Relativistic particle incoherent scattering in oriented crystals

Victor V. Tikhomirov

Research Institute for Nuclear Problems,
Belarusian State University, Minsk, Belarus

(Dated: April 14, 2020)

Abstract

The coherent process of particle deflection by aligned atomic strings and planes of oriented crystals is accompanied by the incoherent scattering by atomic cores. While the coherent particle deflection, described by the axial or planar averaged potential, becomes more and more classical, the incoherent scattering remains essentially quantum at relativistic energies. Though the latter reminds the scattering by atoms of amorphous medium at high enough momentum transfers, at the smallest ones the incoherent scattering process in crystals experiences some modification by the influence of the inhomogeneity of the atom distribution in the plane, normal to the crystal axis or plane. Considering the axial case as a more general example, we present a consistent theory of high energy particles incoherent scattering in oriented crystals. The latter takes into consideration both the quantum scattering nature and the atom distribution inhomogeneity, revealing a limited applicability of the scattering cross section notion. A way to incorporate the quantum scattering features into the widely used classical trajectory simulations is elaborated using a specific mean square scattering angle definition.

PACS numbers: 61.85.+p,12.20.Ds
I. INTRODUCTION

High energy particle interaction with oriented crystals makes it possible both to observe many remarkable phenomena and apply them to develop diverse sources of x- and gamma-radiation [1–3], to efficiently deflect high energy particle beams [4–6], to measure and even to modify elementary particle properties, such as magnetic momenta [1], to reduce the thickness of particle detectors as well as to make the latter sensitive to both direction and polarization [7–10]. All the pronounced effects, induced by the coherent particle interaction with oriented crystal lattice, are described by the averaged (continuum) potential of atomic strings/planes [11, 12] introduced by J. Lindhard, who also proved that the particle motion in the averaged potential can be treated classically at high enough energy.

Despite the large strength of the coherent effects in crystals, all their applications are essentially limited by the incoherent scattering effects relational, but not completely similar to the scattering process in amorphous media or randomly oriented crystals. Most severely incoherent scattering by nuclei limits the deflection of negatively charged particles by bent crystals [13, 14] as well as both the channeling [1–3] and crystal undulator [1, 15–17] radiation of the same. That is why, to consider any application of the coherent effects in crystals, it is mandatory both to understand and properly treat the incoherent ones. However neither a consistent theory, nor a commonly recognized view on the nature of high energy particle incoherent scattering still exist.

Channeling effect study began from the classical particle motion simulations by binary collision method [18]. Being correct for MeV-energy ions, the latter is inapplicable in relativistic case, as, following [11, 19–21], we remind in Section 2. This way both a fundamental problem and practical necessity of treating quantum effects in the incoherent scattering of high energy particles, moving along classical trajectories in the averaged crystal potential, arise. Following [22], the multiple scattering theory in homogeneous medium was initially applied [23] to sample the angles of classically moving particle scattering on the atomic planes. However this approach was not completely satisfactory since the plane/string atomic density is strongly inhomogeneous at the scale of \( u_1 < 0.1 \text{Å} \), which makes it inadequate to use a fixed density value for impact parameters \( b \) from the interval \( u_1 \leq b \leq R \), where 0.1 Å < \( R \leq 0.5 \text{Å} \) are atomic radii.

The recently observed [24] influence of crystal atom density inhomogeneity on incoherent
particle scattering was predicted along with the development of coherent bremsstrahlung theory [25], which also described the incoherent radiation and pair production reduction, caused by the same of incoherent scattering. Being developed in the quantum nature plane wave [25] and reproduced in the classical straight-line approximations [2, 3], coherent bremsstrahlung theory remains valid at particle incident angles, at least, a few times exceeding the critical channeling angle, involving only the incoherent scattering intensity averaged over the uniform particle flux implied by both approximations.

However, at channeling and close to channeling conditions, particles spend different time at different locations in the plane of transverse motion or even do not reach some of them at all. The uniform flux approximation, accordingly, loses its applicability, making necessary to describe incoherent particle scattering at each point individually, taking into consideration the scattering by nuclei at the far distances $R > u_1$ from the trajectory. This problem, in principle, is solved by the full quantum treatment of transverse particle motion [26, 27], which, in fact, is both really necessary and practically feasible only at the electron and positron energies of a few dozen MeV and less. However most of the current investigations are conducted at GeV [13, 14, 28] and higher [1–10, 15–17, 29–35] energies, at which the quantum description of particle motion in the averaged crystal field becomes both redundant and cumbersome, revealing the necessity of the introduction of classical particle motion features into the treatment of their incoherent scattering by the inhomogeneously distributed nuclei. Till now, a redefinition of the scattering impact parameter upper limit $R \to u_1$ [29–32, 36] has been used, which did not take into consideration the incoherent scattering dependence on transverse particle coordinate, giving, thus, mostly a qualitative estimate.

To develop a really quantitative approach, the Wigner function of the transverse particle motion phase space [37] is applied for the local treatment of the incoherent scattering in Section 3, in which an essentially novel formula for local probability of incoherent scattering of a classically moving high energy particle is derived in the axial case. A method of consistent inclusion of the quantum scattering features into the simulations of relativistic particle classical motion in the averaged atomic string/plane potential is detailed in Section 4. We reveal, that the strong enough inhomogeneity of the string atom nuclei distribution in the plane of transverse particle motion results in impossibility to introduce a local scattering probability for the small angles and, to preserve the classical trajectory simulations, suggest to apply the newly introduced mean scattering angles. Considerable attention is also payed
FIG. 1: Comparison of diffractive wave packet divergence (dashed) and classical particle deflection (solid line) in quantum (left) and classical cases.

both to the interrelation and individual roles of single and multiple scattering processes, quite differently treated for decades.

This Preprint presents the revised version of the paper [38], both corrected and simplified according to Erratum [39] in order to make the developed approach to the high-energy particle incoherent scattering in oriented crystals more exact and available for implementation into simulations.

