transversal motion E_{tr} with regard to the Doppler effect in LabRS.

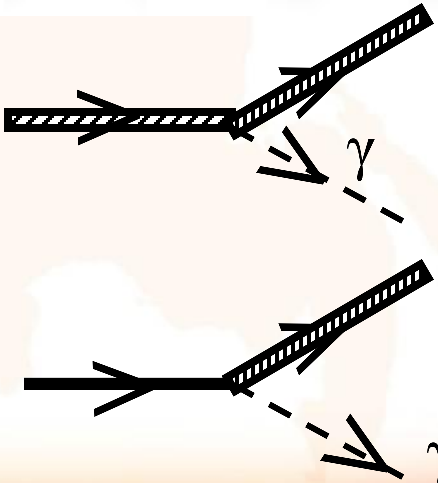
$$\hbar\omega = \Delta E_{tr}/(\theta^2 + m^2c^4/E^2) \sim (E/mc^2)^2 \Delta E_{tr}$$

Here θ is the angle of radiation relative to the channeling direction.

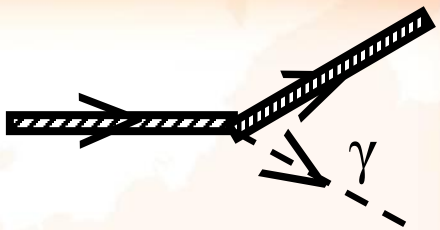
The average energy difference between discrete levels of transversal motion ΔE_{tr} can be estimated as the ratio of the potential depth U_0 and the total number of discrete states *N*.

In Lab.RS: $\Delta E_{tr} \sim U_0 / N \sim= (hc/R)(U_0/2E)^{1/2}$,

$=> \hbar\omega \sim (E/mc^2)^{3/2} (hc/R)(U_0/2mc^2)^{1/2}$

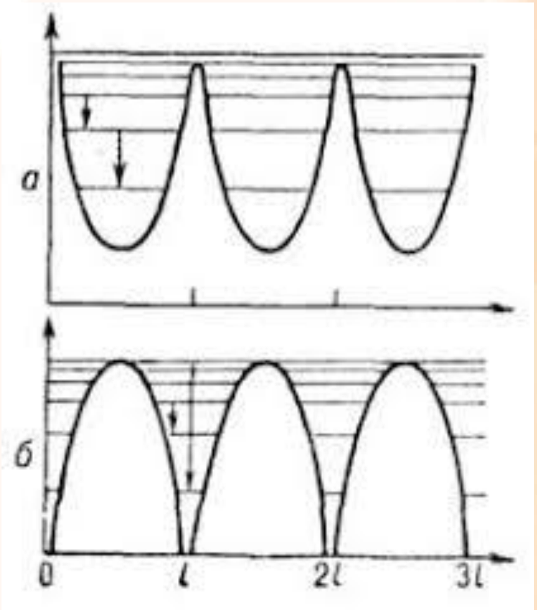


2. The *intensity* of electromagnetic radiation)

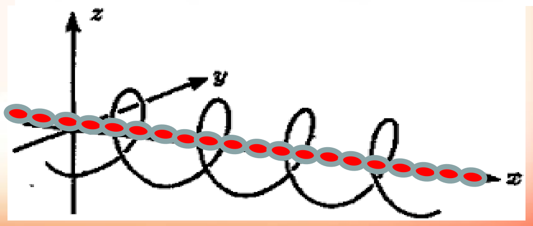


The easiest way to estimate the intensity of electromagnetic radiation is to apply the classical electrodynamic approach The intensity P of dipole radiation from the moving particle, is proportional to its acceleration w squared:

$$P = (e^2/2\pi\varepsilon_0 c^3)w^i$$



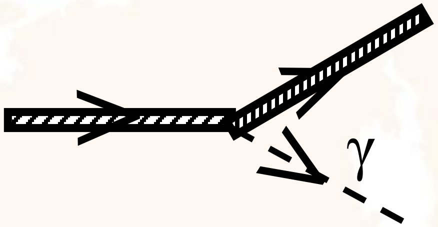
In classical approach the electron in the realistic inverse parabolic potential in CMRS moves with average acceleration $w = \sim EU_0 / m^2c^2R$. The same estimation is valid for the centripetal acceleration of electron, moving in cone model potential in axial channel.



