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Динамико-статистический подход к описанию движения быстрых частиц сквозь кристалл

Получено кинетическое уравнение для функции распределения частицы большой энергии, каналирующей сквозь кристалл.

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A Dynamical Statistical Approach for Description of Motion of a Fast Particle Through a Crystal

A general scheme for the description of a fast charged particle motion through a crystal is suggested. The starting point for the theoretical investigation in this approach is the distribution function $f(z\psi s_{\perp})$. The parameters ψ, z, $s_{\perp}$ are phase-space variables of this problems. As a result an exact formal equation for $f(z\psi s_{\perp})$ is obtained. The small parameters which occur in this problem are considered.

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A great variety of physical phenomena arises when an energetic charged particle falls into a crystal at a small angle with respect to a crystal axis (axis channeling) or to a crystal plane (plane channeling)[1]. Since the angle ψ and the across momentum of the incident particle are very small, the particle wave vector corresponding to motion perpendicular to the direction of channeling is very small too. In other words the phenomenon of motion of a fast particle in channeling is due to the near - forward scattering. That is why this motion can be very well described within classical mechanics[2]. This allows us to develop an approach for the description of channeling using the distribution function for the "small" subsystem and the Hamilton equations of motion. Relativistic effects can easily be included in this approach. They lead only to renormalization of some parameters of the considered problem. Therefore we consider here the commonly suggested scheme for the description of a fast charged particle motion through a crystal neglecting the relativistic effects.

The starting point for the theoretical investigation in this approach is the distribution function $f_t(z,\psi,S_\perp)$. It can be obtained from the distribution function of the whole system by integrating over the variables of the crystal subsystem

$$f_t(z,\psi,S_\perp) = \int d\Sigma\, f_t(z,\psi,S_\perp,\Sigma), \qquad (1)$$

where Σ is the set of phase-space variables of the crystal subsystem, i.e., $\{\vec{v}_i, \vec{z}_i\}$, $i = 1, 2, \ldots, N$, $\vec{v}_i$ is the velocity of an ion in the i-th lattice site and $\vec{z}_i$ is its space coordinate. $S_\perp$ is the set of phase-space variables of the incident particle in the plane perpendicular to the direction of channeling, ψ is a parameter describing the energy distribution of incident particles and t is the time.

The dynamics of the whole system is determined by the Hamiltonian function H.

$$H = \frac{M\vec{v}^2}{2} + \sum_{i=1}^{N} V(\vec{R} - \vec{z}_i) + H_{kp}, \tag{2}$$

where M is the incident particle mass; $\vec{v}$, its velocity, H_{kp} is the Hamiltonian function of the crystal subsystem, V is the interaction potential between the incident particle and an ion of the crystal. The time evolution of the ($S+\Sigma$) system is discribed by the whole Liouville equation:

$$\frac{\partial}{\partial t} f_t(S_\perp \psi z \Sigma) = \Lambda f_t(S_\perp \psi z \Sigma), \tag{3}$$

where Λ is Liouville's operator of the ($S+\Sigma$) system, defined as $\{H, \}$, where $\{\ ,\ \}$ are Poisson's brackets. The aim of the present paper is to obtain a closed equation for the distribution function $f_t(z \psi S_\perp)$. The stationary case of this problem is considered here, i.e., $f_t(z \psi S_\perp) = f(z \psi S_\perp)$ does not depend on time.

Let us introduce the new phase-space variables $\psi, z, \vec{R}_\perp, \vec{v}_\perp$; $\vec{R} = (z, \vec{R}_\perp)$; $\vec{v} = (v_0 \cos\psi, \vec{v}_\perp)$. v_0 is the velocity determined by the initial energy E_0 of the incident particle. $v_0 = \sqrt{\frac{2E_0}{M}}$; By using the relation $\frac{\partial}{\partial t} = -\frac{1}{v_0 \sin\psi} \frac{\partial}{\partial \psi}$ we can rewrite the stationary form of equation (3) in the following way

$$\frac{\partial}{\partial z} f(z, \psi, S_\perp, \Sigma) = -\sqrt{\frac{M}{2E_0}} \frac{1}{\cos\psi} \vec{v}_\perp \frac{\vec{\partial}}{\partial \vec{R}} f(z \psi S_\perp \Sigma) + \left[\Lambda'_{kp} + \Lambda'_z + \Lambda'_\perp\right] f(z \psi S_\perp \Sigma), \tag{4}$$

