# RELATION BETWEEN THE BLOCKING EFFECT AND RUTHERFORD SCATTERING IN THE NONLOCAL-STATISTICAL THEORY OF THE INTERACTION OF CHARGED PARTICLES WITH SINGLE CRYSTALS

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The relation between blocking and Rutherford scattering is investigated in Vlasov and Kuraev's nonlocal-statistical theory of orientation effects. A solution is obtained for the initial equation system of the theory in the second approximation, and it is shown that Rutherford scattering emerges in the second approximation, while blocking effects are obtained in the first approximation with respect to the charge of the beam particles. The calculation was made without consideration of the screening factor.

## 1. FORMULATION OF PROBLEM AND SOLUTION METHOD. DERIVATION OF FORMULAS FOR THE SECOND APPROXIMATION

In [1-4], Vlasov and Kuraev developed a statistical theory of the interaction of fast charged particles with a single crystal, and it was shown in [5] that the observed effects can be studied on the basis of Vlasov's equation and a crystal model with freely mobile atoms.

Let the charged-particle source be described by the function $Q(\mathbf{r}, \mathbf{v})$. $Q(\mathbf{r}, \mathbf{v})dt$ is the probability density that a particle will be produced at the point $(\mathbf{r}, \mathbf{v})$ of phase space during a time dt. The actual form of the function $Q(\mathbf{r},\mathbf{v})$ depends on the physical conditions under which the beam particles are produced.

The present paper considers scattering of fast charged particles on a single crystal after they have been ejected from sources inside the crystal. As an example of such a source we might cite interstitial radioactive atoms emitting charged particles, for example α-particles, in a crystal lattice. Excited nuclei that emit charged particles, such as protons, on their return to the ground state furnish another example. Such nuclei may be formed by irradiating a crystal with high-energy particles. In all of these cases, we can speak of the production of charged particles by these sources. We shall henceforth assume that $Q(\mathbf{r},\mathbf{v})$ can be presented in the form $Q(\mathbf{r}, \mathbf{v}) = q\Phi(|\mathbf{v}|)Q(\mathbf{r})$.

The equation system for the beam particle distribution function $f(\mathbf{r},\mathbf{v},t)$, based on statistical description of the beam particles and nonlocal crystal theory, will be

$$\begin{aligned}
&\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_{\mathbf{r}} f - \frac{1}{m}\nabla_{\mathbf{r}}\{U_f(\mathbf{r}) + \\
&+ Ze\varphi(\mathbf{r}, t)\}\cdot\nabla_{\mathbf{v}} f = Q(\mathbf{r}, \mathbf{v}), \\
&U_f(\mathbf{r}) = \int K_f(|\mathbf{r} - \mathbf{r}'|)\rho(\mathbf{r}')\,d\mathbf{r}', \\
&\rho(\mathbf{r}) = C\exp\left\{-\frac{U_f(\mathbf{r})}{\theta}\right\}, \\
&\Delta\varphi = -4\pi Ze\int\limits_{(\infty)} f(\mathbf{r}, \mathbf{v}, t)\,d\mathbf{v},
\end{aligned} \tag{1}$$

where $U_f(\mathbf{r})$ is the potential energy of the interaction of a beam particle situated at point $\mathbf{r}$ with the entire crystal, θ is the temperature of the crystal, m is the mass of the beam particle and Ze is its charge, $C \equiv \text{const}$, and $K_f(|\mathbf{r}-\mathbf{r}'|)$ is the kernel that describes the interaction between the beam particles and the entire crystal.

For the case of scattering of high-energy charged particles by a crystal, $K_f(|\mathbf{r}-\mathbf{r}'|)$ can be narrowed down to the form of the screened Coulomb potential

$$K_f(|\mathbf{r}-\mathbf{r}'|) = \frac{ZZ_1e^2}{|\mathbf{r}-\mathbf{r}'|}\exp(-\varkappa|\mathbf{r}-\mathbf{r}'|),$$

where Ze and $Z_1e$ are the charges of the beam particles and the atomic nuclei of the crystal and $\varkappa^{-1}=a_B\cdot 0{,}8853\ (Z^{2/3}+Z_1^{2/3})^{-1/2}$ ($a_B$ is the Bohr radius).

It was shown in [2] that a solution of system (1) can be found in the form of a series in a parameter proportional to the beam-particle charge. Putting

$$U_f \to \varepsilon U_f, \quad e\varphi \to \varepsilon e\varphi,$$
$$f = f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + \ldots, \quad \varphi = \varepsilon\varphi_1 + \varepsilon^2\varphi_2 + \ldots,$$

we obtain an expression for the particle distribution density in the first approximation

$$\tilde{\rho}_f^1(\mathbf{r}, \mathbf{r}_0, t) = \int_{(\infty)} \tilde{f}^1(\mathbf{r}, \mathbf{r}_0, \mathbf{v}, t)\,d\mathbf{v},$$

when they are emitted by a point source

$$Q(\mathbf{r}, \mathbf{v}) = q\Phi(|\mathbf{v}|)\delta(\mathbf{r}-\mathbf{r}_0):$$

$$\tilde{\rho}_f^1(\mathbf{r}, \mathbf{r}_0, t) = \frac{q}{|\mathbf{r}-\mathbf{r}_0|^2}\int_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\,\xi\,d\xi + \tag{2}$$

$$+\frac{q}{m}\int_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{at}{\xi}\int_0^1\Delta U_f[(\mathbf{r}-\mathbf{r}_0)(1-\eta)+\mathbf{r}_0]\,\eta(1-\eta)\,d\eta.$$

The function $\tilde{\rho}_f^1(\mathbf{r}, \mathbf{r}_0, t)$ gives a good explanation for the blocking of the incident-particle beam by the single crystal, but it does not describe Rutherford scattering.