II. QUANTUM NATURE OF RELATIVISTIC PARTICLE SINGLE ATOM SCATTERING

First of all, remind, why, on the contrary to the coherent, the incoherent scattering becomes quantum at relativistic energies [11, 19–21]. The inapplicability of classical mechanics to relativistic elementary (with a unit charge $|z| = 1$) particle scattering by nuclei, in fact, directly follows from a comparison of the quantum (diffractional) angular uncertainty $\Delta \theta \sim \hbar/pb$, where $p$ is particle momentum and $b$ impact parameter, with the classical deflection angle $\theta_{cl} = 2Z\alpha/\beta v b$, where $Z$ is atomic number, $\alpha$ fine structure constant and $v = \beta c$ particle velocity. Indeed, since $\Delta \theta >> \theta_{cl}$ at both $Z\alpha/\beta << 1$ and $\beta \simeq 1$, the scattering angle uncertainty exceeds the classical deflection angle, making the trajectory notion inapplicable for relativistic elementary particles, as Fig. 1 qualitatively illustrates. In other words, while the usage of classical trajectories in the averaged crystal potential becomes more and more justified with the energy increase (above several dozen MeV for electrons
FIG. 2: The ratio of "quantum" to "classical" cross sections vs the scattering angle for Si atom ($\alpha Z = 0.102$).

and positrons) [11], classical binary collision method [18], on the opposite, becomes inapplicable.

To illustrate the difference of quantum and classical predictions, let us compare the corresponding cross sections, evaluated for Yukawa atomic potential, characterized by the adopted from [40, 41] and implemented into GEANT4 screening radius $R = a_{TF}[1.13 + 3.76(\alpha Z/\beta)^2]^{-1/2}$, where $a_{TF} = 0.8853a_BZ^{-1/3}$ and $a_B$ are, respectively, Thomas-Fermi screening and Bohr radii. Fig. 2 presents the angular dependence of the ratio of "quantum" to "classical" cross sections, the latter of which was evaluated following [42] in the relativistic case. These cross sections, as is well known [20], coincide at large transverse momentum transfers $q \gg h/R$, corresponding to the scattering angles $\theta \gg \theta_{\text{min}} = h/pR$. However at $q \leq h/R$ or $\theta \leq \theta_{\text{min}}$, when the screening effect considerably modifies Coulomb potential, classical approach overestimates [43] the scattering intensity, demonstrating the loss of its applicability. Note, that both the cross sections, compared in Fig. 2, have been calculated under the assumption of a uniform incident particle flux, for which classical mechanics overestimates the total cross section by the factor $(2Z\alpha)^{-1}$, reaching 25 for Si atom. At the same time, on the opposite to the classical particle deflection in binary collisions model, quantum mechanics can not be directly applied to quantify the deflection of a particle moving along a classical trajectory.

It will be shown below, that the correlations of particle collisions with string atoms result in the incoherent scattering reduction similar, in a sense, to a screening at momentum
FIG. 3: Transverse radius-vector $\rho$ and the directions $n_\rho, n_\phi$ of extremal scattering intensities at the background of the string field. The double-sided arrows portray the excess of radial scattering over the azimuthal one.

Transfers $q \leq \hbar/u_1$, corresponding to the scattering angles $\theta_{u_1} \leq \hbar/pu_1$, where $u_1$ is the root mean square amplitude of atom thermal vibrations. Since $\theta_{u_1}$ usually two-three times exceeds $\theta_{\text{min}}$, one can expect [26, 36] (see also [29–32]) that collision correlations have to result in an incoherent scattering reduction which will be numerically described below, taking for the first time into consideration its dependence on transverse coordinates.

To have a natural measure of the difference of incoherent scattering in crystals from the scattering in amorphous medium, we will introduce a Kitagawa-Ohtsuki ansatz ("KO ansatz" below)

$$\frac{d\Sigma_{KO}(\rho)}{dq} = \frac{4Z^2\alpha^2n_n(\rho)}{\nu^2(g^2 + \kappa_{sc}^2)^2},$$

(1)

inspired by the paper [22] of M. Kitagawa and Y. H. Ohtsuki to be equal to the product of the unperturbed microscopic scattering cross section (relativistic cross section for the screened Coulomb (Yukawa) potential here) by either planar or, considered below as an example, axial

$$n_n(\rho) = \exp(-\rho^2/2u_1^2)$$

(2)

nuclear number density, were $\rho$ is the distance from the atomic string symmetry axis (see Fig. 3) and $d$ interatomic distance in the string. One can mention that Eq. (1) reminds macroscopic cross sections, widely used in the reactor physics, in which the nuclear number density can also vary widely.

However, KO ansatz (1) combines a classical particle coordinate $\rho$ with the quantum cross section only formally, neglecting the nuclear number density (2) variation, which exceeds
100% for the largest substantial impact parameters $b \sim R > u_1$, as well as missing both the effect of incoherent scattering reduction by correlations \(24, 26, 29, 32, 36\) and azimuthal asymmetry of the same \(36, 47\). To take the influence of the nuclear density inhomogeneity into consideration, we also introduce below some "macroscopic cross section", which, formally reminding the same in reactor physics, possesses, in a sense, a deeper meaning, combining in its general form the inseparable characteristics of scattering probability and scatterers’ density distribution. At the same time, in the high transfer momentum limit, the same macroscopic cross section reduces to the product of nuclear density by a modified microscopic cross section, preserving the effect of the density (2) inhomogeneity and allowing one to incorporate quantum scattering effects in classical trajectory simulations.