2. The ***intensity*** of electromagnetic radiation)

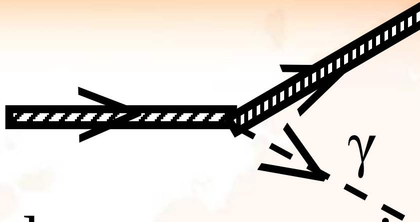
For both planar and axial channeling cases the intensity of radiation thus may be estimated as

$$P = \sim (e^2/2\pi\varepsilon_0 c^3)(EU_0 / m^2c^2R)^i$$



In typical channeling conditions the effective length, where each channeling electron emits at least 1 photon, equals ~several *mm*,

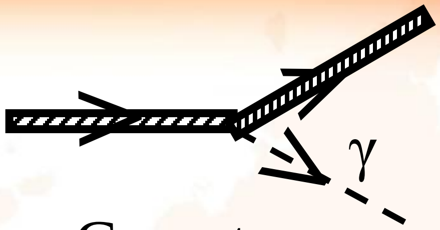
3. Conversion of electron energy into a photon (inverse Compton scattering)



The crystal axis potential generally can be presented as an expansion in series: $U(r) = U_0 + U_1 cos(2\pi z/d) + Re[U_n \exp(i2\pi nz/d)]$, $n = 2, 3,$ U_0 Is the averaged channeling potential. The periodical component with U_1 `U_0 in CMRS can be interpreted as electromagnetic wave or flow of photons with wavelength $\lambda = (mc^2/E)d$, hitting the resting (in CMRS) electron. The Lorenz factor shows up in CMRS due to the Doppler effect.

The scattered photon, as we know from Compton effect theory, may change the direction of propagation for inverse practically without loosing energy (if $\lambda << mc^2$). In LabRS the Doppler effect will act again, making the photon wavelength even shorter $\lambda' = (mc^2/E)^2 d$,

3. Conversion of electron energy into a photon (inverse Compton scattering)



The real photon, produced as the result of the inverse Compton scattering of the “as-if photon” (*$U_1 cos(2\pi z/d)$ 0)* may carry away the considerable part of the relativistic energy of electron in LabRS:

$$\hbar\omega' =\sim (E/mc^2)^2(hc/d) \sim (E/mc^2)^2 \text{ keV} ,$$

If E > GeV the inverse Compton scattering may result in converting of nearly all the electron energy into one photon.

$$\hbar\omega' =\sim (hc/d) \; / \; [(mc^2/E)^2 + (hc/Ed)\,] \;\text{->}\; \sim E - m^2c^3d/h$$

$$\Psi(\boldsymbol{\rho}, z) = \exp\left(\frac{ip_z z}{\hbar}\right)\Psi_{nm}(\boldsymbol{\rho}),$$

$$\Psi_{nm}(\boldsymbol{\rho}) = e^{im\varphi}\begin{cases} C_1 J_m(k_n\rho), & \rho < a; \\ C_2 K_m(\eta_n\rho), & \rho > a, \end{cases}$$

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Some conclusions.

Simplifying analytical approaches, such as

- using co-moving reference system (CMRS)
- re-using known results from quantum and atomic physics, like Bohr - quantization rule or Compton effect analyses
- mixing quantum and classical approaches
- interpreting the crystal lattice potential as a flow of ‘photons’ in CMRS
- etc…

..do really help to obtain substantial analytical results when considering the channeling effect aspects, **such as** ……

- calculating the values of the the transversal motion energy levels and radiation spectra

- Estimating the Intensity of radiation from channeling particles
- Considering the Inverse Compton scattering of crystal lattice ‘photon flow,
- etc, etc…

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Kalashnikov N.P. . Olchak A.S.

National Nuclear Research University MEPhI.
Moscow, RF

Thank You for Attention!