This paper investigates the relation between the blocking effect and Rutherford scattering in the nonlocal-statistical theory of the interaction of charged particles with a crystal. For this purpose, we obtain a solution of system (1) in the second approximation, assuming that the interaction of the particles with one another can be neglected. For this purpose, system (1) is simplified to

$$\begin{aligned}
&\frac{\partial f_0(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r f_0 = q\Phi(|\mathbf{v}|)Q(\mathbf{r}),\\
&\frac{\partial f_1(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r f_1 = \frac{1}{m}\nabla_r U_f \nabla_v f_0,\\
&\frac{\partial f_2(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r f_2 = \frac{1}{m}\nabla_r U_f \nabla_v f_1,\\
&\ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned} \tag{3}$$

Since (3) is a system of linear equations, it is first necessary to find a solution due to a small volume of the source, i.e., to represent the source and solution in the form

$$\begin{aligned}
Q(\mathbf{r}) &= \int_{(\infty)} d\mathbf{r}_0 Q(\mathbf{r}_0)\delta(\mathbf{r}-\mathbf{r}_0),\\
\tilde{f}(\mathbf{r}, \mathbf{v}, t) &= \int_{(\infty)} d\mathbf{r}_0 Q(\mathbf{r}_0)\tilde{f}(\mathbf{r}, \mathbf{r}_0, \mathbf{v}, t).
\end{aligned} \tag{4}$$

We then obtain the following equation system for $\tilde{f} = \tilde{f}_0 + \varepsilon\tilde{f}_1 + \varepsilon^2\tilde{f}_2 + \ldots$:

$$\begin{aligned}
&\frac{\partial \tilde{f}_0(\mathbf{r}, \mathbf{r}_0, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r\tilde{f}_0 = q\Phi(|\mathbf{v}|)\delta(\mathbf{r}-\mathbf{r}_0),\\
&\frac{\partial \tilde{f}_1(\mathbf{r}, \mathbf{r}_0, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r\tilde{f}_1 = \frac{1}{m}\nabla_r U_f \nabla_v \tilde{f}_0,\\
&\frac{\partial \tilde{f}_2(\mathbf{r}, \mathbf{r}_0, \mathbf{v}, t)}{\partial t} + \mathbf{v}\nabla_r\tilde{f}_2 = \frac{1}{m}\nabla_r U_f \nabla_v \tilde{f}_1,\\
&\ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned} \tag{5}$$

Since the function

$$\tilde{f}(\mathbf{r},\ \mathbf{v},\ t)=\int\limits_0^t Q(\mathbf{r}-\mathbf{v}(t-t_1),\ \mathbf{v},\ t_1)\,dt_1,$$

is a solution of the differential equation $\frac{\partial \tilde{f}}{\partial t}+\mathbf{v}\nabla_{\mathbf{r}}\tilde{f}=Q(\mathbf{r},\ \mathbf{v},\ t)$, we find from (5)

$$\tilde{f}_0(\mathbf{r},\ \mathbf{r}_0,\ \mathbf{v},\ t)=\int\limits_0^t q\Phi(|\mathbf{v}|)\,\delta(\mathbf{r}-\mathbf{r}_0-\mathbf{v}(t-t_3))\,dt_3,$$

$$\tilde{f}_1(\mathbf{r},\ \mathbf{r}_0,\ \mathbf{v},\ t)=\int\limits_0^t\frac{1}{m}\nabla U_f(\mathbf{r}-\mathbf{v}(t-t_2))\,\nabla_{\mathbf{v}_2}\Big|_{\mathbf{v}_2=\mathbf{v}}\int\limits_0^{t_2}\delta(\mathbf{r}-\mathbf{r}_0-\mathbf{v}(t-t_2)-$$
$$-\mathbf{v}_2(t_2-t_3))\,q\Phi(|\mathbf{v}_2|)\,dt_2dt_3,$$

where $\nabla_{\mathbf{v}_2}|_{\mathbf{v}_2=\mathbf{v}}$ is the symbolic notation for differentiation of the expression following this operator with respect to $\mathbf{v}_2$, after which it is necessary to put $\mathbf{v}_2=\mathbf{v}$.