III. WIGNER FUNCTION APPLICATION TO SINGLE ATOM SCATTERING

To introduce quantum features of incoherent scattering consistently into the classical picture of high energy particle motion in the averaged crystal potential, the Wigner function approach is most adequate \(37\). Taking the axial case as an example, let us consider the Wigner function

$$W(\rho, q) = \frac{1}{\pi} \int \psi^*(\rho + \chi)\psi(\rho - \chi) \exp(2i q \chi) d^2 \chi,$$  \hspace{1cm} (3)

determined in the two-dimensional phase space \((\rho, q)\). \(\rho = (x, y), q = (q_x, q_y)\), of the impact parameter plane nearly parallel to that of transverse motion of a particle, scattered by the residual atomic potential \(26, 27\)

$$\delta U_{at}(\rho, \rho_n, z) = U_{at}(\rho, \rho_n, z - z_n) - \int U_{at}(\rho, \rho_n, z - z_n)n_n(\rho_n) d^2 \rho_n dz_n,$$  \hspace{1cm} (4)

emerging after the substraction of the averaged one, already taken into consideration by the axial potential, which determines the classical particle motion. The potential (4) is small and localized enough to leave the three terms

$$\psi(\rho, \rho_n) = 1 - i \int \delta U_{at}(\rho, \rho_n, z) \frac{dz}{v} - \frac{1}{2} \left[ \int \delta U_{at}(\rho, \rho_n, z) \frac{dz}{v} \right]^2,$$  \hspace{1cm} (5)

of the eikonal wave function expansion, in which

$$\int \delta U_{at}(\rho, \rho_n, z) \frac{dz}{v} = \frac{Z \alpha}{\pi \nu} \int \exp(i \kappa \rho) \frac{\exp(-i \kappa \rho_n) - \exp(-\kappa^2 u_1^2/2)}{\kappa^2 + \kappa^2 s} d^2 \kappa.$$  \hspace{1cm} (6)
Assuming a purely classical particle motion in the averaged potential both before and after the incoherent scattering at the point $\rho$ in transverse plane, we will evaluate the distribution in momentum $q$, transferred to the particle at this point, being that of catenation of the classical trajectories before and after the incoherent scattering. Substituting the wave function product

$$
\psi^*(\rho + \chi, \rho_n)\psi(\rho - \chi, \rho_n) = 1 + i \int \delta U_{at}^*(\rho + \chi, \rho_n, z) \frac{dz}{v} - i \int \delta U_{at}(\rho - \chi, \rho_n, z) \frac{dz}{v} + \frac{1}{2} \int \delta U_{at}^*(\rho + \chi, \rho_n, z) \frac{dz}{v} \int \delta U_{at}(\rho - \chi, \rho_n, z) \frac{dz}{v} \int \delta U_{at}(\rho - \chi, \rho_n, z) \frac{dz}{v} \int \delta U_{at}(\rho - \chi, \rho_n, z) \frac{dz}{v}$$

into Eq. (3) and assuming, that the unity in Eq. (7) corresponds to the particle propagation in the absence of incoherent scattering, one arrives to the "scattering" Wigner function

$$W_{\rho_n}(\rho, q) = -\frac{8Z\alpha}{\pi v} \left\{ \frac{\cos 2q(\rho - \rho_n) - \cos(2q\rho) \exp(-2q^2u_1^2)}{4q^2 + \kappa_{sc}^2} \right\} \exp\left[-i(q + \kappa)\rho_n\right] \exp\left[-(q + \kappa)^2u_1^2/2\right] \times \left\{ \frac{\exp[i(q - \kappa)\rho_n] - \exp[-(q - \kappa)^2u_1^2/2]}{(q - \kappa)^2 + \kappa_{sc}^2} \right\} d^2\kappa$$

$$-\frac{4Z^2\alpha^2}{\pi^2v^2} \exp(2iq\rho) \int \exp\left[-i(q + \kappa)\rho_n\right] \exp\left[-(q + \kappa)^2u_1^2/2\right] \times \left\{ \frac{\exp[-i(q - \kappa)\rho_n] - \exp[-(q - \kappa)^2u_1^2/2]}{(q - \kappa)^2 + \kappa_{sc}^2} \right\} d^2\kappa$$

describing particle incoherent scattering at the point $\rho$ by an atom having a transverse radius vector $\rho_n$. In general, Eq. (8) can be applied to an arbitrary instant nuclear distribution in thermal vibration coordinates $\rho_n$, as is discussed in Refs. 46, 48. However, a probabilistic interpretation of Eq. (8) does not look straightforward, since the leading, linear in $\alpha$, term strongly oscillates between positive and negative values. At the same time, the rest quadratic terms in Eq. (8) reduce to the expected high momentum transfer limit of the relativistic Rutherford (Mott) cross section multiplied by delta function $\delta(\rho - \rho_n)$ at $qu_1 >> 1$.

To simplify the problem realistically, we choose here the traditional way 25, 26 of Eq. (8) convolution with the scattering nuclei distribution (2), which nullifies the linear in $\alpha$ contribution, leaving only the quadratic ones in (8). Owing to the Fourier integral presence in Eq. (6), the double integration in Eq. (3) results in the two-dimensional delta function, trivializing the double integration over $\kappa$ in one of the potentials (6), leaving the same in
the another one the sole integral in the resulting expression
\[
\frac{d\Sigma(\rho)}{dq} = \langle W_{\rho n}(\rho, q) \rangle = \frac{4Z^2\alpha^2}{\pi^2\nu_0^2} \int \cos(2\kappa \rho) \exp(-2\kappa^2u_1^2) \exp[-(q^2 + \kappa^2)u_1^2] \frac{d^2\kappa}{[(q + \kappa)^2 + \kappa_{sc}^2][(q - \kappa)^2 + \kappa_{sc}^2]}
\]
\[
- \cos(2q\rho) \left[ \pi \ln\left( \sqrt{q^2/\kappa_{sc}^2 + 1 + q/\kappa_{sc}} \right) - \frac{q}{\sqrt{q^2 + \kappa_{sc}^2}} \exp[-(q^2 + \kappa^2)u_1^2] \right] \frac{d^2\kappa}{[(q + \kappa)^2 + \kappa_{sc}^2][(q - \kappa)^2 + \kappa_{sc}^2]} \right]. \tag{9}
\]
for Wigner function, for which, just renaming the integration variables, the unitarity condition \( \int dq \langle W_{\rho n}(\rho, q) \rangle = 0 \) can be readily checked. Eq. (9) can be widely used for the quantum treatment of incoherent scattering of high energy particles, classically moving in the average crystal potential.

