Quantum Features of Relativistic Particle Scattering and Radiation in Crystals

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Tuesday, 25 September - Hotel Continental Ischia

Plan

Intoduction. *The need of quantum theory of incoherent scattering in crystals*

Wigner function description of both quantum and classical effects

– *classical motion description by eikonal method*

– *quantum scattering description in Born approximation*

Wigner function of incoherent scattering

– *small angle scattering description by averaged angle*

– *large angle scattering description by Moss cross-section modification*

Incoherent scattering contribution to radiation and pair production

Observed effects predicted by Prof. V.G. Baryshevsky and his School

Parametric radiation

Channeling radiation

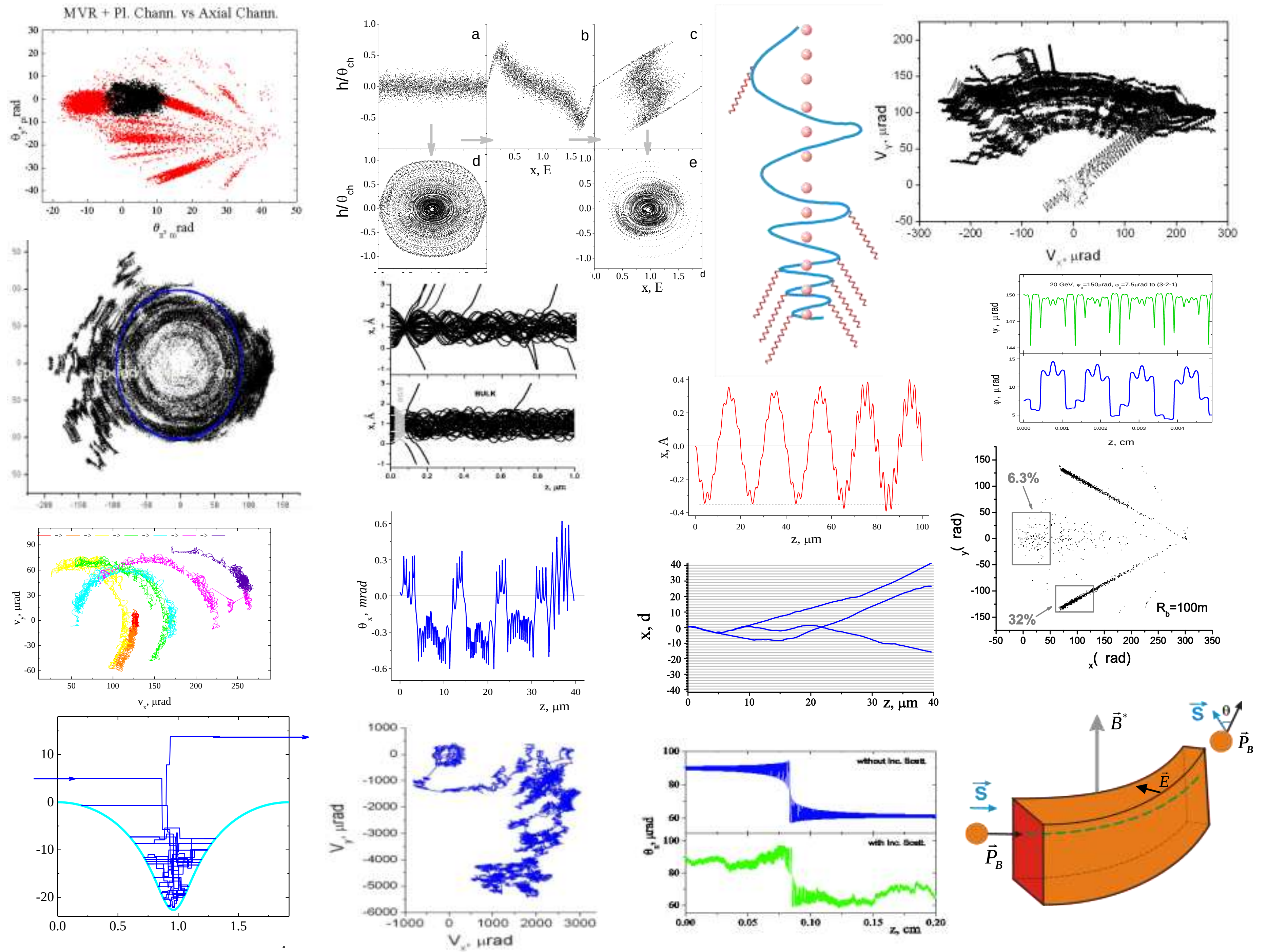
Spin rotation in crystals

Radiative cooling

Synchrotron-type $e^+ e^-$ pair production

Multiple volume reflection in one crystal

Quasichanneling oscillations



MVR + Pl. Chann. vs Axial Chann.
h/θ_ch
x, E
a
b
c
d
e
BULK
x, Å
z, μm
θ_x, mrad
V_y, μrad
V_x, μrad
v_y, μrad
v_x, μrad
x, A
x, d
20 GeV, ψ0=150μrad, φ0=7.5μrad to (3-2-1)
ψ, μrad
φ, μrad
z, cm
6.3%
32%
R_b=100m
without inc. Scatt.
with inc. Scatt.
θ_x, μrad
S
B*
E
P_B
θ

The main thing

still ubiquitously **missed**

is **quantum** incoherent

scattering theory

Det Kgl. Danske Videnskabernes Selskab.
Mathematisk-fysiske Meddelelser **XVIII**, 8.

THE PENETRATION OF ATOMIC PARTICLES THROUGH MATTER

BY

NIELS BOHR

KØBENHAVN
I KOMMISSION HOS EJNAR MUNKSGAARD
1948

Bohr condition $Z\alpha/\beta >> 1$

or, according to (1.1.4) and (1.3.2),

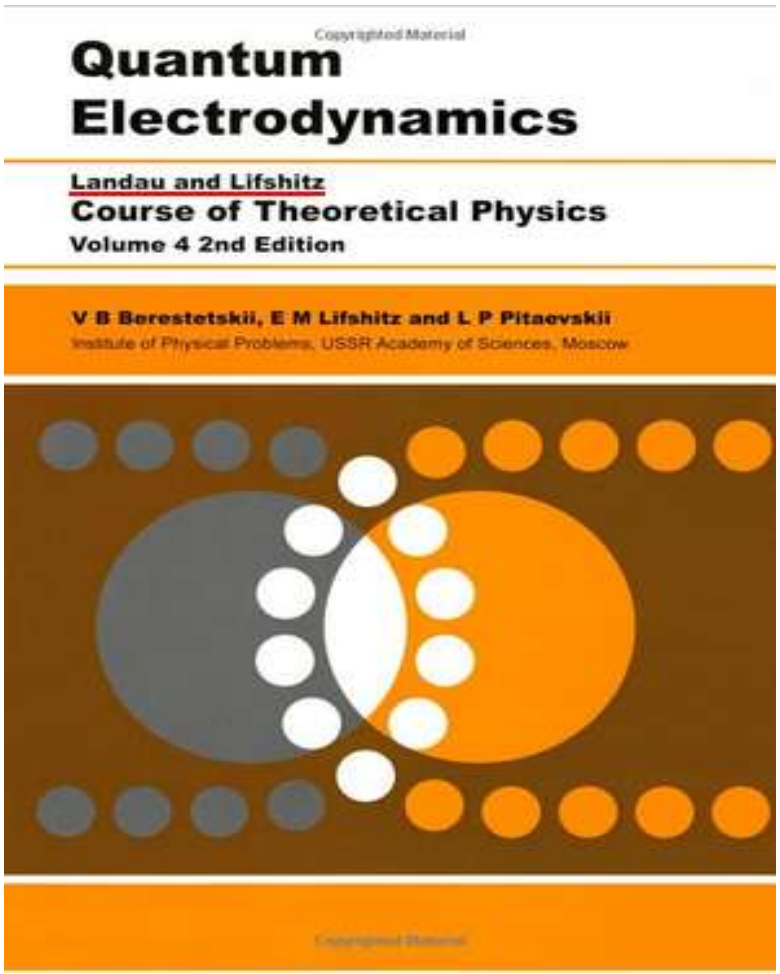
$$\varkappa = \frac{2\,|e_1 e_2|}{\hbar v}, \qquad (1.3.8)$$

we thus have

$$\varkappa \gg 1 \qquad (1.3.9)$$

as the necessary and sufficient condition for the justification of the classical considerations

Landau and Lifshitz about quantum nature of particle scattering by atoms



QUANTUM ELECTRODYNAMICS

by

V. B. BERESTETSKII, E. M. LIFSHITZ

and

L. P. PITAEVSKII

Institute of Physical Problems, U.S.S.R. Academy of Sciences

Volume 4 of *Course of Theoretical Physics*
Second edition

Translated from the Russian by

J. B. SYKES and J. S. BELL

§126. The quasi-classical case

It is of interest to investigate the manner in which the passage occurs from the quantum-mechanical theory of scattering to the limit of the classical theory.

If we can speak of classical scattering through an angle θ when the particle is incident at an impact parameter ρ, it is necessary that the quantum-mechanical indeterminacies of these two quantities should be relatively small: $\Delta\rho \ll \rho$, $\Delta\theta \ll \theta$. The indeterminacy in the scattering angle is of the order of magnitude $\Delta\theta \sim \Delta p/p$, where p is the momentum of the particle and Δp is the indeterminacy in its transverse component. Since $\Delta p \sim \hbar/\Delta\rho \gg \hbar/\rho$, we have $\Delta\theta \gg \hbar/p\rho$, and thus

$$\boxed{\theta \gg \hbar/\rho m v.} \tag{126.6}$$

The classical angle of deviation of the particle can be estimated as the ratio of the transverse momentum increment Δp during the "collision time" $\tau \sim \rho/v$ and the original momentum mv. The force acting on the particle at a distance ρ is $U'(\rho)$; hence $\Delta p \sim |U'(\rho)|\rho/v$, so that $\theta \sim |U'(\rho)|\rho/mv^2$.

Substitution in (126.6) gives the condition for quasi-classical scattering in the form

$$\boxed{|U'(\rho)|\rho^2 \gg \hbar v.} \tag{126.7}$$

For a Coulomb field, $U = \alpha/r$, the condition (126.7) is satisfied if $\boxed{\alpha \gg \hbar v.}$ This is the opposite condition to that for which the Coulomb field can be regarded as a perturbation. We shall see, however, that the quantum theory of scattering in a Coulomb field leads to a result which, as it happens, is always in agreement with the classical result.

Since $\dfrac{Z\alpha}{\beta} \approx \dfrac{14}{137} \ll 1$ **the single-atom scattering is "quantum" and can be treated as a perturbation**

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Bind 34, nr. 14

Mat. Fys. Medd. Dan. Vid. Selsk. 34, no. 14 (1965)

INFLUENCE OF CRYSTAL LATTICE ON MOTION OF ENERGETIC CHARGED PARTICLES

BY

JENS LINDHARD

København 1965
Kommissionær: Ejnar Munksgaard

Appendix B

Quantal Corrections to Classical Description

Single Collision

The total uncertainty, $\delta\vartheta$, in scattering angle can be obtained in a way analogous to that used by BOHR[12].