Substituting this expression for $\tilde{f}_1(\mathbf{r},\ \mathbf{r}_0,\ \mathbf{v},\ t)$ into the last equation of system (5), we obtain

$$\tilde{f}_2(\mathbf{r},\ \mathbf{r}_0,\ \mathbf{v},\ t)=\frac{q}{m^2}\int\limits_0^t dt_1\int\limits_0^{t_1}dt_2\int\limits_0^{t_2}dt_3\dot{\nabla}U_f(\mathbf{r}-\mathbf{v}(t-t_1))\times$$
$$\times\dot{\nabla}_{\mathbf{v}_1}\Big|_{\mathbf{v}_1=\mathbf{v}}\{\ddot{\nabla}U_f(\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{v}_1(t_1-t_2))\times \tag{6}$$
$$\times\ddot{\nabla}_{\mathbf{v}_2}\Big|_{\mathbf{v}_2=\mathbf{v}_1}[\Phi(|\mathbf{v}_2|)\,\delta(\mathbf{r}-\mathbf{r}_0-\mathbf{v}(t-t_1)-\mathbf{v}_1(t_1-t_2)-\mathbf{v}_2(t_2-t_3))]\},$$

where $\nabla$ is the operator for differentiation of the function immediately following this operator with respect to the entire argument.

Vectors over which equal numbers of dots are placed are subject to scalar multiplication by one another (for example, $\dddot{\mathbf{a}}\dddot{\mathbf{b}}\ddot{\mathbf{c}}\ddot{\mathbf{d}}=(\mathbf{ac})(\mathbf{bd})$, where $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d}$ are arbitrary vectors).

We obtain the scattered-particle distribution density $\tilde{\rho}_f^{(2)}(\mathbf{r},\ \mathbf{r}_0,\ t)$ from the formula

$$\tilde{\rho}_f^{(2)}(\mathbf{r},\ \mathbf{r}_0,\ t)=\int\limits_{(\infty)}\tilde{f}_2(\mathbf{r},\ \mathbf{r}_0,\ \mathbf{v},\ t)\,d\mathbf{v},$$

i.e.,

$$\tilde{\rho}_f^{(2)}(\mathbf{r},\ \mathbf{r}_0,\ t)=\frac{q}{m^2}\int\limits_{(\infty)}d\mathbf{v}\int\limits_0^t dt_1\int\limits_0^{t_1}dt_2\int\limits_0^{t_2}dt_3\dot{\nabla}U_f(\mathbf{r}-\mathbf{v}(t-t_1))\times$$
$$\times\dot{\nabla}_{\mathbf{v}_1}\Big|_{\mathbf{v}_1=\mathbf{v}}\{\ddot{\nabla}U_f(\mathbf{r}-\mathbf{v}(t-t_1)-\mathbf{v}_1(t_1-t_2))\times \tag{7}$$
$$\times\ddot{\nabla}_{\mathbf{v}_2}\Big|_{\mathbf{v}_2=\mathbf{v}_1}[\Phi(|\mathbf{v}_2|)\,\delta(\mathbf{r}-\mathbf{r}_0-\mathbf{v}(t-t_1)-v_1(t_1-t_2)-v_2(t_2-t_3))]\}.$$

Since the $\delta$-function $\delta(\mathbf{r}-\mathbf{r}_0-\mathbf{v}(t-t_1)-\mathbf{v}_1(t_1-t_2)-\mathbf{v}_2(t_2-t_3))$, appears under the integral sign, integration can be carried out over the velocities in (7). After reduction of similar terms, this yields

$$\tilde{\rho}_f^{(2)}(\mathbf{r},\ \mathbf{r}_0,\ t)=\frac{q}{m^2}\int\limits_0^t dt_1\int\limits_0^{t_1}dt_2\int\limits_0^{t_2}dt_3\frac{(t-t_1)}{(t-t_3)^5}\{\Phi\cdot(t_2-t_3)\times$$
$$\times[(t-t_2)(t_1-t_3)\,\Delta U_{f_1}\cdot\Delta U_f+(t-t_1)(t_1-t_3)\ddot{\nabla}\,\Delta U_{f_1}\cdot\ddot{\nabla}U_f+$$
$$+(t-t_2)(t_2-t_3)\,\dot{\nabla}U_{f_1}\cdot\dot{\nabla}\Delta U_f+(t-t_1)(t_2-t_3)\,\dot{\nabla}\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f]+ \tag{8}$$
$$+\dot{\nabla}\Phi[(t_2-t_3)(t-t_2)\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f+(t_1-t_3)(t-t_2)\,\Delta U_{f_1}\cdot\dot{\nabla}U_f+$$
$$+(t-t_1)(t_2-t_3)\,\dot{\nabla}\ddot{\nabla}U_{f_1}\cdot\ddot{\nabla}U_f+(t-t_2)(t_2-t_3)\,\dot{\nabla}U_{f_1}\cdot\Delta U_f]+$$
$$+\dot{\nabla}\ddot{\nabla}\Phi(t-t_2)\,\dot{\nabla}U_{f_1}\cdot\ddot{\nabla}U_f\};$$

where

$$\Phi \equiv \Phi\left(\left|\frac{[\mathbf{r}-\mathbf{r}_0}{t-t_3}\right|\right), \text{ a } \nabla\Phi \equiv \nabla_{\frac{\mathbf{r}-\mathbf{r}_0}{t-t_3}}\Phi\left(\left|\frac{\mathbf{r}-\mathbf{r}_0}{t-t_3}\right|\right),$$

$$U_{f_1} \equiv U_f\left((\mathbf{r}-\mathbf{r}_0)\frac{t_1-t}{t-t_3}+\mathbf{r}\right),$$

$$U_f \equiv U_f\left((\mathbf{r}-\mathbf{r}_0)\frac{t_2-t}{t-t_3}+\mathbf{r}\right).$$