As will be shown in Section 4, Eq. (9) predicts quite peculiar behavior at momentum transfers \( q < h/u_1 \), quickly approaching at \( q > 2h/u_1 \) its asymptote
\[
\frac{d\sigma_{mod}(\rho)}{dq} \approx \frac{1}{n_n(\rho)} \frac{d\Sigma(\rho)}{dq} \left[ 1 - \frac{\rho^2}{2q^2u_1^4} \left( 1 - 8e^{-\rho^2/2u_1^2} - q^2u_1^2 \right) \right] \frac{2(q\rho)^2}{q^2\rho^2} - 1 \tag{10}
\]
which will be used to clarify the nature of the considered effects. At still larger momenta \( q >> h/u_1 \), corresponding to the impact parameters \( b \sim h/q << u_1 \), at which the influence of the nuclear distribution inhomogeneity on scattering process must vanish, Eq. (9) reduces to the product
\[
\left( \frac{d\Sigma(\rho)}{dq} \right)_{q >> h/u_1} \rightarrow \frac{4Z^2\alpha^2}{q^4} \frac{d\sigma_{Ruth}(\rho)}{dq} = \frac{d\sigma_{Ruth}}{dq} \frac{n_n(\rho)}{\rho} \tag{11}
\]
of Rutherford cross section by the nuclear density. Note, that this "natural" limit takes place owing to both the residual incoherent scattering potential (4) introduction and averaging over the nuclei distribution (2).

### IV. QUANTUM INCOHERENT SCATTERING FEATURES AND THEIR INCORPORATION INTO CLASSICAL TRAJECTORY SIMULATIONS

#### A. Local scattering probability and mean square angles

Since both Eq. (9) and (10) demonstrate a strong scattering asymmetry, also emphasized in [36, 47], we will consider Wigner function (9) properties for both radial \( q = (q_\rho, 0) \) and
FIG. 4: Modified cross section dependence on momentum transfer for radial ($i = \rho$) and azimuthal ($i = \phi$) scattering directions, evaluated using the general (9) (solid) and asymptotic (10) (dashed lines) formulae for the radial coordinates $\rho = 0$ (top left), $\rho = u_1$ (top right), $\rho = 2u_1$ (bottom left) and $\rho = 3u_1$ (bottom right) of the scattering point.

azimuthal $q = (0, q_\phi)$ transferred momenta (see Fig. 3). Fig. 4 illustrates the diversity of the low-momentum (9) behavior at different radial coordinates, corresponding to both various nuclear densities and relative numbers - see Fig. 5. The incoherent scattering modification considerably affects, in fact, solely the smallest momentum transfers $q \lesssim \hbar/u_1$, only $R/u_1 \div 2 - 3$ times exceeding the minimal effective angle $1/Rp$ of particle scattering by a single atom. At such small momentum transfers the incoherent scattering differential probability drops below the normalization value, demonstrating the effect of incoherent scattering reduction by collision correlations [24–26, 29, 32, 36], and even becomes negative.

A capability to attain negative values is an essential property of Wigner function, reflecting its quantum nature. The Wigner function negativity does not allow one to unconditionally treat it as a scattering probability. To retain, nevertheless, the possibility to simulate quantum incoherent scattering of classically moving particles, we put forward here a more indirect way, resembling formally the ”multiple scattering approach”, applied here, however,
FIG. 5: Radial dependence of both the nuclear number density $n(\rho)/n(0)$ and, proportional to the latter, number of the nuclei $N(\rho' > \rho)$, situated at the radial distances $\rho' > \rho$, exceeding the plotted $\rho$ value, both measured in units of their maximum values reached at $\rho = 0$.

in the absence of positively determined scattering probability (cross section). The point is that, since Rutherford cross section peaks at the lowest $q$, the small angle particle deflection often manifests itself as a multiple scattering process, characterized by the mean square scattering angle per unit length \[^{[40, 41, 43]}\]. One can, similarly, use Eq. (9) to introduce the same for both radial $i = \rho$ and azimuthal $i = \varphi$ scattering directions

$$
\frac{d\theta^2_i(\rho)}{dz} = \int_{q < q_{max}^{MS}} \frac{d\Sigma(\rho)}{dq} \frac{q_i^2}{p^2} d^2q. \tag{12}
$$

Fig. 6 illustrates the dependence of the latter on the momentum integration limit $q_{max}^{MS}$, demonstrating again the drastic scattering asymmetry, which can be further taken into consideration by making $q_{max}^{MS}$ dependent on both radial coordinate and transferred momentum direction. Since the cross section approaches the Rutherford $q^{-4}$-type behavior at large $q$, for which the values (12) are definitely positive, one can expect that large enough $q_{max}^{MS}$ value will assure (12) positivity, making possible routine scattering angle sampling. Suggesting here to use the positively determined mean square angles (12), we have in mind that, despite the absence of the local probabilistic interpretation, in general, Wigner function is applicable to evaluate the consistent integral values of both scattering probability and mean square scattering angle, validating suggested sampling method. Note also that the complicated by the distant interference effects quite large Eq. (9) contribution to the Eq. (12) integrand is, in fact, strongly suppressed by the $q^3$ factor.
FIG. 6: Mean square angles of the scattering in both radial ($i = \rho$) and azimuthal ($i = \varphi$) directions along with their average ($i = \text{av.}$) versus the Eq. (12) momentum limit $q_{\text{MS}}^{\text{max}}$ at $\rho = 0$ (top left), $\rho = 2u_1$ (top right), $\rho = 2.5u_1$ (bottom left) and $\rho = 3u_1$ (bottom right), plotted as a ratio to the analogous positive values, evaluated using KO anzats (1).

Figs. 4 and 6 reveal considerably different transferred momentum dependence at small $\rho < 2u_1$ and large $\rho > 2u_1$ distances. Indeed, the asymptote (10) demonstrates that Wigner function contains both the nuclear density proportional, and the cosine-dependent disproportionate parts, describing, respectively, the local, high momentum and the distant, interference-sensitive, low-momentum transfers. The interference effects, naturally, induce Wigner function (9) oscillations at $\rho > au_1$, where, say, $a > 1.5$, demonstrating the distant action of the region $\rho \sim au_1 - b$ of the high nuclear density $n_n (au_1 - b) \gg n_n (au_1)$, becoming pronounced at collision parameters $u_1 \leq b \leq R$. The same interference part of Eq. (9) also gives rise to the strong scattering asymmetry in the region $2 \div 3u_1$ of about 10% of the nuclei.