With a wave packet of width δr there are two contributions to $\delta\vartheta$, one from diffraction and one from classical uncertainty in position, i.e.

$$(\delta\vartheta)^2 = \frac{\lambda\!\!\!^{-2}}{4(\delta r)^2} + (\delta r)^2 \cdot (\vartheta'(p))^2. \tag{B.1}$$

In order to obtain a well-defined orbit, we may demand $(\delta\vartheta)^2 < \vartheta^2$, or

$$\lambda\!\!\!^{-} \frac{d}{dp}\left(\frac{1}{\vartheta(p)}\right) < 1, \tag{B.3}$$

which formula in the case of Rutherford scattering, $\vartheta = b/p$, leads to the inequality of BOHR[12]

$$\boxed{\varkappa = \frac{2Z_1 Z_2 e^2}{\hbar v} > 1.} \tag{B.4}$$

3.C:6.B *Nuclear Physics* **A96** (1967) 481—504;

QUANTAL TREATMENT OF DIRECTIONAL EFFECTS FOR ENERGETIC CHARGED PARTICLES IN CRYSTAL LATTICES

PHILIP LERVIG, JENS LINDHARD and VIBEKE NIELSEN
Institute of Physics, University of Aarhus, Denmark

in continuation of previous work [1,2]

1) J. Lindhard, Phys. Lett. 12 (1964) 126

2) J. Lindhard, Mat. Fys. Medd. Dan. Vid. Selsk. 34, No. 14 (1965).

single scattering of a charged particle by an atom is to be described by **quantal** perturbation methods when the **velocity** is sufficiently **high**, in particular at small angles of deflection 3).

3) **N. Bohr**, Mat. Fys. Medd. Dan. Vid. Selsk. 18, No. 8 (1948).

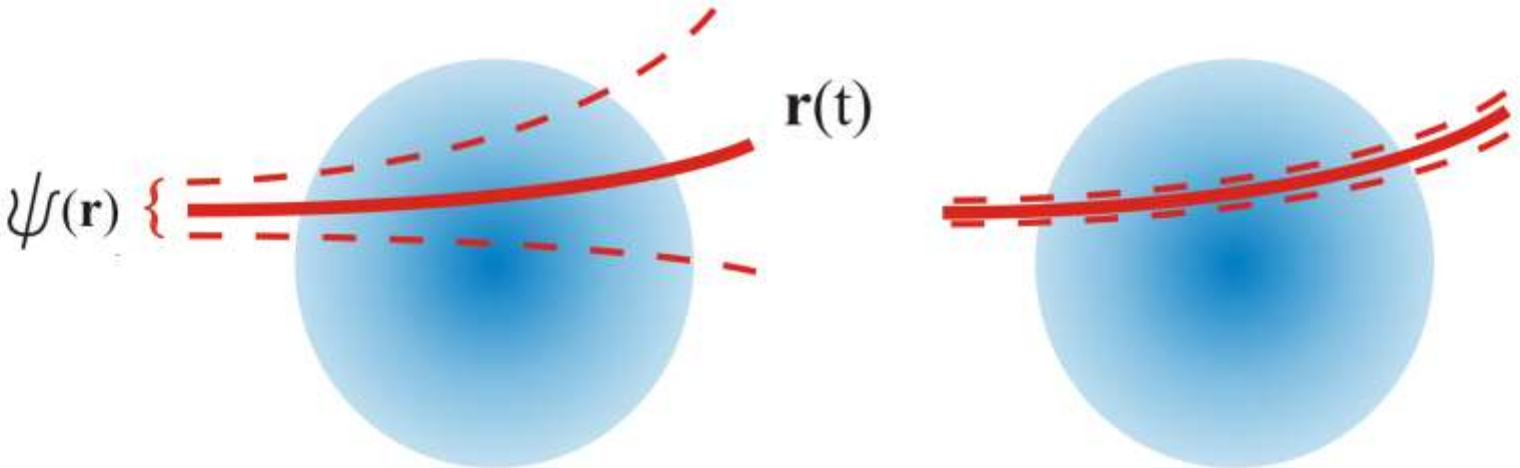
Xavier ARTRU

This conference talk:

Quantum Versus Classical Approach of Dechanneling and Other Incoherent Processes at High Energy in Aligned Crystals

We discuss whether it can be treated classically, like in the binary collision model, or if it should be treated **quantum-mechanically**. **We give arguments for the latter** opinion. We show that the quantum approach predicts a slower dechanneling than the classical one.

classical *vs* quantum scattering



$$\frac{Z\alpha}{\beta} << 1$$

quantum

$$\frac{Z\alpha}{\beta} >> 1$$

classical

Quantum *vs* classical cross sections

Relativistic analog to

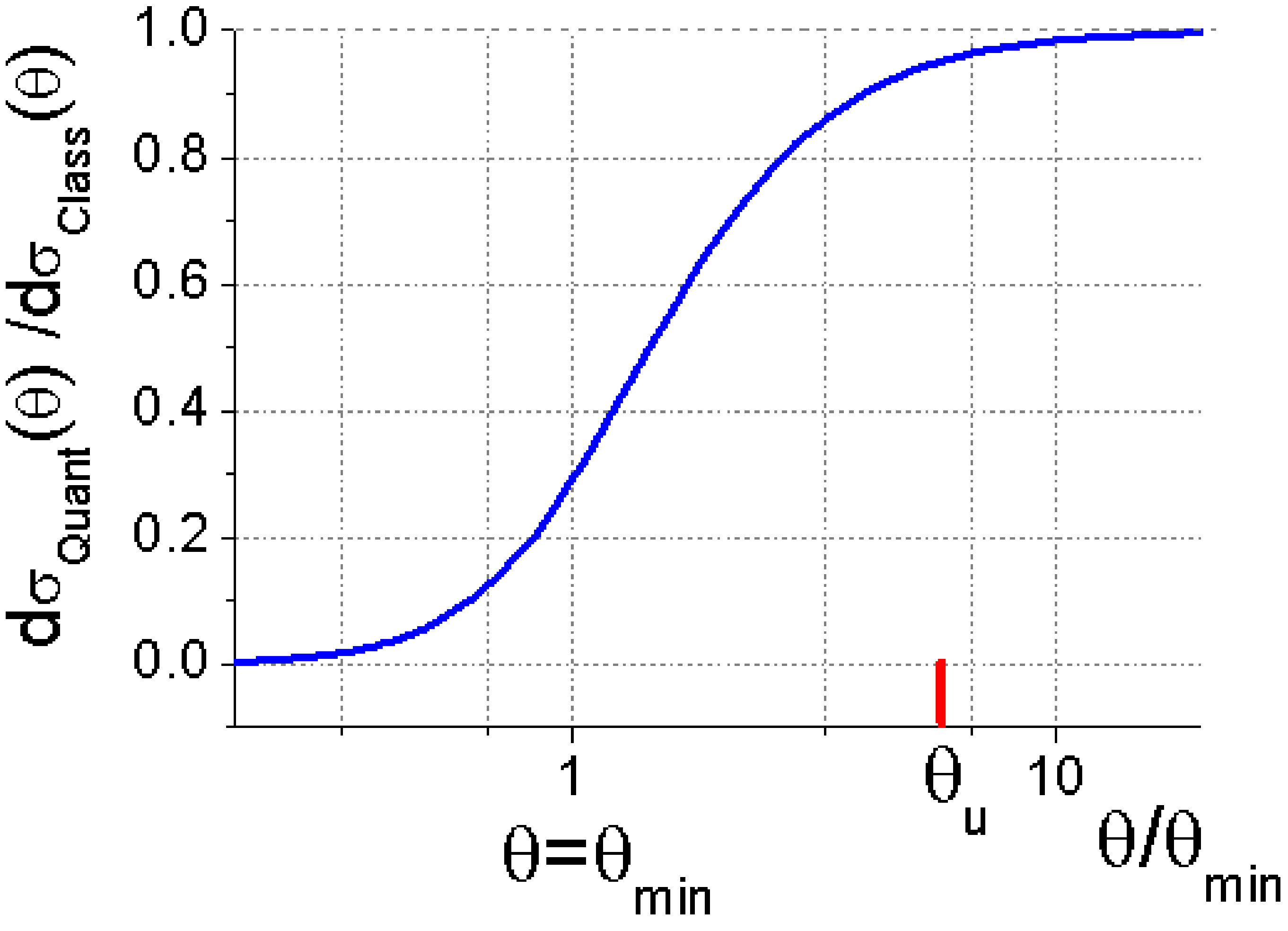
C. LEHMANN and G. LEIBFRIED. Higher order momentum approximations in classical collision theory. Zeitschrift fiir Physik 172, 465--487 (1963).

$$\theta(\rho) \approx \frac{2Z\alpha}{\varepsilon a \rho} \int_{\rho}^{\infty} \frac{\exp(-r/a)}{\sqrt{r^2-\rho^2}} r\,dr = \frac{2Z\alpha}{\varepsilon a} K_1(\rho/a)$$

$$\frac{d\sigma_{Class}}{d\Omega} \approx \frac{\rho(\theta)}{\theta} \left| \frac{d\theta(\rho)}{d\rho} \right|^{-1} = \frac{4Z^2\alpha^2}{\varepsilon^2\theta^4} \left[\frac{b}{K_1'(b)K_1^3(b)} \right], \qquad b = \rho/a$$

$$\frac{d\sigma_{Quant}}{d\Omega} \approx \frac{4Z^2\alpha^2}{\varepsilon^2\theta^4} \frac{1}{\left(1+\hbar^2/\theta^2 p^2 a^2\right)^2} = \frac{4Z^2\alpha^2}{\varepsilon^2\theta^4} \left(1+\hbar^2/\theta^2 p^2 a^2\right)^{-2}$$

Indeed, classical approach **overestimates** scattering



Typical scattering angles $\theta_{\min}$ and θ_u

Momentum transfer $q_\perp = \hbar Z^{1/3} / a_0$

and scattering angle $\theta_{\min} = \hbar Z^{1/3} / a_0 p$

are determined by the **atom screening** radius $a_0 / Z^{1/3}$

Momentum transfer $q_\perp = \hbar / u_1$

and scattering angle $\theta_u = \hbar / u_1 p \approx (2 \div 3)\,\theta_{\min}$

are determined by atomic vibration amplitude u_1

which determines **additional effective screening**

(scattering suppression by correlations)

PHYSICAL REVIEW B VOLUME 8, NUMBER 7 1 OCTOBER 1973

Modified Dechanneling Theory and Diffusion Coefficients

M. Kitagawa and Y. H. Ohtsuki
Department of Physics, Waseda University, Nishi-Ohkubo 4, Shinjuku, Tokyo, Japan
(Received 20 February 1973)