where

$$\Lambda'_{kp} = \sqrt{\frac{M}{2E_0}} \frac{1}{\cos\psi} \Lambda_{kp};$$

$$\Lambda_{kp} = -\sum_{i=1}^{N} \vec{v}_i \frac{\vec{\partial}}{\partial \vec{z}_i} + \sum_{i<j}^{N} \frac{\partial}{\partial \vec{z}_i} \Phi(\vec{z}_i - \vec{z}_j)\left(\frac{1}{m_i}\frac{\vec{\partial}}{\partial \vec{v}_i} - \frac{1}{m_j}\frac{\vec{\partial}}{\partial \vec{v}_j}\right).$$

is the Liouville operator of the crystal subsystem

$$\Lambda'_z = -\sum_{i=1}^{N} \frac{\partial}{\partial z} V(\vec{R} - \vec{z}_i) \left[\frac{1}{E_0 \sin 2\psi} \frac{\partial}{\partial \psi} + \sqrt{\frac{M}{2E_0}} \frac{1}{m_i \cos\psi} \frac{\partial}{\partial v_i^z}\right]$$

is the z-component of the operator describing the interaction between the incident particle and lattice.

$$\Lambda'_\perp = \sqrt{\frac{M}{2E_0}} \frac{1}{\cos\psi} \Lambda_\perp;$$

$$\Lambda_\perp = \sum_{i=1}^{N} \frac{\vec{\partial}}{\partial \vec{R}_\perp} V(\vec{R} - \vec{z}_i) \left[\frac{1}{M} \frac{\vec{\partial}}{\partial \vec{v}_\perp} - \frac{1}{m_i} \frac{\partial}{\partial v_i^\perp}\right]$$

is the transverse component of the same operator. Equation (4) is like an ordinary Liouville equation in which z coordinate plays the role of the evolution parameter. Now, we shall use a modified version of the approach/3/ suggested in paper/4/ to obtain a closed form equation for the distribution function $f(z \psi S_\perp)$. The projective operator $\hat{P}_0$ is defined by the initial conditions which are obvious for the present problem:

$$f(z \psi S_\perp \Sigma)\Big|_{z=0} = f(\psi S_\perp)\, \mathcal{D}_0(\Sigma), \tag{5}$$

where $f(\psi S_\perp)$ is the incident particle distribution function in $z=0$, i.e., the initial distribution function of the particle. $\mathcal{D}_c(\Sigma)$ is the Gibbs distribution function for the crystal subsystem.

So, as in/4/, the projective operators are

$$\hat{P} = \int d\Sigma (\cdot\,\cdot) \; ; \quad \hat{P}_o = \mathcal{D}_o(\Sigma)\hat{P} \tag{6}$$

and the function is

$$\Delta(z\psi S_\perp \Sigma) = [1-\hat{P}_o]\, f(z\psi S_\perp \Sigma). \tag{7}$$

Notice that

$$f(z\psi S_\perp) = \hat{P} f(z\psi S_\perp \Sigma). \tag{8}$$

Using equation (4) and definitions (6)-(8), we can easily obtain the following system of equations.

$$\begin{aligned} \frac{\partial}{\partial z} f(z\psi S_\perp) &= -\sqrt{\frac{M}{2E_0}}\,\frac{\vec{v}_\perp}{\cos\psi}\frac{\partial}{\partial \vec{R}_\perp} f(z\psi S_\perp) + \\ & [\bar{\Lambda}_z + \bar{\Lambda}_\perp] f(z\psi S_\perp) + \hat{P}[\Lambda_z+\Lambda_\perp]\Delta(z\psi S_\perp\Sigma); \end{aligned} \tag{9}$$

$$\begin{aligned} \frac{\partial}{\partial z}\Delta(z\psi S_\perp\Sigma) &= -\sqrt{\frac{M}{2E_0}}\,\frac{\vec{v}_\perp}{\cos\psi}\frac{\partial}{\partial \vec{R}_\perp}\Delta(z\psi S_\perp\Sigma) + \\ & + [\Lambda'_{zp}+\Lambda'_z+\Lambda'_\perp]\Delta(z\psi S_\perp\Sigma) + [\Lambda'_z - \bar\Lambda_z + \Lambda'_\perp - \bar\Lambda_\perp]\times \\ & \times \mathcal{D}_o(\Sigma) f(z\psi S_\perp) - \hat{P}_o[\Lambda_z+\Lambda_\perp]\Delta(z\psi S_\perp\Sigma), \end{aligned}$$

where

$$\Lambda_z = -\sum_{i=1}^{N} \frac{\partial}{\partial z} V(\vec R - \vec z_i)\frac{1}{E_c \sin 2\psi}\frac{\partial}{\partial\psi}, \quad \Lambda_\perp = \sum_{i=1}^{N} \frac{\partial}{\partial \vec R_\perp} V(\vec R-\vec z_i)\times$$

$$\frac{1}{\sqrt{2E_0M}}\,\frac{1}{\cos\psi}\,\frac{\partial}{\partial \vec v_\perp}, \quad \bar\Lambda_a = \hat P[\Lambda_a \mathcal{D}_c(\Sigma)], \quad a = z,\perp.$$

The initial conditions for the system of equations (9) are:

$$f(z\psi S_\perp)_{z=0} = \varphi(\psi S_\perp), \quad \Delta(z\psi S_\perp\Sigma)_{z=0} = 0. \tag{10}$$

Now, we solve this system of equations with initial conditions (10) for the function $f(z\psi S_\perp)$, i.e., exclude the function Δ from equations (9). As a result we obtain the closed equation for the distribution function $f(z\psi S_\perp)$.