These two qualitatively different Eq. (10) parts correspond to Kitagawa-Ohtsuki [22] and Lindhard [11] diffusion coefficients, respectively. Despite the former neglects the incoherent scattering reduction by correlations [24, 26, 29, 32, 36], it describes the incoherent scattering
in the dense nuclear region with an accuracy of 5-10%. However the strong nuclear density (2) decrease at \( \rho > 2u_1 \) makes the Kitagawa-Ohtsuki ansatz (1) inapplicable \cite{44, 45} for treating the ultimate channeling stability problem for which both Lindhard’s transverse energy diffusion and electron scattering are primarily important. The free from introduction of any approximate limit local nuclear dechanneling treatment is provided by Eqs. (8) and (9), taking into consideration all the peculiarities of both large-angle single and small-angle multiple scattering addressed below.

B. The necessity of consideration and relative role of single and multiple scattering in simulations

Incoherent scattering treatment is crucial for both accuracy and efficiency of simulations of particle propagation through crystals. However, the really polar approaches of simulating all the incoherent channeling effects by using solely the mean square angle definition \cite{22, 23, 49} on the one hand, and of the sampling successive single scatterings either classically \cite{18, 48} or quantumly \cite{31, 32} on the other, coexist in the literature for decades.

Our approach \cite{31}, verified in \cite{9, 10, 13, 14, 17, 28, 35, 50} and other investigations, includes the features of both of them, combining the sampling of both small angle multiple and large angle single scattering, the latter of which is most consonant to \cite{32} in the necessity of its quantum treatment. The introduced Eq. (9) delivers both the firm grounds and calculation capabilities to the method \cite{31}. However, before going to the latter, let us remind the peculiarities of multiple Coulomb scattering theory \cite{40, 41, 51} application to the simulations of particle propagation in crystals, which are still under discussion.

Though multiple Coulomb scattering theory \cite{40, 41, 51} (see also \cite{25, 43, 52}) is thoroughly developed and widely tested experimentally, its formal application to the channeling simulations is highly questionable \cite{41}. First of all, remind that the former predicts a nearly Gaussian angular distribution, characterized by the mean square angle

\[
\theta_s^2(l) = 8\pi n Z^2 \alpha^2 \ln \left( \frac{\theta_{\text{max}}}{\theta_{\text{min}}} \right) \left\{ 16\pi n Z^2 \alpha^2 \ln \left( \frac{204 Z}{10} \right) \right\},
\]

where \( n \) is a nuclear number density and \( l \) a scattering length. We consider here only the ultra-relativistic small angle limit and adopt the slightly arbitrary numerical coefficients from \cite{43}. Proceeding from the quantum principles, the theory \cite{40, 41, 51} introduces both
FIG. 7: Particle number (left) and deflection angle square (right) distributions of 150 GeV electrons, scattered within a typical trajectory simulation step (17): simulated directly (solid, red) and evaluated using Gaussian polar angle distribution with mean square angles determined by the usual (13) (dash-dot, black), Williams’s (dashed, blue) and Molière’s (dotted, green lines) formulae.

the lower

\[ \theta_{\text{min}} = \frac{Z^{1/3} m}{192 p}, \]  

where \( m \) and \( p \) are particle mass and momentum, and the upper

\[ \theta_{\text{max}} = \frac{274 m}{Z^{1/3} p} \]  

scattering angle limits for high energy particles. Essential point of both [26, 29, 32, 36] and the present paper is the widely discussed above need of redefinition of the lower integration limit (14) in the presence of coherent scattering in crystals.

However, the upper one (15), being often formally used with both the mean square angle (13) and Gaussian distribution, is also mostly inapplicable to the trajectory simulations in crystals [31]. Instead of the coherent scattering effect at the small scattering angles, Eq. (13) inapplicability at the large ones is related with the unaccustomed short length of trajectory simulation steps, the case of which finds relatively specific complex treatment in Molière scattering theory [40, 41, 43, 52]. The latter elucidates that single scattering does not play considerable role if only \( 2.5 \theta_s > \theta_{\text{max}} \), as in a target with many radiation lengths thickness. However, if \( 2.5 \theta_s < \theta_{\text{max}} \), the Gaussian distribution is applicable solely at the angles \( \theta < 2.5 \theta_s \), while at \( 2.5 \theta_s < \theta < \theta_{\text{max}} \) single Coulomb scattering dominates.

The point is that the submicron length scale of simulated particle trajectories in crystals results in the root mean square angles \( \theta_s \), being drastically smaller than the maximal angle.
\( \theta_{\text{max}} \) (15) and making both the single scattering essential and the application of the angle \( \theta_{\text{max}} \) as an upper limit in Eq. (13) highly inconsistent. Indeed, Eq. (13) involves a very wide single scattering angle interval \( \theta_s \leq \theta \leq \theta_{\text{max}} \) into the evaluation of the width \( \theta_s \) of the Gaussian distribution, covering, at the same time, only a much smaller interval \( 0 < \theta < \theta_s \), which does not include the angles \( \theta_s \ll \theta \leq \theta_{\text{max}} \), quite contradictory involved in \( \theta_s \) evaluation through Eq. (15) at the same time. That is why, taken with the upper limit (15), Eq. (13) considerably overestimates the mean square angle, making the Gaussian unphysically wide – see Fig. 7. The book [43] elucidates accordingly that at less than 200 collisions the true distribution, simulated here by an elemental Monte Carlo for Fig. 7, ”is more sharply peaked at zero angle than a Gaussian” [43, 52], as one can indeed see in Fig. 7. That is why all the single scattering angles \( \theta_s \leq \theta \leq \theta_{\text{max}} \) should be disregarded in the mean scattering angle evaluation by redefining the upper limit in (15) according to the implicit condition \( \theta_{\text{max}} \simeq \theta_s(\theta_{\text{max}}) \) [31, 40, 41].