We have for an arbitrary function $\varphi(t_1, t_2, t_3)$

$$\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \varphi(t_1, t_2, t_3) =$$

$$= \int_0^t dt_3 \int_{t_3}^t dt_2 \int_{t_2}^t dt_1 \varphi(t_1, t_2, t_3).$$

We can therefore write

$$\tilde{\rho}_f^{(2)}(\mathbf{r}, \mathbf{r}_0, t) = \frac{q}{m^2}\int_0^t \frac{dt_3}{(t-t_3)^5}\int_{t_3}^t dt_2 \int_{t_2}^t dt_1 (t-t_1)\mathcal{R},$$

where $\mathcal{R}$ stands for the expression in the braces in (8). Making the substitution of variables

$$\eta = \frac{t-t_2}{t-t_3}, \quad \eta_1 = \frac{t-t_1}{t-t_3}, \quad \xi = \frac{|\mathbf{r}-\mathbf{r}_0|}{t-t_3},$$

in this expression, we obtain

$$\begin{aligned}
\tilde{\rho}_f^{(2)}(\mathbf{r}, \mathbf{r}_0, t) = \frac{q}{m^2}|\mathbf{r}-\mathbf{r}_0|^2 \int_{\left|\frac{\mathbf{r}-\mathbf{r}_0}{t}\right|}^{\infty} \Phi(\xi)\frac{d\xi}{\xi^3}\int_0^1 (1-\eta)d\eta \int_0^\eta \eta_1 d\eta_1 \times \\
\times [\eta(1-\eta_1)\Delta U_{f_1}\Delta U_f + \eta_1(1-\eta_1)\dot{\nabla}\Delta U_{f_1}\cdot\dot{\nabla}U_f + \\
+ \eta(1-\eta)\dot{\nabla}U_{f_1}\dot{\nabla}\Delta U_f + \eta_1(1-\eta)\dot{\nabla}\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f] + \\
+ \frac{q}{m^2}|\mathbf{r}-\mathbf{r}_0| \int_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty} \dot{\nabla}_\xi\Phi(\xi)\frac{d\xi}{\xi^2}\int_0^1 d\eta \int_0^\eta \eta_1 d\eta_1 \times \\
\times [\eta(1-\eta)\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f + \eta(1-\eta_1)\Delta U_{f_1}\cdot\dot{\nabla}U_f + \\
+ \eta_1(1-\eta)\dot{\nabla}\ddot{\nabla}U_{f_1}\ddot{\nabla}U_f + \eta(1-\eta)\dot{\nabla}U_{f_1}\cdot\Delta U_f] + \\
+ \frac{q}{m^2}\int_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty} \dot{\nabla}_\xi\ddot{\nabla}_\xi\Phi(\xi)\frac{d\xi}{\xi}\int_0^1 d\eta\eta\int_0^\eta d\eta_1\eta_1\dot{\nabla}U_{f_1}\cdot\ddot{\nabla}U_f,
\end{aligned} \tag{9}$$

where

$$U_{f_1} \equiv U_f((\mathbf{r}-\mathbf{r}_0)(1-\eta_1)+\mathbf{r}_0),$$
$$U_f \equiv U_f((\mathbf{r}-\mathbf{r}_0)(1-\eta)+\mathbf{r}_0).$$

Further transformations are made with consideration of the fact that

$$\nabla_\xi\Phi(\xi) = \Phi'(\xi)\frac{\xi}{\xi},$$

and since $\frac{\xi}{\xi} = \frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|} = \mathbf{n}$ is the unit vector in the direction of the vector $\mathbf{r} - \mathbf{r}_0$, we have

$$\nabla_\xi\Phi(\xi) = \Phi'(\xi)\mathbf{n}, \quad \left(\Phi'(\xi) \equiv \frac{d}{d\xi}\Phi(\xi)\right); \quad \dot{\nabla}_\xi\ddot{\nabla}_\xi\Phi(\xi) = \Phi''(\xi)\dot{\mathbf{n}}\ddot{\mathbf{n}} - \Phi'(\xi)[\dot{\mathbf{n}}\ddot{\mathbf{n}} - \dot{\nabla}_\xi(\ddot{\xi})]\frac{1}{\xi},$$

with $\dot{\mathbf{a}}\dot{\nabla}_{\xi}(\ddot{\xi})\ddot{\mathbf{b}} = \mathbf{ab}$, where $\mathbf{a}$ and $\mathbf{b}$ are arbitrary vectors;

$$\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty} \dot{\nabla}_{\xi}\Phi(\xi)\frac{d\xi}{\xi^2} = 2\dot{\mathbf{n}}\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi^3},$$

$$\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty} \dot{\nabla}_{\xi}\ddot{\nabla}_{\xi}\Phi(\xi)\frac{d\xi}{\xi} = 2\dot{\nabla}_{\xi}(\ddot{\xi})\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi^3}.$$