A new type of dechanneling theory is presented by constructing a Fokker-Planck equation. The damping term, which is not renormalized to the diffusion coefficient, and a new term in addition to the usual diffusion equation appear in the Fokker-Planck equation. Making use of the general expression of the diffusion coefficient given by Ohtsuki, some simple analytic expressions for diffusion coefficients due to the many-phonon excitations, the one-electron excitation, and the plasmon excitation are presented.

$$\boxed{\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle \cong \left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle_{\text{random}} P(r_\perp),} \tag{3.8}$$

where $\langle \Delta p_\perp^2/\Delta z\rangle_{\text{random}}$ is the diffusion coefficient in random case given by Bohr,[21]

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle_{\text{random}} = \frac{8\pi Z_1^2 Z_2^2 e^4 N}{v_z^2} L_n , \tag{3.9}$$

and $P(r_\perp)$ is the distribution function of the atom in thermal motion at the (x, y) plane,

$$P(r_\perp) = \sum_{h_\perp} e^{-M(\vec{h}_\perp)} e^{i\vec{h}_\perp \cdot \vec{r}_\perp} = \frac{r_0^2}{\rho_\perp^2} \exp\left(-\frac{r_\perp^2}{\rho_\perp^2}\right). \tag{3.10}$$

Diffusion coefficients for the planar case are also derived from Eq. (3.1) with same assumptions taking into account $\vec{h}_\perp = (0, h_y)$,

$$\boxed{\langle \Delta p_y^2/\Delta z\rangle = \langle \Delta p_y^2/\Delta z\rangle_{\text{random}} P(y),} \tag{3.11}$$

where $P(y)$ is the distribution function of the atom at y from the channeling plane,

$$P(y) = \frac{d_y}{(2\pi)^{1/2}\rho_y} \exp\left(-\frac{y^2}{2\rho_y^2}\right) , \tag{3.12}$$

Presently used:

Kitagawa-Ohtsuki approximation

$$\left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle \cong P(r_\perp) \times \left\langle \frac{\Delta p_\perp^2}{\Delta z} \right\rangle_{\text{random}}$$

$$P(r_\perp) = \frac{r_0^2}{\rho_\perp^2} \exp\left(-\frac{r_\perp^2}{\rho_\perp^2}\right), \qquad P(y) = \frac{d_y}{(2\pi)^{1/2}\rho_y} \exp\left(-\frac{y^2}{2\rho_y^2}\right).$$

we: + *suppression by coherent scattering*

$$\langle d\vartheta_s^2(z)/dz \rangle = n \int_0^{\vartheta_2} \int_0^{2\pi} \vartheta^2 \frac{d\sigma}{d\Omega} [1 - \underline{\exp(-p^2\vartheta^2 u_1^2)}] d\varphi \vartheta d\vartheta$$

Kitagawa-**O**htsuki approximation

$$d\Sigma_{KO} \equiv n(\rho) \cdot d\sigma_{Mott}(\vec{q}_\perp) =$$

$$\frac{\exp\left(-\rho^2 / 2u_1^2\right)}{2\pi u_1^2} \times \frac{4\alpha^2 Z^2 d\,\vec{q}_\perp}{\left(q_\perp^2 + \hbar^2 / a_F^2\right)^2}$$

– is, in fact, **refined** in the present talk

– is used everywhere for **normalization**

Single-atom scattering modification in crystals (M. L. Ter-Mikaelian)

$$\varphi = \sum_i \frac{Ze}{|\mathbf{r}-\mathbf{r}_i|} \exp\left(\frac{-|\mathbf{r}-\mathbf{r}_i|}{R}\right).$$

$$d\sigma = d\sigma_{\mathrm{BH}} \left| \sum_i \exp\left(\frac{i\mathbf{q}\mathbf{r}_i}{\hbar}\right) \right|^2, \qquad q = \mathbf{p}_1 - \mathbf{p}_2 - \hbar\mathbf{k}$$

averaging over thermal vibrations:

$$\overline{\left| \sum_i \exp\left(\frac{iq\mathbf{r}_i}{\hbar}\right) \right|^2} = N\left[1 - \exp\left(\frac{-q^2\bar{u}^2}{\hbar^2}\right)\right] + \exp\left(\frac{-q^2\bar{u}^2}{\hbar^2}\right) \left| \sum_i \exp\left(\frac{i\mathbf{q}\mathbf{r}_{i0}}{\hbar}\right) \right|^2.$$

Using this equality, we obtain for bremsstrahlung cross section in a crystal the expression [see formulas (3) and (12) in Ref. 4]

$$d\sigma = d\sigma_{\mathrm{BH}} \left\{ \underbrace{N\left[1 - \exp\left(\frac{-q^2\overline{u^2}}{\hbar^2}\right)\right]} + \exp\left(\frac{-q^2\bar{u}^2}{\hbar^2}\right) \left| \sum_i \exp\left(\frac{i\mathbf{q}\mathbf{r}_{i0}}{\hbar}\right) \right|^2 \right. \qquad (7.4)$$

M. L. Ter-Mikaelian approach

is equivalent to the

plane wave approximation

and does not take into consideration

both **particle and nuclei**

transverse distribution **nonuniformity**

Essential points for KO refining:

- Strong particle *transverse* **localization** (trajectories)
- Strong **nonuniformity** of transverse distriburion of the scatterers

Our approach is founded on

Wigner function (WF) as well as

both eikonal and Born approximations

and ***quantum-mechanically*** *describes*

incoherent *particle scattering*

in non-uniform media

of atomic strings and planes

This new approach:

– **refines K**itagawa**-O**htsuki approximation

– **Uses ideas/works** of W.R. Hamilton, N. Bohr, E. Wigner, J. Lindhard , M. L. Ter-Mikeilian

Has something **common** with works of A.I. Akhiezer & **N.F. Shul´ga** and **X. Artru**

Primary formulae

$$P(z, z_0, \vec{\rho}, \vec{q}_\perp) =$$

$$\pi^{-2} \int \Psi^*(z, z_0, \vec{\rho} + \vec{\chi}) \Psi(z, z_0, \vec{\rho} - \vec{\chi}) \exp(2i\vec{q}_\perp \vec{\chi}) d^2\chi$$

$$\Psi \approx \Psi_{eik}(\vec{r}) \left[1 - i \int \delta U_{at}(\vec{\rho}' - \vec{\rho}_{at}, z') \frac{dz'}{\upsilon} \right]$$

Eikonal ($\approx$ "classical") wave function and Wigner function

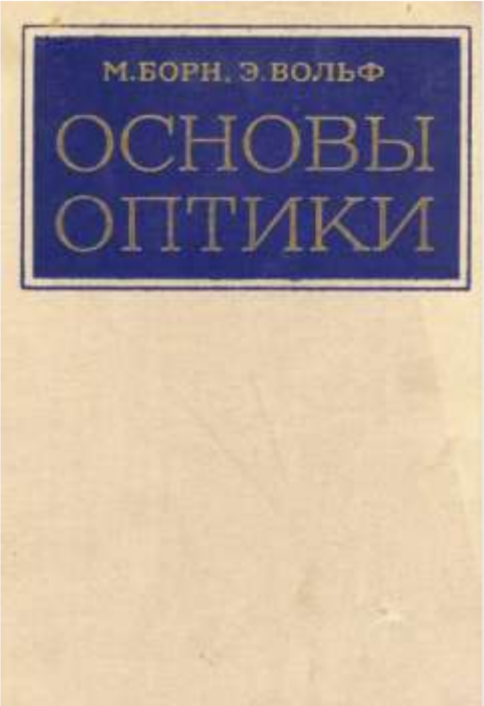
Dirac equation solution by optic eikonal method

$$\left[\Delta + p^2 - 2\varepsilon U(\vec{r})\right]\psi(\vec{r}) = \left[\Delta + p^2 n^2\right]\psi(\vec{r}) = 0$$

$$\psi(\vec{r}) = f(\vec{r})\exp\left(ip\mathfrak{I}(\vec{r})\right)$$

$$n^2 = 1 - 2\varepsilon U / p^2$$

$$\left(\vec{\nabla}\mathfrak{I}\right)^2 = n^2$$



Light rays *vs* particle trajectories

$$\left(\vec{\nabla}\Im\right)^2 = n^2 \qquad\qquad n^2 = 1 - 2\varepsilon U / p^2$$

$$\vec{s} = \frac{d\vec{r}}{d\,s} = \frac{\vec{\nabla}\Im}{\left|\vec{\nabla}\Im\right|}$$

$$n\frac{d\vec{r}}{ds} = \vec{\nabla}\Im \qquad\qquad \frac{d}{ds}\left(n\frac{d\vec{r}}{ds}\right) = \vec{\nabla}n$$

$$\varepsilon\frac{d^2\vec{r}}{d\,t^2} = -\vec{\nabla}U + \left(\vec{\upsilon}\,\vec{\nabla}U\right)\vec{\upsilon} \quad \rightarrow \qquad \varepsilon\frac{d^2\vec{r}}{dt^2} = -\vec{\nabla}U + \left(\vec{s}\,\vec{\nabla}U\right)\vec{s},$$

$$\Im\left(\vec{r}\right) = \Im\left(\vec{r}(s, s_0)\right) = \int_{s_0}^{s} n\left(\vec{r}(s')\right)ds' \approx -\int_{s_0}^{s} U\left(\vec{r}(s')\right)ds' / \upsilon$$

Pre-exponential factor in $\psi(\vec{r}) = f(\vec{r})\exp\left(ip\Im(\vec{r})\right)$

$$\frac{\partial f}{\partial s} = \frac{1}{n}\left(\vec{\nabla} f\right)\vec{\nabla}\Im = \left(\vec{\nabla} f\right)\frac{d\vec{r}}{ds} = -\frac{1}{2n} f\Delta\Im + \frac{i\Delta}{2n} f$$

$$f(\vec{\rho}, s) = \frac{p}{2\pi i s}\int \exp\left(-\frac{p}{2is}\left(\vec{\rho} - \vec{\rho}(s)\right)^2\right) f\left(\vec{\rho}_0\right) d\vec{\rho}_0$$ diffraction

$$f = \exp\left(-\frac{1}{2}\int_0^s \nabla^2\Im\, ds\right)$$ focusing / defocusing

Eikonal WF asymptotically (only!) reduces to a delta-function corresponding to the classical limit

!

$$1D:\quad \int \exp\left(i\int \left[U(x+\chi,z)-U(x-\chi,z)\right]\frac{dz}{v}\right)\exp(2iq_x\chi)d\chi =$$

$$2\pi\left(\int U^{'''}dz/v\right)^{-1/3} Ai\left(2\left(q+\int U^{'}dz/v\right)\left(\int U^{'''}dz/v\right)^{-1/3}\right)\approx \pi\delta\left(q+\int U^{'}dz/v\right)$$

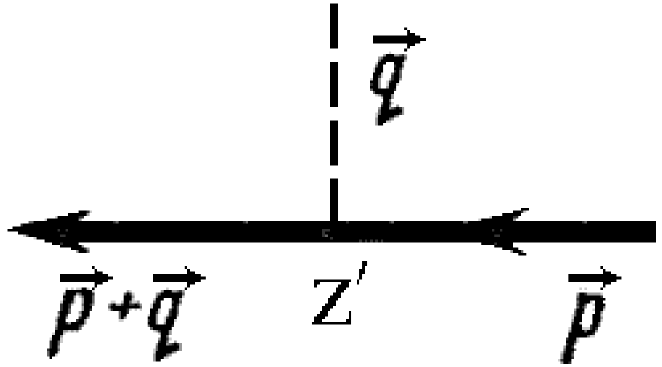
$$P_{eik}(\vec{\rho},\vec{q}_\perp,z,z_0)\approx \frac{d}{d\,\vec{q}_\perp}n\left(\vec{q}_\perp+\int_{z_0}^{z}\vec{\nabla}U(\vec{\rho},z')dz'\right)\neq n\delta\left(\vec{q}_\perp+\int_{z_0}^{z}\vec{\nabla}U(\vec{\rho},z')dz'\right)\textbf{!}$$

where $\vec{q}_\perp=-\int_{z_0}^{z}\vec{\nabla}U(\vec{\rho},z')dz'$ corresponds to classical motion

however $\vec{q}_\perp$ uncertainty is not zero !