The first realistic estimate [51]

\[
\theta_c = \frac{Ze}{\nu p} \sqrt{4\pi nl}
\]  

(16)
of the actual width of the Gaussian distribution was introduced by equating the scattering probability at the angles \( \theta > \theta_c \) to unity. However, the value (16), in fact, underestimates the angular distribution width (see Fig. 7), since a few scatterings by the angles \( \theta < \theta_c \) often result in a multiple scattering angle \( \theta > \theta_c \). The correct estimate \( B\theta_c \), which contained a coefficient \( B \), determined from some implicit condition, was finally introduced in [40, 41] along with the involved formula for the more exact angular distribution.

To avoid the usage of the latter, we suggested [31] to sample both the small angle multiple and large angle single scattering jointly within each trajectory step. At that, the minimal angle of single scattering can be chosen to be either equal or smaller than the root mean square multiple scattering angle, evaluated using an estimate of the same as the upper integration limit. This seemingly loose choice of the latter is, in fact, validated by the adjustment of the single scattering process, self-adapting to the choice of the minimal single scattering angle. The multiple scattering simulation is, in fact, optional for this method, being used to avoid the simulation of some number of single scattering events. However, since the latter is quite modest for the short trajectory steps, the multiple scattering consideration can be reasonably abandoned in favor of the single scattering simulations with the properly
chosen lower cutoff $[29, 31, 32]$. 

To compare the different mean square angle definitions, we have simulated the particle scattering in the screened Coulomb potential by the angles $0 < \theta \leq \theta_{max} \simeq 300 \mu\text{rad}$ for the 150 GeV energy used in the first experiment [53] on negatively charged particle multiple volume reflection [50]. Fig. 7, left, presents the simulated angular distribution along with the three Gaussians, built for the mean square angles determined, respectively, by Eqs. (13)-(15); (16) and $\theta_s = B\theta_c$. All the four distributions were evaluated for the typical trajectory step length

$$\Delta l = 0.02 \hat{A}/\theta_{ch} \sim 0.05 \mu\text{m}. \quad (17)$$

Fig. 7, left, demonstrates, that, being applied with the upper limit (15), the definition (13) drastically overestimates the true width of the angular distribution, correctly predicted by Moliere theory and reproduced by simulations.

At the same time, starting from $5\mu\text{rad}$, the Gaussian distribution with any mean square angle definition essentially underestimates the single scattering distribution tail, which both gives considerable contribution to the mean square angle up to the maximum single scattering angle $\theta_{max} \simeq 300 \mu\text{rad}$ and determines the actual, generally stochastic appearance of the scattering particle trajectories. Also, since $\theta_{ch} \sim 40 \mu\text{rad} \gg 5\mu\text{rad}$, the single scattering processes is completely responsible for the effects of instant dechanneling and rechanneling. At the same time, owing both to the fast cross section decrease with angle and small trajectory steps length, single scattering simulations are not time consuming, free from the problem with the logarithm in the mean square angle formula (13) and readily reproduce both the not completely Gaussian small angle, the single scattering large angle, and the most difficult to handle intermediate angle regions of Moliere angular distribution, highly unappropriate for efficient sampling. By this reason we have mostly relied in our simulations [9, 10, 13, 14, 17, 28, 31, 33, 50] on the single scattering sampling, while the multiple scattering one was applied only optionally to accelerate the simulation process.

Instead of the previously known average estimates, the above consideration treats the effect of incoherent scattering reduction in crystals [24–26, 29, 32, 36] quantitatively at any arbitrary point in the impact parameter plane. Both Eqs. (8)-(12) and Figs. 4 and 6 reveal the indispensable role of the multiple scattering consideration describing its nontrivial characteristics (12) in the presence of collision correlations. Indeed, Fig. 4 highlights the impossibility to introduce the positive small angle scattering probability or cross section.
However, according to Fig. 6, the multiple scattering angles (12) can be made positive by the high enough integration limit $q_{max}^{MS}$ choice, in order to be appropriate for scattering angle sampling. Figs. 4, 6 demonstrate that both scattering probability (9) and mean square angles (12) becomes positive starting from the rather small momentum transfer $q_{max}^{MS} \approx \bar{h}/u_1$.

The most direct way to consistently combine single scattering with multiple one within an arbitrary trajectory step is to simulate the ”small” angle scattering as a cumulative multiple process of all the momentum transfers $q < q_{max}^{MS}$ using the mean angle squares (12) and to perform further the single scattering sampling using the local probability (9), being positive at $q_{max}^{MS} < q < \theta_{max} p$.

However, being the most straightforward, this approach includes two relatively laborious step of both (9) and (12) evaluation, the former of which can be avoided, including the difference of Eq. (9) predictions from the ones of Kitagawa-Ohtsuki ansatz into the integrals of Eq. (12) type.

According to the central limit theorem a loose choice of the momentum transfer limit $q_{max}^{MS}$ will have negligible influence on the simulated angular distribution, provided both the small $q_{max}^{MS}$ value and thoroughly evaluated mean squared angles (12) use.

The above consideration, undertaken here for the axial case, can be extend to the planar one by either a direct derivation, analogous to Eqs. (3)-(8), or through the averaging of Eqs. (9)-(12) along straight trajectories traversing atomic strings. If to picture crystal planes as the ones being assembled from atomic strings, it becomes clear, that the scattering intensity increase in the radial direction, illustrated by both Figs. 4 and 6, has to result in the same of the nuclear dechanneling rate in the region of $2.5 u_1 \sim 0.2\text{Å}$, critical for positively charged particle dechanneling.

Besides the numerous particle beam manipulation problems, the developed approach can be applied to refine both the radiation and pair production simulation methods of Refs. [9, 10, 17, 28, 35].

V. CONCLUSIONS

A theory of incoherent particle scattering in oriented crystals in the high energy limit, in which relativistic particle motion in the averaged field of atomic strings and planes is mostly classical, is developed. Quantum interference effects of scattering by the atomic cores along
a classical trajectory are treated through applying the Wigner function, determined in the phase space of transverse particle motion. The recently observed effect of incoherent scattering reduction in the presence of atom distribution inhomogeneity is, for the first time, described precisely on a classical particle trajectory. An impossibility to introduce the local small-angle scattering probability is revealed and a novel definition of mean square scattering angle is introduced to incorporate the quantum scattering features into the classical trajectory simulations. A considerable excess over the Kitagawa-Ohtsuki diffusion coefficient is numerically demonstrated in the region of negligible nuclear density. In general, present theory makes it possible to refine a numerical treatment of any experiment on high energy particle scattering and radiation in crystals ever conducted or planned.