Then, applying (2) also, we obtain a solution of system (1) in the second approximation for the distribution density $\tilde{\rho}_f^{II}(\mathbf{r}, \mathbf{r}_0, t)$ of the particles emitted by the source $Q(\mathbf{r}, \mathbf{v}) = q\Phi(|\mathbf{v}|)\delta(\mathbf{r}-\mathbf{r}_0)$:

$$\begin{aligned}
\tilde{\rho}_f^{II}(\mathbf{r}, \mathbf{r}_0, t) = {} & \frac{q}{|\mathbf{r}-\mathbf{r}_0|^2}\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\,\xi d\xi + \\
& + \frac{q}{m^2}\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi}\int_0^1 \Delta U_f\cdot\eta(1-\eta)\,d\eta + \\
& + \frac{q}{m^2}\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi^3}\Big\{|\mathbf{r}-\mathbf{r}_c|^2\int_0^1(1-\eta)\,d\eta\int_0^{\eta}\eta_1 d\eta_1\times \\
& \times[\eta(1-\eta_1)\Delta U_{f_1}\cdot\Delta U_f + \eta_1(1-\eta_1)\nabla\Delta U_{f_1}\cdot\nabla U_f + \\
& + \eta(1-\eta)\nabla U_{f_1}\cdot\nabla\Delta U_f + \eta_1(1-\eta)\,\dot{\nabla}\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f] + \\
& + 2|\mathbf{r}-\mathbf{r}_c|\int_0^1 d\eta\int_0^{\eta}\eta_1 d\eta_1[\eta(1-\eta)\,\dot{\nabla}U_{f_1}\cdot(\mathbf{n}\nabla)\,\dot{\nabla}U_f + \\
& + \eta(1-\eta_1)\Delta U_{f_1}\cdot(\mathbf{n}\nabla)U_f + \eta_1(1-\eta)\,\dot{\nabla}U_f\cdot(\mathbf{n}\nabla)\,\dot{\nabla}U_{f_1} + \\
& + \eta(1-\eta)(\mathbf{n}\nabla)U_{f_1}\cdot\Delta U_f] + 2\int_0^1\eta d\eta\int_0^{\eta}\eta_1 d\eta_1\nabla U_{f_1}\cdot\nabla U_f\Big\},
\end{aligned} \tag{10}$$

where

$$U_{f_1} \equiv U_f((\mathbf{r}-\mathbf{r}_0)(1-\eta_1)+\mathbf{r}_0),$$
$$U_f \equiv U_f((\mathbf{r}-\mathbf{r}_0)(1-\eta)+\mathbf{r}_0), \quad \mathbf{n} = \frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|}.$$

The integrals over $\eta$ in (10) do not depend on t. Only the integrals

$$\int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\,\xi d\xi, \qquad \int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi}, \qquad \int\limits_{\frac{|\mathbf{r}-\mathbf{r}_0|}{t}}^{\infty}\Phi(\xi)\frac{d\xi}{\xi^3},$$

depend on t in this formula; at $t \to \infty$ and $|\mathbf{r}-\mathbf{r}_0| < \infty$, they become

$$\int_0^{\infty}\Phi(\xi)\,\xi d\xi, \qquad \int_0^{\infty}\Phi(\xi)\frac{d\xi}{\xi}, \qquad \int_0^{\infty}\Phi(\xi)\frac{d\xi}{\xi^3}. \tag{*}$$

Obviously, the convergence or divergence of these integrals is fully determined by the function $\Phi(\xi)$, which is nothing other than the velocity distribution of the particles emitted by the charged-particle source. The case that is most frequently encountered in practice and therefore most important, in which the velocity distribution function $\Phi(\xi)$ is delta-shaped ($\Phi(\xi) = \frac{1}{4\pi v_0^2}\delta(\xi - v_0)$) or nearly so. The integrals (*) obviously converge for this class of functions $\Phi(\xi)$.

## 2. CONDITIONS FOR EMERGENCE OF BLOCKING EFFECT AND RUTHERFORD SCATTERING

To analyze the solution (10) obtained above, let us examine the particular case in

which the particle beam is monoenergetic, i.e., when the velocity distribution function $\Phi(|\mathbf{v}|)$ has the form

$$\Phi(|\mathbf{v}|) = \frac{1}{4\pi v_0^2}\,\delta(|\mathbf{v}| - v_0).$$

Let us consider how $\tilde{\rho}_f^{\mathrm{II}}(\mathbf{r}, \mathbf{r}_0, t)$ depends on $\mathbf{r}$, $\mathbf{r}_0$, and $\mathbf{v}_0$ at great distances from the crystal. The dependence on $\mathbf{r}$ and $\mathbf{r}_0$ can be obtained in explicit form by analyzing, for example, the second term of the sum in (10). The integral

$$J = \int_0^1 d\eta\,(1-\eta)\,\Delta U_f\,((\mathbf{r}-\mathbf{r}_0)(1-\eta) + \mathbf{r}_0).$$

depends on $\mathbf{r}$ and $\mathbf{r}_0$. We make the substitution of variable $\gamma = (1-\eta)|\mathbf{r}-\mathbf{r}_0|$ and bear in mind that $\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|} = \mathbf{n}$. Then

$$J = \frac{1}{|\mathbf{r}-\mathbf{r}_0|^2}\int_0^{|\mathbf{r}-\mathbf{r}_0|} \gamma d\gamma \left(1 - \frac{\gamma}{|\mathbf{r}-\mathbf{r}_0|}\right)\Delta U_f\,(\mathbf{n}\gamma + \mathbf{r}_0).$$