Resulting WF undergoes factorization in the classical :

$$P(z > z', z_0, \vec{\rho}, \vec{q}_\perp) =$$



$$P_{eik}(z, z'_{+0}, \vec{\rho}, \vec{q}_\perp) \times P_{at}(\vec{\rho}(z'), \vec{q}_\perp) \times P_{eik}(z'_{-0}, z_0, \vec{\rho}, \vec{q}_\perp)$$

making it possible to introduce local WF of incoherent scattering :

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Wigner function of incoherent scattering

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Incoherent scattering contribution to radiation and pair production

Wigner function of incoherent scattering

$$P_{at}(\vec{\rho}-\vec{\rho}_{at}(z'),\vec{q}_{\perp}) \square\, P_{Born}(\vec{\rho}-\vec{\rho}_{at}(z'),\vec{q}_{\perp}) = \int \left[1 + i \int_{z'-0}^{z'+0} \delta U_{at}(\vec{\rho}+\vec{\chi}-\vec{\rho}_{at}(z'), z'') \frac{dz''}{\upsilon} \right]$$

$$\times \left[1 - i \int_{z'-0}^{z'+0} \delta U_{at}(\vec{\rho}-\vec{\chi}-\vec{\rho}_{at}(z'), z'') \frac{dz''}{\upsilon} \right] \exp(2i\vec{q}_{\perp}\vec{\chi}) \frac{d^2\chi}{\pi^2}$$

$$\frac{d\Sigma(\vec{\rho})}{d\vec{q}_{\perp}} \equiv n_{nucl}(\vec{\rho}) \frac{d\sigma(\vec{\rho})}{d\vec{q}_{\perp}} = \frac{1}{n_p}\frac{d}{dz}\frac{dn_p(\vec{\rho})}{d\vec{q}_{\perp}} = \int \left[P_{at}(z',\vec{\rho}-\vec{\rho}_{at},\vec{q}_{\perp}) - 1 \right] \exp\left(-\frac{\rho_{at}^2}{2u_1^2} \right) \frac{d^2\rho_{at}}{2\pi u_1^2 d}$$

$$= \left(\frac{2Z\alpha}{\pi v} \right)^2 \frac{1}{d} \int_{-\infty}^{\infty} \cos(2\vec{\kappa}\vec{\rho}) \frac{\exp(-2\kappa^2 u_1^2) - \exp[-(q^2+\kappa^2)u_1^2]}{[(\vec{q}+\vec{\kappa})^2+\kappa_s^2][(\vec{q}-\vec{\kappa})^2+\kappa_s^2]} d\vec{\kappa}$$

Single nucleus limit $q_{\perp} >> \hbar / u_1$

$$\frac{d\Sigma(\vec{\rho})}{d\vec{q}_{\perp}} \;\to\; n_{nucl}(\vec{\rho}) \frac{d\sigma_{Mott}(\mathrm{q}_{\perp})}{d\vec{q}_{\perp}} = \left(\frac{2Z\alpha}{v q^2} \right)^2 \frac{1}{2\pi u_1^2 d_{inat}} \exp\left(-\frac{\rho^2}{2u_1^2} \right)$$

Essential expression of the presentation

$$\frac{d\Sigma(\vec{\rho})}{d\vec{q}_\perp} \equiv \frac{d}{dz}\frac{dn(\vec{\rho})}{n\,d\vec{q}_\perp} = \left(\frac{2Z\alpha}{\pi\upsilon}\right)^2 \frac{1}{d} \times$$

$$\int \cos(2\vec{\kappa}\vec{\rho}) \frac{\exp(-2\kappa^2 u_1^2) - \exp[-(q^2+\kappa^2)u_1^2]}{[(\vec{q}+\vec{\kappa})^2+\kappa_s^2][(\vec{q}-\vec{\kappa})^2+\kappa_s^2]}\, d\vec{\kappa}$$

describes Coulomb scattering by nonuniformly distributed screened nuclei

$$\frac{d\Sigma(\vec{\rho})}{d\vec{q}_\perp} \equiv \frac{d}{dz}\frac{dn(\vec{\rho})}{n\,d\vec{q}_\perp} = \left(\frac{2Z\alpha}{\pi\upsilon}\right)^2 \frac{1}{d} \times$$

$$\int \cos(2\vec{\kappa}\vec{\rho}) \frac{\exp(-2\kappa^2 u_1^2) - \exp[-(q^2+\kappa^2)u_1^2]}{[(\vec{q}+\vec{\kappa})^2+\kappa_s^2][(\vec{q}-\vec{\kappa})^2+\kappa_s^2]}\, d\vec{\kappa}$$

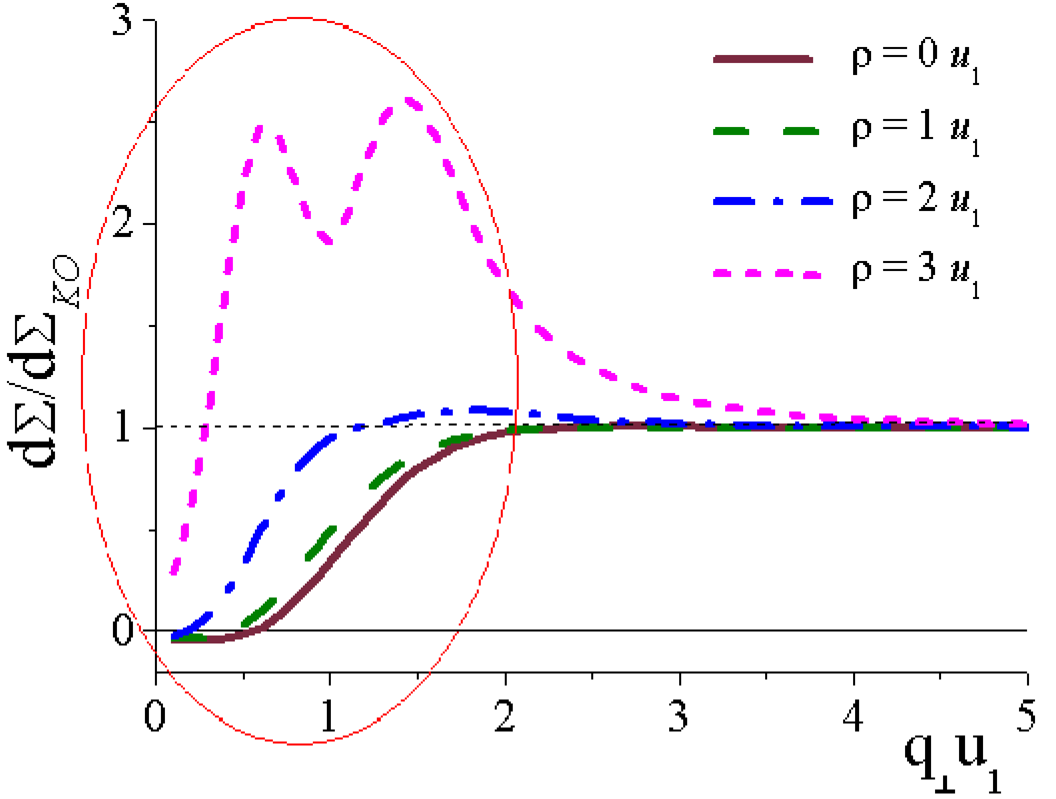
versus

$$d\Sigma_{KO} \equiv n(\rho)\cdot d\sigma(\vec{q}_\perp) =$$

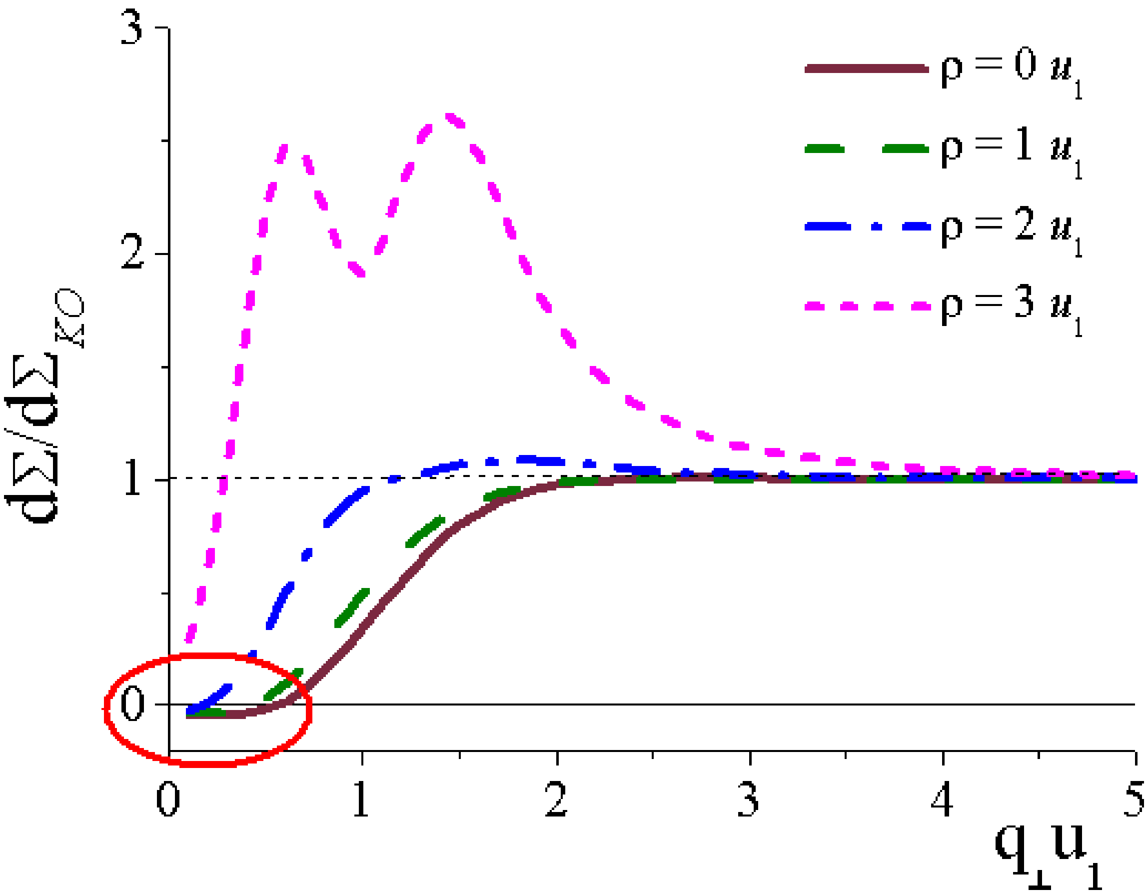
$$\frac{\exp\left(-\rho^2/2u_1^2\right)}{2\pi u_1^2} \times \frac{4\alpha^2 Z^2 d\,\vec{q}_\perp}{\left(q_\perp^2 + \hbar^2/a_F^2\right)^2}$$