A. Acknowledgments

Financial support by the European Commission through the PEARL Project, GA 690991, is gratefully acknowledged.

The author is obliged to both the anonymous referee and X. Artru for sharing the understanding of importance of the treated problem.

[1] V.G. Baryshevsky, High-Energy Nuclear Optics of Polarized Particles. World Press, 2012. 640 p. https://doi.org/10.1142/7947
[2] A.I. Akhiezer, N.F. Shul’ga, High Energy Electrodynamics in Matter. Gordon and Breach, New York, 1996.
[3] V.N. Baier, V.M. Katkov, and V.M. Strakhovenko, Electromagnetic Processes at High Energies in Oriented Single Crystals (World Scientific, Singapore, 1998).
[4] E.N. Tsyganov, Some aspects of the mechanism of a charged particle penetration through a monocystal, Fermilab TM-682 (1976).
[5] V.M. Biryukov, Yu.A. Chesnokov, and V.I. Kotov, Crystal channeling and its application at high-energy accelerators. (Springer, Berlin, Germany, 1997).
[6] W. Scandale, Use of crystals for beam deflection in particle accelerators, Mod. Phys. Lett. A. 27 (2012) 1230007.
[7] V.A. Baskov, V.A. Khablo, V.V. Kim, V.I. Sergienko, B.I. Luchkov, and V.Yu. Tugaenko, Electromagnetic showers in aligned crystals, Nucl. Instrum. Methods Phys. Res., Sect. B 122 (1997) 194.

[8] V.G. Baryshevskii, V.V. Tikhomirov, Synchrotron-type radiation processes in crystals and polarization phenomena accompanying them, Usp. Fiz. Nauk 159 (1989) 529; [Sov. Phys. Usp. 32 (1989) 1013].

[9] L. Bandiera, E. Bagli, V. Guidi, A. Mazzolari, A. Berra, D. Lietti, M. Prest, E. Vallazza, D. De Salvador, and V. Tikhomirov, Broad and intense radiation accompanying multiple volume reflection of ultrarelativistic electrons in a bent crystal, Phys. Rev. Lett. 111 (2013) 255502.

[10] L. Bandiera, V.V. Tikhomirov, M. Romagnoni, N. Argiolas, E. Bagli, G. Ballerini, A. Berra, C. Brizzolani, R. Camattari, D. De Salvador, V. Haurylavets, V. Mascagna, A. Mazzolari, M. Prest, M. Soldani, A. Sytov and E. Vallazza, Strong reduction of the effective radiation length in an axially oriented scintillator crystal, Phys. Rev. Lett. 121 (2018) 021603.

[11] J. Lindhard, Influence of crystal lattice on motion of energetic charged particles, Phys. Lett. 12, 126 (1964); Kgl. Dan. Vidensk. Selsk. Mat. Fys. Medd. 34 (1965) 1.

[12] M.W. Thompson, Effects of proton channeling at 2.8 MeV of the \(\text{Cu}^{65}(p, n)\text{Zh}^{65}\) reaction rate in a single crystal of Cu, Phys. Rev. Lett. 13 (1964) 756.

[13] A. Mazzolari, E. Bagli, L. Bandiera, V. Guidi, H. Backe, W. Lauth, V. Tikhomirov, A. Berra, D. Lietti, M. Prest, E. Vallazza, and D. De Salvador, Steering of a sub-GeV electron beam through planar channeling enhanced by rechanneling, Phys. Rev. Lett. 112 (2014) 135503.

[14] A.I. Sytov, L. Bandiera1, D. De Salvador, A. Mazzolari1, E. Bagli1, A. Berra, S. Carturan, C. Durighello1, G. Germogli1, V. Guidi1, P. Klag, W. Lauth, G. Maggioni, M. Prest, M. Romagnoni, V. V. Tikhomirov, E. Vallazza, Steering of Sub-GeV electrons by ultrashort Si and Ge bent crystals, Eur. Phys. J. C. 77 (2017) 901.

[15] A.V. Korol, A.V. Solov’yov, W. Greiner, Channeling and Radiation in Periodically Bent Crystals, Springer Series on Atomic, Optical, and Plasma Physica 69, Springer-Verlag Berlin Heidelberg 2013. DOI: 10.1007/978-3-642-31895-5_6.

[16] S. Bellucci, V.A. Maisheev, Radiation of relativistic particles for quasiperiodic motion in a transparent medium, J. Phys.: Condens. Matter 18 (2006) S2083.

[17] V.G. Baryshevsky, V.V. Tikhomirov, Crystal undulators: from the prediction to the mature simulations, Nucl. Instrum. and Methods. B 309 (2013) 30.
[18] M. T. Robinson and O. S. Oen, The channeling of energetic atoms in crystal lattices, Appl. Phys. Lett. 2 (1963) 30.

[19] N. Bohr, The penetration of atomic particles thorough matter, Kgl. Dan. Vidensk. Selsk. Mat. Fys. Medd. 18 (1948) 8.

[20] L.D. Landau, E.M. Lifshitz, Quantum Mechanics: Non-Relativistic Theory, Vol. 3 (3rd ed.) Pergamon Press, 1977.

[21] P. Lervig, J. Lindhard, V. Nielsen, Quantal treatment of directional effects for energetic charged particles in crystal lattices, Nucl. Phys. A96 (1967) 481.

[22] M. Kitagawa, Y.H. Ohtsuki, Modified dechanneling theory and diffusion coefficients, Phys. Rev. B 8 (1973) 3117.

[23] A.M. Taratin and S.A. Vorob’ev, Proton volume capture in channeling regime in bent crystal, Zh. Tekh. Fiz. 55 (1985) 1598 [Sov. Phys. Tech. Phys. 30 (1985) 927].