We are concerned with the beam particle density distribution at large distances $|\mathbf{r}-\mathbf{r}_0|$, distances much larger than the path $|\mathbf{r}_k-\mathbf{r}_0|$, travelled by the beam inside the crystal ($\mathbf{r}_k$ is a point on the boundary of the crystal and on the line connecting the points $\mathbf{r}$ and $\mathbf{r}_0$). Since, like $\nabla U_f(\mathbf{r})$, $\Delta U_f(\mathbf{r}) = 0$ outside of the crystal, we have

$$J \approx \frac{1}{|\mathbf{r}-\mathbf{r}_0|^2}\int_0^{|\mathbf{r}_k-\mathbf{r}_0|} d\gamma\cdot\gamma\Delta U_f\,(\mathbf{n}\gamma + \mathbf{r}_0) = \tag{11}$$

$$= \frac{1}{|\mathbf{r}-\mathbf{r}_0|^2}\,Y_1(\mathbf{n}, \mathbf{r}_0, \mathbf{r}_k, \{U_f\}),$$

where $Y_1(\mathbf{n}, \mathbf{r}_0, \mathbf{r}_k, \{U_f\}) \equiv \int_0^{|\mathbf{r}_k-\mathbf{r}_0|} \gamma d\gamma\Delta U_f\,(\mathbf{n}\gamma + \mathbf{r}_0)$ is an expression that depends only on $\mathbf{n}$, $\mathbf{r}_0$, $\mathbf{r}_k$ and functionally on $U_f$.

The dependence on $\mathbf{r}$ and $\mathbf{r}_0$ at great distances from the crystal can also be expressed in similar fashion in the other terms of formula (10).

Then for a monoenergetic beam

$$\tilde{\rho}_f^{\mathrm{II}}(\mathbf{r}, \mathbf{r}_0, t) \approx \frac{q}{4\pi v_0}\,\frac{1}{|\mathbf{r}-\mathbf{r}_0|^2}\left[1 + \left(\frac{1}{mv_0^2}\,Y_1\right)(\mathbf{n}, \mathbf{r}_0, \mathbf{r}_k, \{U_f\}) + \right.$$
$$\left. + \left(\frac{1}{mv_0^2}\right)^2 Y_2(\mathbf{n}, \mathbf{r}_0, \mathbf{r}_k, \{U_f\}, \{U_{f_1}\})\right], \tag{12}$$

where, for $t > \frac{|\mathbf{r}-\mathbf{r}_0|}{v_0}$ and $|\mathbf{r}-\mathbf{r}_0| \gg |\mathbf{r}_k-\mathbf{r}_0|$,

$$Y_2(\mathbf{n}, \mathbf{r}_0, \mathbf{r}_k, \{U_f\}, \{U_{f_1}\}) \equiv \int_0^{|\mathbf{r}_k-\mathbf{r}_0|} \gamma d\gamma \int_\gamma^{|\mathbf{r}_k-\mathbf{r}_0|} d\gamma_1\,[\gamma_1\Delta U_{f_1}\cdot\Delta U_f +$$
$$+ \gamma_1\nabla\Delta U_{f_1}\cdot\nabla U_f + \gamma\nabla U_{f_1}\cdot\nabla\Delta U_f + \gamma\dot{\nabla}\ddot{\nabla}U_{f_1}\cdot\dot{\nabla}\ddot{\nabla}U_f] +$$
$$+ 2\int_0^{|\mathbf{r}_k-\mathbf{r}_0|} d\gamma \int_\gamma^{|\mathbf{r}_k-\mathbf{r}_0|} d\gamma_1\,[\gamma\nabla U_{f_1}\cdot(\mathbf{n}\nabla)\nabla U_f + \tag{13}$$
$$+ \gamma_1\Delta U_{f_1}\cdot(\mathbf{n}\nabla)U_f + \gamma(\mathbf{n}\nabla)\nabla U_{f_1}\cdot\nabla U_f +$$
$$+ \gamma(\mathbf{n}\nabla)U_{f_1}\cdot\Delta U_f + \nabla U_{f_1}\cdot\nabla U_f],$$
$$(U_{f_1} \equiv U_f(\mathbf{n}\gamma_1 + \mathbf{r}_0),\quad U_f \equiv U_f(\mathbf{n}\gamma + \mathbf{r}_0)).$$