New Wigner function

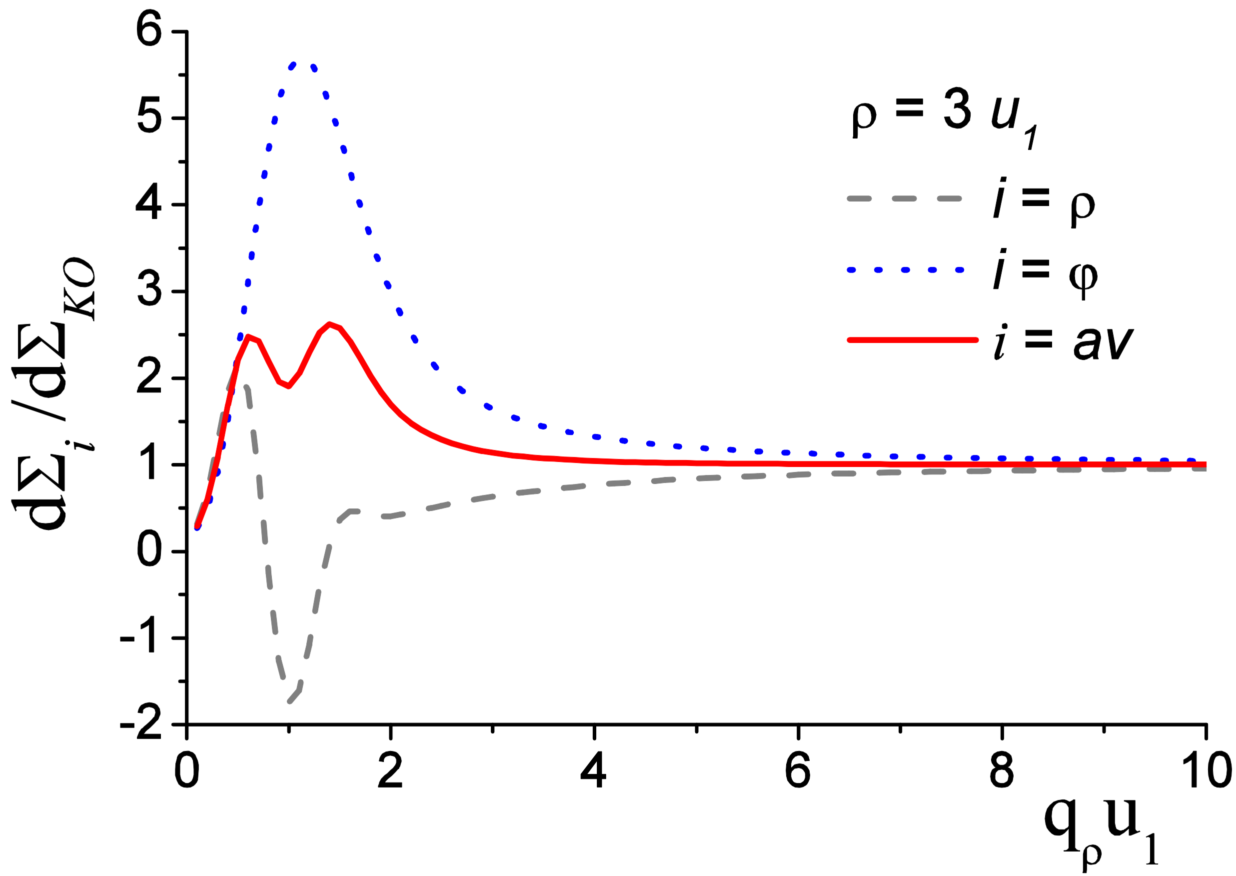
greatly differs from KO at $q_\perp$ about u_1



WF can be negative 1



WF can be negative 2



WF completely looses probabilistic interpretation

at $q_\perp \sim u_1, \quad \rho > 2.5\, u_1$ (< 5 % of particles)

All the effects of

small angle incoherent scattering

boils down

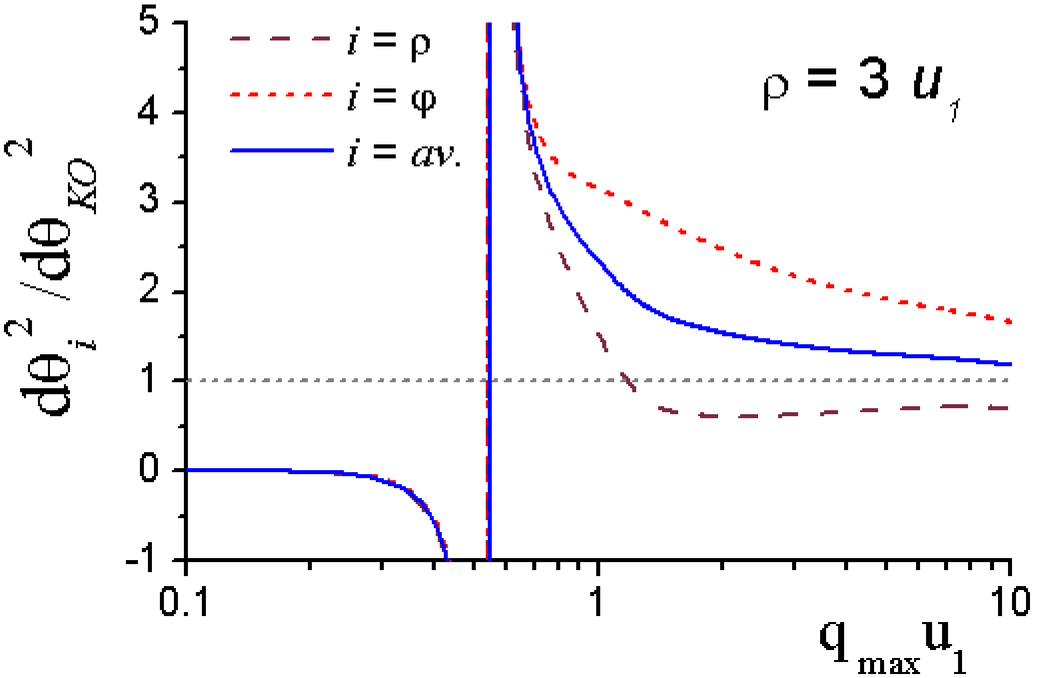
to the **average square**

of the scattering angle

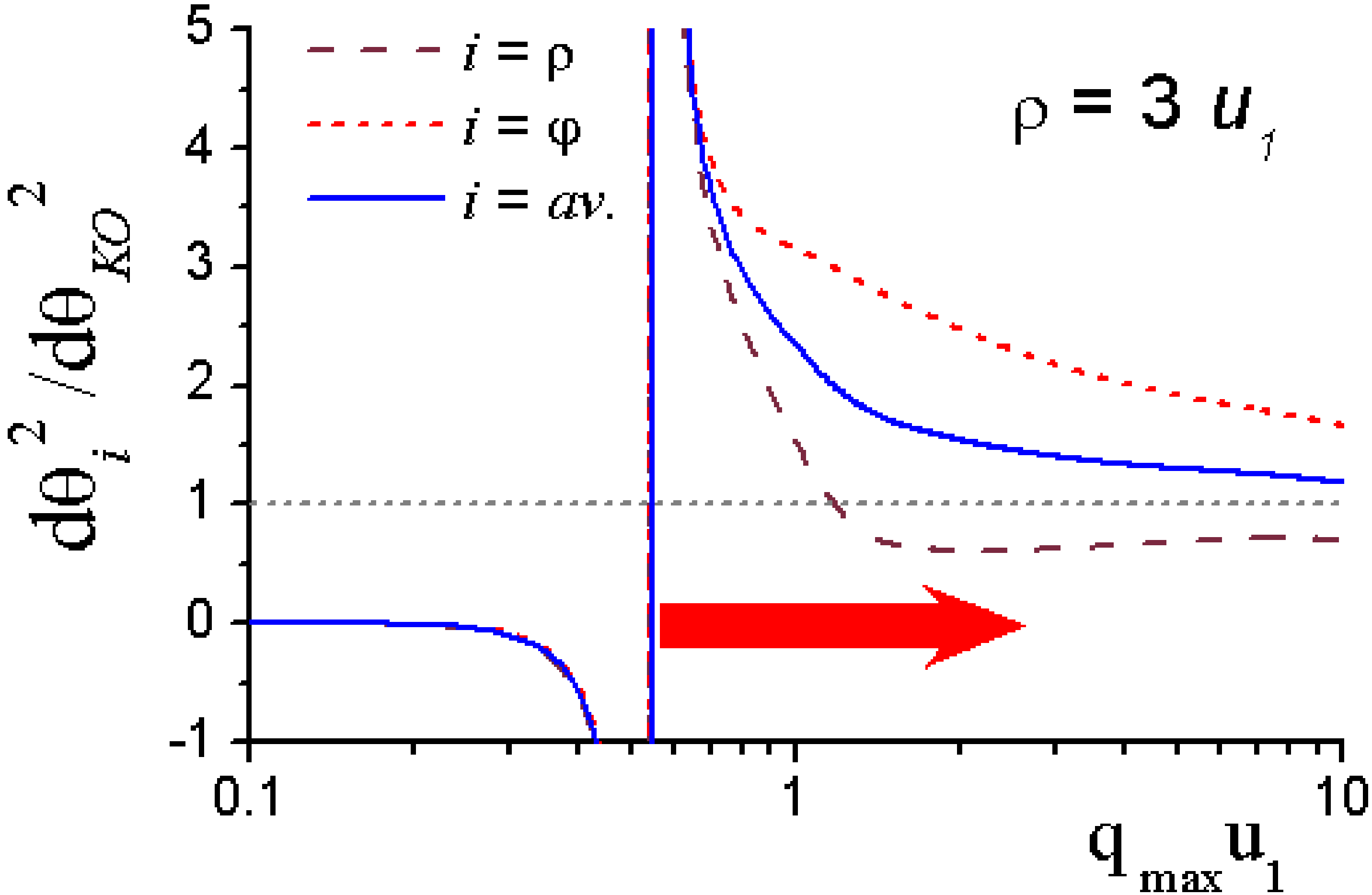
$$\frac{d\theta^2_{\rho,\varphi}(\vec{\rho})}{dz} = \int_{q<q_{\max}} \frac{d\Sigma(\vec{\rho})}{d\vec{q}_\perp} \frac{q^2_{\rho,\varphi}}{p^2} d\vec{q}$$