[24] A. Mazzolari, A. Sytov, L. Bandiera, G. Germogli, M. Romagnoni, E. Bagli, V. Guidi, V.V. Tikhomirov, D. Salvador, S. Carturan, C. Durigello, G. Maggioni, M. Campostrini, A. Berra, V. Mascagna, M. Prest, E. Vallazza, W. Lauth, P. Klag, M. Tamisari, Broad angular anisotropy of multiple scattering in a Si crystal, Eur. Phys. J. C. 80 (2020) 63.

[25] M.L. Ter-Mikaelian, High-energy Electromagnetic Processes in Condensed Media Wiley. New York, 1972.

[26] V.A. Bazylev, V.V. Goloviznin, Quantum theory of channeled electron and positron scattering in a crystal, Zh. Eksp. Teor. Fiz. 82 (1982) 1204; [Sov. Phys. JETP 55 (1982) 700].

[27] V.A. Bazylev, S.B. Dabagov, Electromagnetic radiation under incoherent and incoherent scattering of relativistic electrons in crystals, Zh. Tekh. Fiz. 58 (1988) 1563.

[28] L. Bandiera, E. Bagli, G. Germogli, V. Guidi, A. Mazzolari, H. Backe and W. Lauth, A. Berra, D. Lietti, M. Prest, D. Salvador, E. Vallazza, V. Tikhomirov, Investigation of the electromagnetic radiation emitted by sub-GeV electrons in a bent crystal, Phys. Rev. Lett. 115 (2015) 025504.

[29] V.V. Tikhomirov, On the theory of electron-positron pair production in crystals, J de Physique 48 (1987) 1009.

[30] V.V. Tikhomirov, The position of the peak in the spectrum of 150 GeV electron energy losses in a thin Germanium crystal is proposed to be determined by radiation cooling, Phys. Lett. A 125 (1987) 411.
[31] V.V. Tikhomirov, Simulation of Multi-GeV electron energy losses in crystals, Nucl. Instrum. B 36 (1989) 282.

[32] X. Artru, A simulation code for channeling radiation by ultrarelativistic electroins or positrons, Nucl. Instr. Meth. in Phys. Res. B 48 (1990) 278.

[33] V.V. Tikhomirov, Quantitative theory of channeling particle diffusion in transverse energy in the presence of nuclear scattering and direct evaluation of dechanneling length, Eur. Phys. J. C. 77 (2017) 483.

[34] V.G. Baryshevsky, V.V. Tikhomirov, The role of incoherent scattering in radiation processes at small angles of incidence of particles on crystallographic axes or planes, Zh. Eksp. Teor. Fiz. 90, 1908 (1986); [Sov. Phys. JETP 63 (1986) 1116].

[35] V. Guidi, L. Bandiera, and V. Tikhomirov, Radiation generated by single and multiple volume reflection of ultrarelativistic electrons and positrons in bent crystals, Phys. Rev. A 86 (2012 042903).

[36] V.L. Ljuboshits, M.I. Podgoretsky, Multiple Coulomb scattering of ultrarelativistic charged particles moving at small angles to crystallographic planes, Zh. Eksp. Teor. Fiz. 87, 717 (1984); [Sov. Phys. JETP 60 (1984) 409].

[37] M. Ichikawa, Y.H.Ohtsuki, Inelastic-scattering theory for dechanneling, Phys. Rev. B 10 (1974) 1129.

[38] V.V. Tikhomirov, Quantum features of high energy particle incoherent scattering in crystals, Phys. Rev. Accel. Beams. 22 (2019) 054501.

[39] V.V. Tikhomirov, Erratum: Quantum features of high energy particle incoherent scattering in crystals [Phys. Rev. Accel. Beams 22, 054501 (2019)], Phys. Rev. Accel. Beams. 23 (2020) 039901(E).

[40] G. Molière, Theorie der streuung schneller geladener teilchen II mehrfach- und vielfachstreuung I, Z. Naturforschg. 3a (1948) 78.

[41] H.A. Bethe, Moliere’s theory of multiple scattering, Phys. Rev. 89 (1953) 1256.

[42] C. Lehmann, G. Leibfried, Higher order momentum approximations in classical collision theory, Zeitschrift fiir Physik 172 (1963) 465.

[43] J.D. Jackson, Classical Electrodynamics (3rd ed.). New York: John Wiley & Sons, 1999. ISBN 978-0-471-30932-1.

[44] Y. H. Ohtsuki and H. Nitta, Theory of dechanneling. Relatioistic Channeling, edited by R.
Carrigan, Jr. and J. Ellison (Plenum, New York, 1987).

[45] H. Nitta and Y. H. Ohtsuki, Dechanneling and stopping power of relativistic channeled particles, Phys. Rev. B 38 (1988) 4404.

[46] X. Artru, Correlations in thermal vibrations of crystal atoms. Effect on dechanneling and bremsstrahlung, Nucl. Instrum. Meth. B 402 (2017) 21.

[47] X. Artru, Quantum versus classical approach of dechanneling and incoherent electromagnetic processes in aligned crystals, arXiv:2003.03818v1 [quant-ph].

[48] I.A. Solov’yov, A.V. Korol, A.V. Solov’yov, Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer, Springer International Publishing, 2017.

[49] W. Scandale et al., Dechanneling of high energy particles in a long bent crystal, Nucl. Instrum. B 438 (2019) 38.

[50] V.V. Tikhomirov, Multiple volume reflection from different planes inside one bent crystal, Phys. Lett. A., 655 (2007) 217.

[51] E.J. Williams, Multiple scattering of fast electrons and alpha-particles, and “curvature” of cloud tracks due to scattering, Phys. Rev. 58 (1940) 292.

[52] P. Sigmund, K.B. Winterborn, Small-angle multiple scattering of ions in the screening Coulomb region, Nucl. Instrum. and Methods, 119 (1974) 541.

[53] W. Scandale et al., Observation of multiple volume reflection by different planes in one bent silicon crystal for high-energy negative particles, Europhys. Lett., 93 (2011) 56002.

[54] M. Tanabashi et al., (Particle Data Group), The Review of Particle Physics (2018), Phys. Rev. D 98 (2018) 030001.