We introduce the quantity $\bar{U}_f$, which is related to the potential $U_f$ by $U_f = ZZ_1e^2\bar{U}_f$. We can then write with (11) and (13)

$$\tilde{\rho}_f^{II}(\mathbf{r},\ \mathbf{r}_0,\ t) \approx \frac{q}{4\pi v_0}\frac{1}{|\mathbf{r}-\mathbf{r}_0|^2}\left[1+\frac{zz_1e^2}{mv_0^2}Y_1(\mathbf{n},\ \mathbf{r}_0,\ \mathbf{r}_k,\ \{\bar{U}_f\})+\right.$$
$$\left.+\left(\frac{zz_1e^2}{mv_0^2}\right)^2 Y_2(\mathbf{n},\ \mathbf{r}_0,\ \mathbf{r}_k,\ \{U_f\},\ \{U_{f_1}\})\right]. \tag{14}$$

It is evident from (14) that for sufficiently high particle energies, the most characteristic features of the effects observed during passage of the particles through the single crystal should be described even by the first approximation (3) of the solution of equation system (1).

Let us use (10) in a calculation for the particular case in which a beam of parallel-incident particles is scattered by a Coulomb potential, i.e., let us put $U_f(\mathbf{r})=\frac{zz_1e^2}{|\mathbf{r}|}$.

Denoting $\mathbf{R}=(\mathbf{r}-\mathbf{r}_0)(1-\eta)+\mathbf{r}_0$, we have $\Delta U_f(\mathbf{R})=\Delta\left(\frac{zz_1e^2}{|\mathbf{R}|}\right)=0$ at all points R except R = 0, or, introducing the angle $\vartheta$ between the vectors r and $\mathbf{r}-\mathbf{r}_0$:

$$\Delta U_f(\mathbf{R})=0 \quad \text{for} \quad \vartheta\neq 0. \tag{15}$$

Applying (15) and making the substitution of variables $\eta|\mathbf{r}-\mathbf{r}_0|=\gamma$, $\eta_1|\mathbf{r}-\mathbf{r}_0|=\gamma_1$, in the integrals of (10), we obtain

$$\tilde{\rho}_f^{II}(\mathbf{r},\ \mathbf{r}_0,\ t)=\frac{1}{4\pi v_0}\frac{q}{|\mathbf{r}-\mathbf{r}_0|^2}\left\{1+\right.$$
$$+\int_0^{|\mathbf{r}-\mathbf{r}_0|}d\gamma\left(1-\frac{\gamma}{|\mathbf{r}-\mathbf{r}_0|}\right)^2\int_0^{\gamma}d\gamma_1\gamma_1^2\times$$
$$\times\dot{\nabla}\ddot{\nabla}\left(\frac{zz_1e^2}{|\mathbf{R}|}\right)\dot{\nabla}\ddot{\nabla}\left(\frac{zz_1e^2}{|\mathbf{R}_1|}\right)+$$
$$+\frac{2}{|\mathbf{r}-\mathbf{r}_0|}\left[\int_0^{|\mathbf{r}-\mathbf{r}_0|}d\gamma\cdot\gamma\left(1-\frac{\gamma}{|\mathbf{r}-\mathbf{r}_0|}\right)\int_0^{\gamma}d\gamma_1\cdot\gamma_1\times\right.$$
$$\times(\mathbf{n}\nabla)\nabla\left(\frac{zz_1e^2}{|\mathbf{R}|}\right)\cdot\nabla\left(\frac{zz_1e^2}{|\mathbf{R}_1|}\right)+\int_0^{|\mathbf{r}-\mathbf{r}_0|}d\gamma\left(1-\frac{\gamma}{|\mathbf{r}-\mathbf{r}_0|}\right)\times \tag{16}$$
$$\left.\times\int_0^{\gamma}d\gamma_1\cdot\gamma_1^2\nabla\left(\frac{zz_1e^2}{|\mathbf{R}|}\right)\cdot(\mathbf{n}\nabla)\nabla\left(\frac{zz_1e^2}{|\mathbf{R}_1|}\right)\right]+$$
$$\left.+\frac{2}{|\mathbf{r}-\mathbf{r}_0|^2}\int_0^{|\mathbf{r}-\mathbf{r}_0|}d\gamma\cdot\gamma\int_0^{\delta}d\gamma_1\cdot\gamma_1\nabla\left(\frac{zz_1e^2}{|\mathbf{R}|}\right)\nabla\left(\frac{zz_1e^2}{|\mathbf{R}_1|}\right)\right\}.$$
$$(\mathbf{R}=(\mathbf{r}-\mathbf{r}_0)(1-\eta)+\mathbf{r}_0,\quad \mathbf{R}_1=(\mathbf{r}-\mathbf{r}_0)(1-\eta_1)+\mathbf{r}_0).$$