.. which WF allows one to readily evaluate

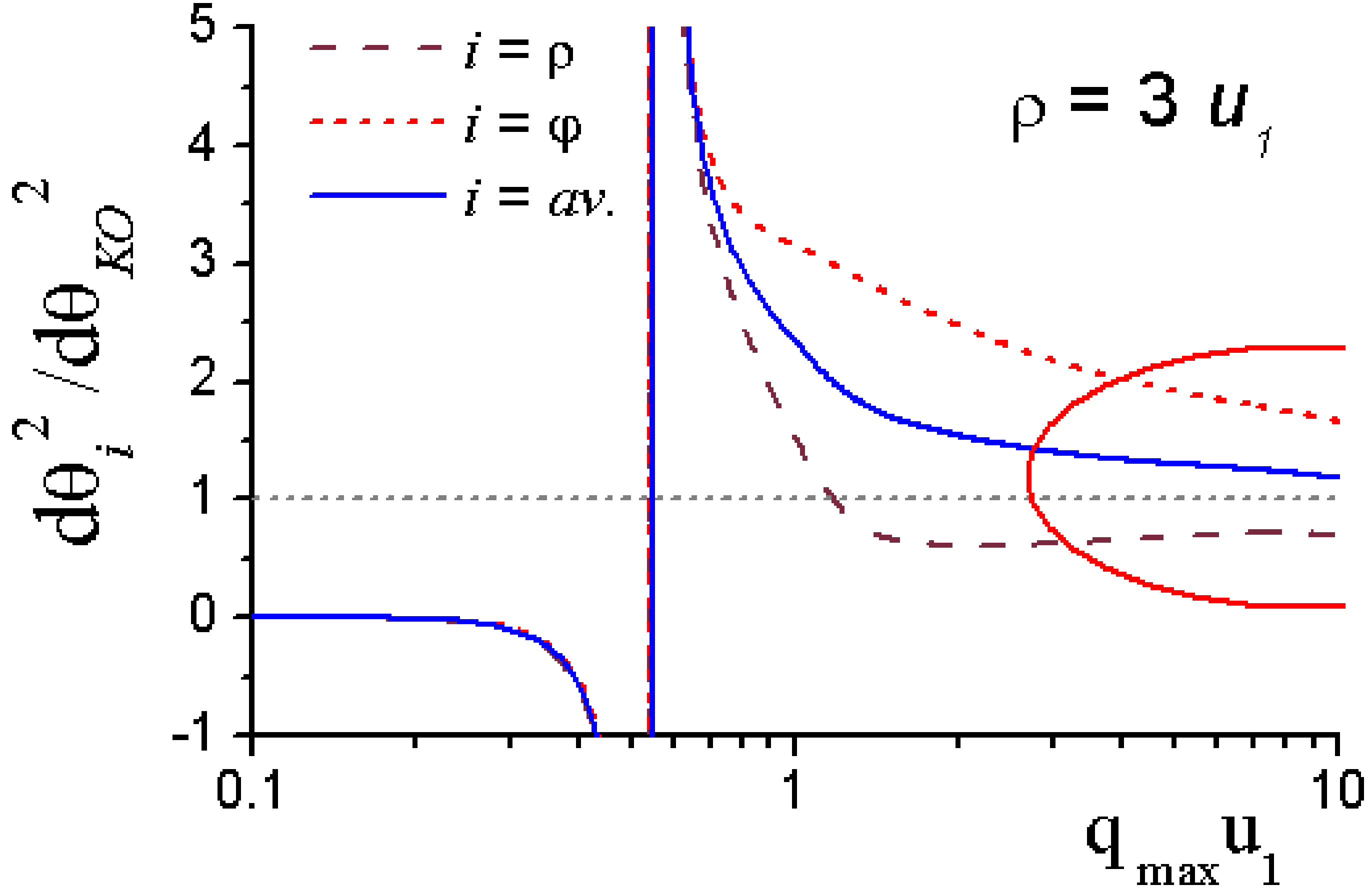
$$\frac{d\theta^2_{\rho,\varphi}(\vec{\rho})}{dz} = \int\limits_{q<q_{\max}} \frac{d\Sigma(\vec{\rho})}{d\vec{q}_\perp} \frac{q^2_{\rho,\varphi}}{p^2} d\vec{q}$$



Average scattering angle **square** becomes **positively** determined at small momentum transfer



Average scattering angle square considerable **exceeds KO** limit at large q and ρ



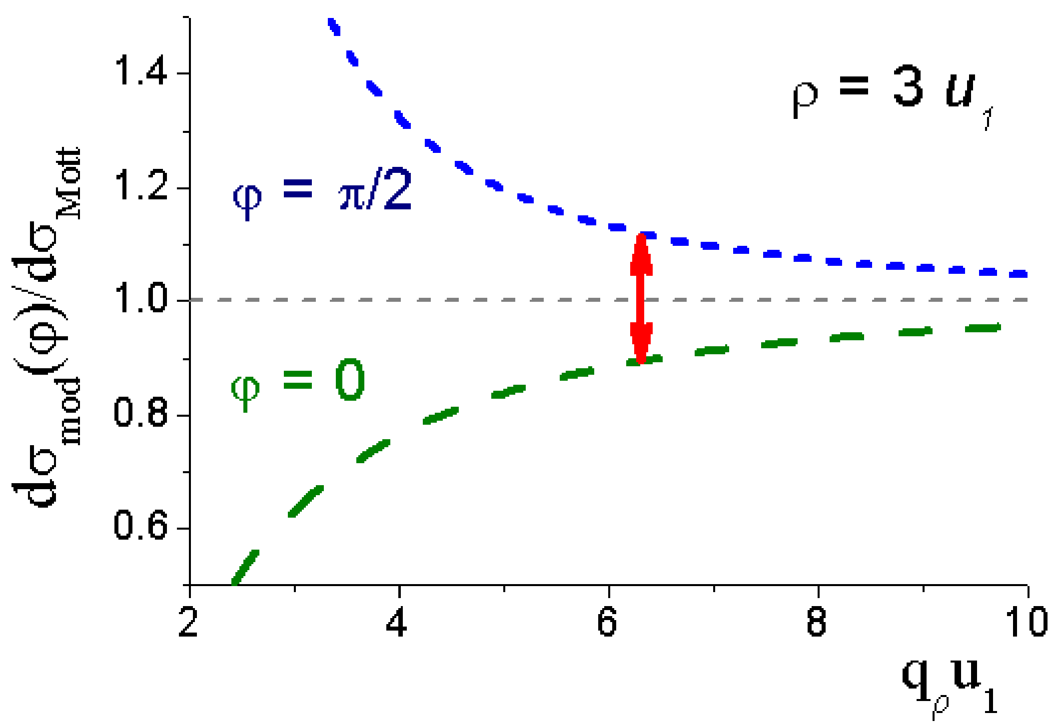
WF high $q_\perp$ Mott limit:

$$d\Sigma \xrightarrow{q_\perp \gg \frac{\hbar}{u_1}} d\Sigma_{KO}$$

$$\equiv n_{nucl}(\rho)\cdot d\sigma(\vec{q}_\perp) = \frac{\exp\left(-\rho^2/2u_1^2\right)}{2\pi u_1^2} \times \frac{4\alpha^2 Z^2 d\,\vec{q}_\perp}{\left(q_\perp^2 + \hbar^2/a_F^2\right)^2}$$

Mott cross section modification by nonuniformity of string atom distribution

$$d\sigma_{\text{mod}} = d\sigma_{Mott}\left\{1-\frac{\rho^2}{2q^2u_1^4}\exp\left(-\frac{\rho^2}{2u_1^2}\right)\left[2(\vec{q}\vec{\rho})^2/\rho^2p^2-1\right]+..\right\}$$



Plan

Intoduction. *The need of quantum theory of incoherent scattering in crystals*

Wigner function description of both quantum and classical effects

– *classical motion description by eikonal method*

– *quantum scattering description in Born approximation*

Wigner function of incoherent scattering

– *small angle scattering description by averaged angle*

– *large angle scattering description by Moss cross-section modification*

Incoherent scattering contribution to radiation and pair production

Development of the consistent **theory** of relativistic particle incoherent scattering in crystals will mean the same for **radiation** and **pair production** processes

Key points

Radiation (pair production),

accompanying single scattering:

− has to be simulated separately

− is suppressed by coherent scattering;

coherent scattering also suppresses

Landau-Pomeranchuk effect

Key simulation points:

Trajectory simulations in most **realistic potentials**

Simulation of **incoherent scattering** on both nuclei and electrons

Separate simulation of **single** and **multiple** scattering

Direct integration of **Baier-Katkov formula**

Infinite trajectories, **density** effect…

Radiation process simulations from the *"First Principles"*

The general expression for radiation intensity

$$\frac{d^2I}{d\omega d^2\theta} = \frac{\alpha\omega^2 d\omega}{8\pi^2\varepsilon'^2} \times \int\int dt_1 dt_2 \left[(\varepsilon^2+\varepsilon'^2)(\mathbf{v}_\perp(t_1)-\boldsymbol{\theta})(\mathbf{v}_\perp(t_2)-\boldsymbol{\theta})+\omega^2/\gamma^2\right]$$

$$\exp\left\{i\frac{\omega\varepsilon}{2\varepsilon'}\left[\int_{-\infty}^{t_1}\left(\gamma^{-2}+(\mathbf{v}_\perp(t')-\boldsymbol{\theta})^2\right)dt' + \int_{-\infty}^{t_2}\left(\gamma^{-2}+(\mathbf{v}_\perp(t'')-\boldsymbol{\theta})^2\right)dt''\right]\right\}$$

contains two integrals

$$A = \int \exp\left\{i\frac{\omega\varepsilon}{2\varepsilon'}\int_{-\infty}^{t}\left[\gamma^{-2}+(\mathbf{v}_\perp(t')-\boldsymbol{\theta})^2\right]dt'\right\}dt,$$

$$\mathbf{B} = \int (\mathbf{v}_\perp(t)-\boldsymbol{\theta})\exp\left\{i\frac{\omega\varepsilon}{2\varepsilon'}\int_{-\infty}^{t}\left[\gamma^{-2}+(\mathbf{v}_\perp(t')-\boldsymbol{\theta})^2\right]dt'\right\}dt$$

and slowly decreases with radiation angle $\boldsymbol{\theta}$, complicating its numerical integration.

Radiation at sharp change of particle trajectory

$$\frac{d\mathcal{E}}{d\omega do} = \frac{e^2}{4\pi^2 c}[\boldsymbol{k}, \boldsymbol{I}]^2,$$

$$\boldsymbol{I} = \frac{ic}{\omega}\int_{-\infty}^{\infty} dt\, e^{i(\omega/c)[ct-\boldsymbol{n}\cdot\boldsymbol{r}(t)]}\frac{d}{dt}\frac{\boldsymbol{v}(t)}{c-\boldsymbol{n}\cdot\boldsymbol{v}(t)}.$$

$$\boldsymbol{I} \approx \frac{ic}{\omega}\left(\frac{\boldsymbol{v}'}{c-\boldsymbol{n}\cdot\boldsymbol{v}'} - \frac{\boldsymbol{v}}{c-\boldsymbol{n}\cdot\boldsymbol{v}}\right),$$

$$\frac{d\mathcal{E}}{d\omega} = \frac{2e^2}{\pi c}\left(\frac{2\xi^2+1}{\xi\sqrt{\xi^2+1}}\ln\left(\xi+\sqrt{\xi^2+1}\right)-1\right).$$

Single scattering effects are treated separately

$$A = \int_{-\infty}^{\infty} \exp\{i\varphi(t)\}dt = \frac{i}{\dot{\varphi}(+0)} - \frac{i}{\dot{\varphi}(-0)} +$$

$$i\sum_{i=1}^{N} \left\{\left[\frac{1}{\dot{\varphi}(t_i+0)} - \frac{1}{\dot{\varphi}(t_i-0)}\right] \exp i\varphi(t_i) - \frac{2\ddot{\varphi}(\bar{t}_i)}{\dot{\varphi}^3(\bar{t}_i)} \sin\left[\frac{\varphi(t_i-0)-\varphi(t_{i-1}+0)}{2}\right] \exp i\varphi(\bar{t}_i)\right\},$$

$$\vec{B} = \int_{-\infty}^{\infty} \left[\vec{v}_\perp(t) - \vec{\theta}\right] \exp\{i\varphi(t)\}dt = \left[\frac{i}{\dot{\varphi}(+0)} - \frac{i}{\dot{\varphi}(-0)}\right] \left(\vec{v}_\perp(0) - \vec{\theta}\right) +$$

$$i\sum_{i=1}^{N} \left\{ \begin{array}{l} \left[\frac{\vec{v}_\perp(t_i)+\vec{\vartheta}_i-\vec{\theta}}{\dot{\varphi}(t_i+0)} - \frac{\vec{v}_\perp(t_i)-\vec{\theta}}{\dot{\varphi}(t_i-0)}\right] \exp i\varphi(t_i) - \\ \frac{2}{\dot{\varphi}^2(\bar{t}_i)} \left[\dot{\vec{v}}_\perp(\bar{t}_i) - \left(\vec{v}_\perp(\bar{t}_i) - \vec{\theta}\right) \frac{\ddot{\varphi}(\bar{t}_i)}{\dot{\varphi}(\bar{t}_i)}\right] \sin\left[\frac{\varphi(t_i-0)-\varphi(t_{i-1}+0)}{2}\right] \exp i\varphi(\bar{t}_i) \end{array} \right\},$$

where $\omega' = \varepsilon/(\varepsilon - \omega)$, $\ddot{\varphi}(t) = \omega'\left(\vec{v}_\perp(t_i) - \vec{\theta}\right) \dot{\vec{v}}_\perp(t)$ and $\bar{t}_i = (t_i + t_{i-1})/2$.

Both surface and refraction effects can be easily included

derivatives of the phase $\varphi(t)$ on the left and on the right of the entrance crystal surface

$$\dot\varphi(-0) = \frac{\omega'}{2}\left[\gamma^{-2} + \left(\vec v_\perp(0) - \vec\theta\right)^2\right],$$

$$\dot\varphi(+0) = \frac{\omega'}{2}\left[\gamma^{-2} + \omega_p^2/\omega^2 + \left(\vec v_\perp(0) - \vec\theta\right)^2\right];$$

on the left and on the right of each inter-step border

$$\dot\varphi(t_i - 0) = \frac{\omega'}{2}\left[\gamma^{-2} + \omega_p^2/\omega^2 + \left(\vec v_\perp(t_i) - \vec\theta\right)^2\right],$$

$$\dot\varphi(t_i + 0) = \frac{\omega'}{2}\left[\gamma^{-2} + \omega_p^2/\omega^2 + \left(\vec v_\perp(t_i) + \vec\vartheta_i - \vec\theta\right)^2\right];$$

and on the right from the exit surface

$$\dot\varphi(t_N + 0) = \frac{\omega'}{2}\left[\gamma^{-2} + \left(\vec v_\perp(T) + \vec\vartheta_N - \vec\theta\right)^2\right].$$

Local approximation, axial case with incoherent scattering for $\vartheta_s(l_{coh}) < m/\varepsilon$

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On the theory of electron-positron pair production in crystals

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Abstract. — The theory describing both coherent and incoherent radiational processes when energetic γ-quanta, electrons or positrons move through crystals in directions nearly parallel to the crystal axes or planes is presented. It is shown that, within the logarithmic approximation, the local probabilities of incoherent radiation processes are proportional to the cross-sections of the same processes pertaining to a separate nucleus placed in a uniform field. When the coherent pair production rate increases, the total probability of incoherent pair production starts to decrease proportionally to the γ-quantum energy to the $-2/3$ power.

Single vs multiple scattering

Multiple

$$\mathbf{v} = v\mathbf{n}(1 - \mathbf{v}_\perp^2(\tau)/2) + \mathbf{v}_\perp(\tau),$$
$$\mathbf{v}_\perp(\tau) = \boldsymbol{\theta} + \mathbf{w}\tau + \delta\mathbf{v}(\mathbf{r} + \mathbf{n}v\tau), \qquad (13)$$

$$|\delta\mathbf{v}| < \vartheta_s(l_{coh}) = (\sigma_s l_{coh})^{1/2}, \qquad (4)$$

$$\left\langle \left(\int_0^\tau \delta\mathbf{v}_\perp \, d\tau' \right)^2 \right\rangle = \sigma_s \tau^2 |\tau|/3, \qquad (19)$$

$$\sigma_s = \sigma_s(\boldsymbol{\rho}) = 8\pi n(\boldsymbol{\rho}) \left(\frac{Ze^2}{\varepsilon_\pm} \right)^2 \underline{\ln(\vartheta_{max}/\vartheta_{min})} \qquad (5)$$

$$\frac{dW_{\mathcal{E},s}}{d\varepsilon_+} = \frac{dW_{\mathcal{E}}}{d\varepsilon_+} + \sigma_s \frac{\alpha \varepsilon_+^2 \, d\varepsilon_+}{30\pi m^2 \omega} F(x, \varepsilon_+/\omega), \qquad (22)$$

Single

$$\delta\mathbf{v}(t) = \begin{cases} \boldsymbol{\vartheta}, & t \geqslant 0, \\ 0, & t < 0, \end{cases} \qquad (26)$$

$$|\boldsymbol{\vartheta}| > \vartheta_s(l_{coh})$$

$$d\sigma(\boldsymbol{\vartheta}) = 8\pi \left(\frac{Z\alpha}{\varepsilon_+} \right)^2 \frac{d\boldsymbol{\vartheta}}{\vartheta^3} \qquad (28)$$

$$\sigma_Z = 8\pi n(\boldsymbol{\rho}) \left(\frac{Ze^2}{\varepsilon_\pm} \right)^2 \underline{\ln(\vartheta_{\mathcal{E}}/\vartheta_{max})}. \qquad (30)$$

$$\frac{dW_{Z,\mathcal{E}}}{d\varepsilon_+} = \sigma_Z \frac{\alpha \varepsilon_+^2 \, d\varepsilon_+}{30\pi m^2 \omega} F(x, \varepsilon_+/\omega), \qquad (29)$$

$$F(x, \varepsilon_+/\omega) = (x^4 Y - 3x^2 Y' - x^3) + (x^4 Y + 3xY - 5x^2 Y' - x^3)(\varepsilon_+^2 + \varepsilon_-^2)/\omega^2,$$

$$Y(x) = \int_0^\infty \sin(ux + u^3/3)\, du, \qquad x = (m^3 \omega / e\mathcal{E}\varepsilon_+ \varepsilon_-)^{2/3}, \quad \kappa = e\mathcal{E}\omega/m^3, \qquad Y'' - xY = -1.$$

Pair production probability in crystals

$$\frac{dW_{\text{loc}}(\boldsymbol{\rho})}{d\varepsilon_+} = \frac{dW_{\mathcal{E},s}}{d\varepsilon_+} + \frac{dW_{Z,\mathcal{E}}}{d\varepsilon_+} = \frac{dW_{\mathcal{E}}}{d\varepsilon_+} + \sigma \frac{\alpha \varepsilon_+^2 \, d\varepsilon_+}{30 \, \pi m^2 \omega} F(x, \varepsilon_+/\omega),$$

$$\sigma = \sigma(\boldsymbol{\rho}) = \sigma_s + \sigma_Z = 8 \pi n(\boldsymbol{\rho}) \left(\frac{Z\alpha}{\varepsilon_+} \right)^2 \ln(\vartheta_{\mathcal{E}}/\vartheta_{\min}).$$

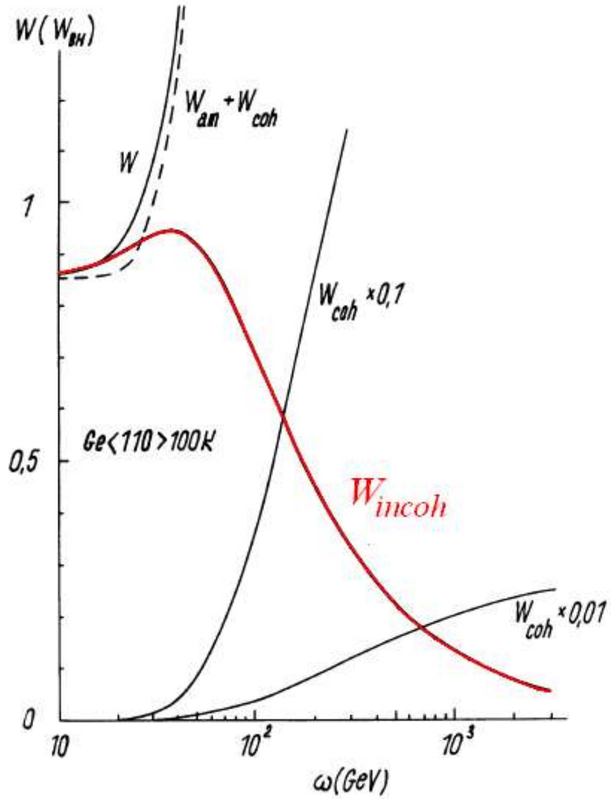
low energy limit:

$$\frac{dW_{\text{am}}}{d\varepsilon_+} = \frac{\ln(183 Z^{-1/3}) - B}{\ln(183 Z^{-1/3})} \cdot \frac{dW_{\text{BH}}}{d\varepsilon_+}, \quad 2B = (1+y)\exp(y) \int_y^\infty \exp(-t) \frac{dt}{t} - 1, \quad y = u^2/a_F^2$$