To obtain a beam of particles in parallel incidence on the scattering center, we let $|\mathbf{r}_0|$ increase without limit. In addition, we introduce the density of the incident beam,

$$\tilde{\rho}_0=\frac{1}{4\pi v_0}\frac{q}{|\mathbf{r}-\mathbf{r}_0|^2}.$$

We then have

$$\tilde{\rho}_f^{II}(\mathbf{r},\ \mathbf{r}_0,\ t)\xrightarrow[|\mathbf{r}_0|\to\infty]{}\tilde{\rho}_\infty^{II}(\mathbf{r})=\tilde{\rho}_0\left[1+\left(\frac{zz_1e^2}{mv_0^2}\right)^2\int_0^{\infty}d\gamma\int_0^{\gamma}d\gamma_1\cdot\gamma_1^2\times\right.$$
$$\left.\times\dot{\nabla}\ddot{\nabla}\left(\frac{1}{|\mathbf{R}|}\right)\cdot\dot{\nabla}\ddot{\nabla}\left(\frac{1}{|\mathbf{R}_1|}\right)\right]. \tag{17}$$

We denote the integral in (17) by $I_\infty$:

$$I_\infty=\int_0^{\infty}d\gamma\int_0^{\gamma}\gamma_1^2d\gamma_1\dot{\nabla}\ddot{\nabla}\left(\frac{1}{|\mathbf{R}|}\right)\cdot\dot{\nabla}\ddot{\nabla}\left(\frac{1}{|\mathbf{R}_1|}\right). \tag{18}$$

Carrying out the differentiation in (18), we obtain

$$I_\infty = \int_0^\infty d\gamma \int_0^\gamma \gamma_1^2 d\gamma_1 \left( \frac{9\,(\mathbf{R}\mathbf{R}_1)^2}{|\mathbf{R}|^5\,|\mathbf{R}_1|^5} - \frac{3}{|\mathbf{R}|^3\,|\mathbf{R}_1|^3} \right)$$

or

$$I_\infty = 9 \int_0^\infty d\gamma \int_0^\gamma d\gamma_1 \frac{\gamma_1^2}{|\mathbf{R}|^5\,|\mathbf{R}_1|^5} \left\{ \gamma_1^2\gamma^2 + \frac{b^2}{4}(\gamma^2+\gamma_1^2) + b(\gamma_1\gamma^2+\gamma\gamma_1^2) + \right.$$
$$\left. + \left(2a+\frac{b^2}{2}\right)\gamma_1\gamma + ab(\gamma+\gamma_1) + a^2 \right\} - 3\int_0^\infty \frac{d\gamma}{|\mathbf{R}|^3} \int_0^\gamma \frac{\gamma_1^2 d\gamma_1}{|\mathbf{R}_1|^3}; \qquad (18')$$

where

$$|\mathbf{R}| = \sqrt{a+b\gamma+\gamma^2},\quad |\mathbf{R}_1| = \sqrt{a+b\gamma_1+\gamma_1^2},$$

$a = r^2$, and $b = -2|\mathbf{r}|\cos\vartheta$ ($\vartheta$ is the angle between the vectors $\mathbf{r}$ and $\mathbf{r} - \mathbf{r}_0$).

On evaluating the integrals in (18'), we obtain

$$I_\infty = \frac{4\,(2\sqrt{a}-b)^2}{\Delta^2},$$

where $\Delta = 4r^2\sin^2\vartheta$, i.e.,

$$I_\infty = \left(4r^2\sin^4\frac{\vartheta}{2}\right)^{-1},\quad (\vartheta \neq 0).$$

Substituting this value for $I_\infty$ in (17), we finally obtain

$$\tilde{\rho}_\infty^{II}(\mathbf{r}) = \tilde{\rho}_0 \left\{ 1 + \left(\frac{zz_1e^2}{2mv_0^2}\right)^2 \frac{1}{r^2\sin^4\frac{\vartheta}{2}} \right\} \quad (\vartheta \neq 0). \qquad (19)$$

Formulas (12) and (19) are approximate formulas obtainable from the exact expression (10). Formula (12) is obtained from (10) in the limiting case in which $|\mathbf{r}-\mathbf{r}_0| \gg |\mathbf{r}_k-\mathbf{r}_0|$, where $|\mathbf{r}_k-\mathbf{r}_0|$ is the path travelled by the particle in the crystal, and formula (19) is obtained from (10) in the limiting case in which $|\mathbf{r}_0|\to\infty$, $|\mathbf{r}| < \infty$.

It is expression (19) which agrees with Rutherford's formula, that is the result of the second approximation in (10).

Analysis of expression (10), which was obtained for the density distribution $\tilde{\rho}_f^{II}(\mathbf{r}, \mathbf{r}_0, t)$ in solution of system (1) in the second approximation, makes it possible to establish the respective cases in which the blocking effects and Rutherford scattering are basic. It was shown in [2] that if the scattering atoms have strictly periodic positions, the blocking effects are strengthened in the directions of the crystallographic axes and planes with small indices. But if the arrangement of the atoms is not periodic, but chaotic (as in polycrystalline targets), the particles will be scattered basically in accordance with the Rutherford law. It follows from (14) that, other conditions being equal, the blocking effects become more distinct as the energy of the beam particles increases.

We note in conclusion that we have obtained a solution of the initial equation system of the theory in the second approximation and shown that Rutherford scattering emerges in the second approximation, while the blocking effects are already in evidence in the first approximation with respect to the charge on the beam particles. The calculation was performed without consideration of the screening factor.

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