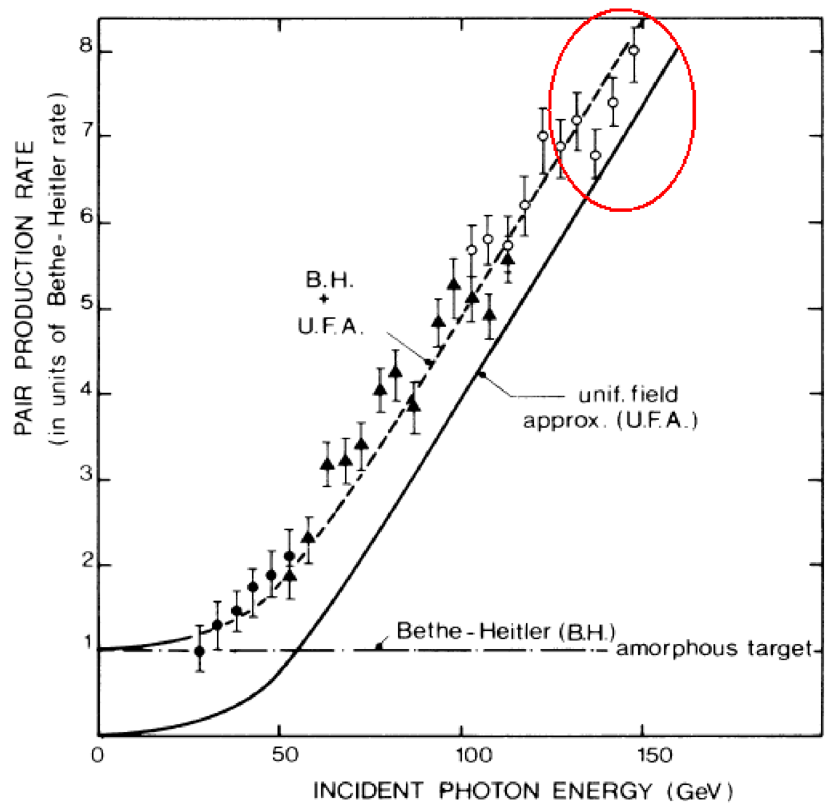
$$\frac{dW_{\text{loc}}(\rho)}{d\varepsilon_+} = \frac{dW_{\mathcal{E}}(\mathcal{E}(\rho))}{d\varepsilon_+} + \frac{2\alpha^3 Z^2 n(\rho)}{15 m^2 \omega} \left[2\ln(183 Z^{-1/3}) - \theta(1-x)\ln x + 1 - (1+y) \times \right.$$
$$\left. \times \exp(y) \int_y^\infty \exp(-t) \frac{dt}{t} \right] [(x^4 Y - 3x^2 Y' - x^3) + (x^4 Y + 3xY - 5x^2 Y' - x^3)(\varepsilon_+^2 + \varepsilon_-^2)/\omega^2],$$

$$\frac{dW}{d\varepsilon_+} = n_0 d \int \frac{dW_{\text{loc}}(\mathcal{E}(\rho), n(\rho))}{d\varepsilon_+} d^2\rho$$

Local approximation, axial case with incoherent scattering:



Coherent and incoherent PP in Ge<110>100K



Experiment on PP in Ge<110>100K

Landau-Pomeranchuk effect suppression by strong crystalline field $\vartheta_s(l_{coh}) > m/\varepsilon$

$$\frac{dW}{d\omega}=\frac{ie^2}{2\pi}\int\limits_{-\infty}^{\infty}\left[\frac{m^2}{\varepsilon^2}+\frac{(\varepsilon^2+\varepsilon'^2)}{4\varepsilon\varepsilon'}\vartheta^2(\tau)\right]\exp(-ia\tau)$$

$$\times\prod_{i=x,y}\exp\left\{\frac{ib}{2}\left[\frac{1}{\tau}\left(\int\limits_0^\tau dt\,\vartheta_i(t)\right)^2-\int\limits_0^\tau dt\,\vartheta_i^2(t)\right]\right\}\frac{d\tau}{\tau},$$

$$a=m^2\omega/2\varepsilon\varepsilon',\quad b=\omega\varepsilon/\varepsilon'.$$

$$d^2\mathcal{P}_N=\frac{d\vartheta_1\ldots d\vartheta_N}{(2\pi\Delta(\sigma_x\sigma_y)^{1/2})^N}\exp\left\{-\left[\frac{(\vartheta_{1x}-w\Delta)^2}{2\sigma_x\Delta}+\frac{\vartheta_{1y}^2}{2\sigma_y\Delta}\right]\right.$$
$$\left.-\ldots-\left[\frac{(\vartheta_{Nx}-w\Delta-\vartheta_{N-1\,x})^2}{2\sigma_x\Delta}+\frac{(\vartheta_{Ny}-\vartheta_{N-1\,y})^2}{2\sigma_y\Delta}\right]\right\}.\quad(9)$$

$$\left\langle\frac{dW}{d\omega}\right\rangle=\int d_w{}^2\vartheta\,\frac{dW\{\vartheta(z)\}}{d\omega}=\lim_{N\to\infty}\int\limits_{-\infty}^{\infty}\ldots\int d^2\mathcal{P}_N\frac{dW\{\vartheta(z)\}}{d\omega},\quad(10)$$

$$\left\langle\frac{dW}{d\omega}\right\rangle=-\frac{e^2}{\pi}\operatorname{Im}\int\limits_0^\infty\left\{\frac{m^2}{\varepsilon^2}+\frac{(\varepsilon^2+\varepsilon'^2)}{2\varepsilon\varepsilon'}\left[\frac{2w^2}{r_x^2}\operatorname{th}^2\left(\frac{r_xz}{2}\right)\right.\right.$$
$$\left.\left.+\sum_{i=x,y}\frac{\sigma_i}{r_i}\operatorname{th}\left(\frac{r_iz}{2}\right)\right]\right\}$$
$$\times\left(\frac{r_xr_y}{\operatorname{sh}r_xz\operatorname{sh}r_yz}\right)^{1/2}\exp\left\{-iaz-\frac{w^2z}{2\sigma_x}+\frac{w^2}{r_x\sigma_x}\operatorname{th}\left(\frac{r_xz}{2}\right)\right\}dz.\quad(16)$$

Landau-Pomeranchuk effect suppression by strong crystalline field

generalizes the expression obtained by Migdal for description of the Landau-Pomeranchuk effect for the probability of emission of a γ ray by $e^{\pm}$ moving in an amorphous beam, and the Klepikov-Nikishov-Ritus expression for the probability of emission of a γ ray by $e^{\pm}$ moving in a uniform electromagnetic field.

$$\left\langle \frac{dW}{d\omega} \right\rangle = -\frac{e^2}{\pi} \operatorname{Im} \int_0^\infty \left\{ \frac{m^2}{\varepsilon^2} + \frac{(\varepsilon^2+\varepsilon'^2)}{2\varepsilon\varepsilon'} \left[\frac{2w^2}{r_x^2} \operatorname{th}^2\left(\frac{r_x z}{2}\right) + \sum_{i=x,y} \frac{\sigma_i}{r_i} \operatorname{th}\left(\frac{r_i z}{2}\right) \right] \right\} \times \left(\frac{r_x r_y}{\operatorname{sh} r_x z \operatorname{sh} r_y z} \right)^{1/2} \exp\left\{ -iaz - \frac{w^2 z}{2\sigma_x} + \frac{w^2}{r_x \sigma_x} \operatorname{th}\left(\frac{r_x z}{2}\right) \right\} dz. \quad (16)$$

The role of incoherent scattering in radiation processes at small angles of incidence of particles on crystallographic axes or planes

V. G. Baryshevskiĭ and V. V. Tikhomirov

Zh. Eksp. Teor. Fiz. **90**, 1908–1921 (June 1986)

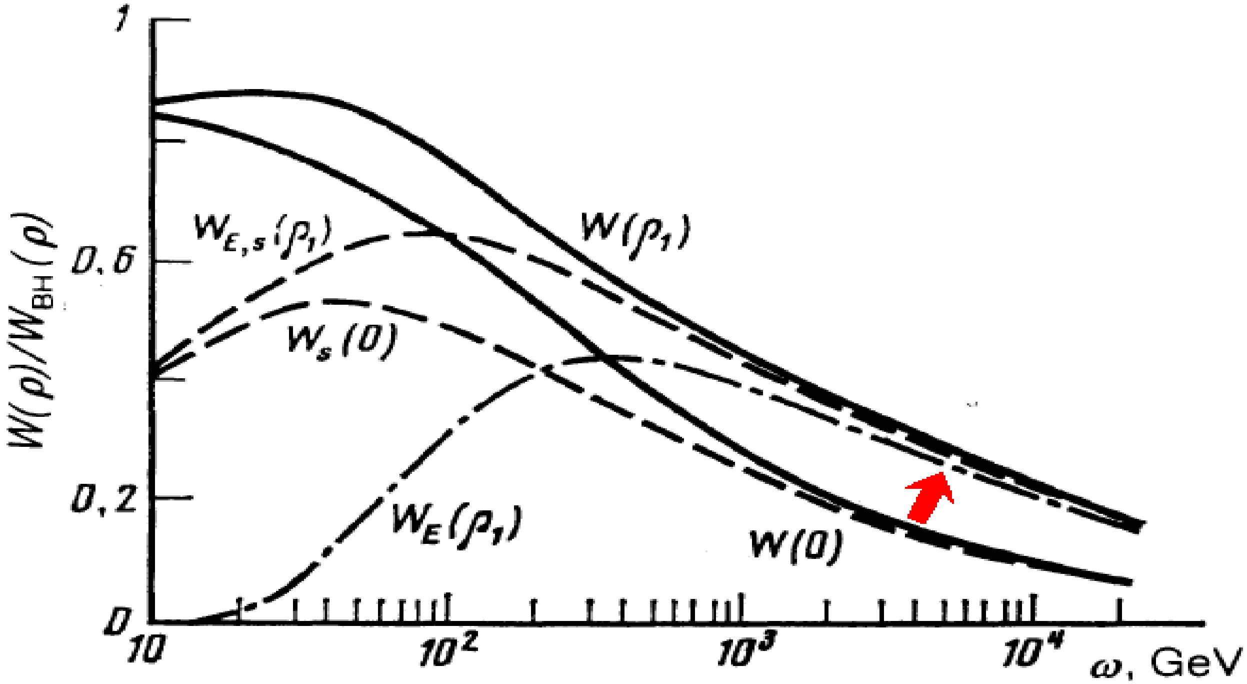


FIG. 2. Pair-production probability obtained after transition to the cross channel and integration over the energy of the e^+ (e^-) in the expressions (18), (22), and (33). The approach of the probability $W(\rho_1)$ to the probability $W_E(\rho_1)$ (and not to the probability $W_s(n(\rho_1)) \approx W_s(n(0))$ (see Eq. (24)) illustrates the absence of the Landua-Pomeranchuk effect.

A consistent theory

of relativistic particle

incoherent scattering

in crystals is suggested

Thank you for your attention!