Let us consider the following equation:

$$\begin{aligned} \frac{\partial}{\partial z}\Delta(z\psi S_\perp\Sigma) &= -\hat{\mathcal L}(z)\Delta(z\psi S_\perp\Sigma), \\ \hat{\mathcal L}(z) &= \sqrt{\frac{M}{2E_0}}\,\frac{\vec v_\perp}{\cos\psi}\frac{\partial}{\partial\vec R_\perp} - [\Lambda'_{zp}+\Lambda'_z+\Lambda'_\perp] \\ & + \hat P_o[\Lambda_z+\Lambda_\perp]; \end{aligned} \tag{11}$$

The solution of this equation can be written using the T-exponent form of the operator $\hat{\mathcal L}(z)$ with respect to the z parameter:

$$\Delta(z\psi S_\perp\Sigma) = T\exp\Big[-\int_0^z \hat{\mathcal L}(\tau)\,d\tau\Big]\Delta_0(\psi S_\perp\Sigma) \tag{12}$$

$\Delta_0(\psi S_\perp\Sigma)$ is any function.

Let us introduce the operator $\hat\Gamma(z)$ which is the inverse from the left T-exponent of the operator $\hat{\mathcal L}(z)$:

$$\hat\Gamma(z)\, T\exp\Big[-\int_0^z \hat{\mathcal L}(\tau)\,d\tau\Big] = 1. \tag{13}$$

Then after this the following change of variables in the system of equation (9) is made

$$\Delta(z\psi S_\perp\Sigma) = T\exp\Big[-\int_0^z\hat{\mathcal L}(\tau)\,d\tau\Big]\,\delta(z\psi S_\perp\Sigma). \tag{14}$$

For the function $\delta(z\psi S_\perp\Sigma)$, we have

$$\frac{\partial}{\partial z}\hat{\delta}(z\psi S_\perp \Sigma) = \hat{\Gamma}(z)\left[\Lambda_z' - \bar{\Lambda}_z + \Lambda_\perp' - \bar{\Lambda}_\perp\right] \times$$
$$\times\ \mathcal{D}_0(\Sigma)\, f(S_\perp \psi z)\ , \qquad \hat{\delta}(z\psi S_\perp \Sigma)_{z=0} = 0\ . \tag{15}$$

And finally for $\Delta(z\psi S_\perp \Sigma)$, we obtain

$$\Delta(z\psi S_\perp \Sigma) = T\exp\left[-\int_0^z \hat{\mathcal{L}}(\tau)d\tau\right] \cdot \int_0^z \Gamma(\tau)\,\times$$
$$\left[\Lambda_\tau' - \bar{\Lambda}_\tau + \Lambda_\perp'(\tau) - \bar{\Lambda}_\perp(\tau)\right] \mathcal{D}_0(\Sigma)\ f(\tau\psi\Sigma)\,d\tau . \tag{16}$$

As a result, the following equation for $f(z\psi S_\perp)$ can be obtained

$$\frac{\partial}{\partial z} f(z\psi S_\perp) = -\sqrt{\frac{M}{2E_0}}\,\frac{\vec{v}_\perp}{\cos\psi}\frac{\vec{\partial}}{\partial R_\perp} f(z\psi S_\perp) + \left[\bar{\Lambda}_z + \bar{\Lambda}_\perp\right]\times$$
$$f(z\psi S_\perp) + \hat{P}\left[\Lambda_z + \Lambda_\perp\right] T\exp\left[-\int_0^z \hat{\mathcal{L}}(\tau)d\tau\right] \cdot \int_0^z \hat{\Gamma}(\tau)\,\times \tag{17}$$
$$\left[\Lambda_\tau' - \bar{\Lambda}_\tau + \Lambda_\perp'(\tau) - \bar{\Lambda}_\perp(\tau)\right] \mathcal{D}_0(\Sigma)\ f(\tau\psi S_\perp)\,d\tau .$$

It is an exact equation describing " z -evolution" of the incident particle. However, it is a formal equation, because it is not clear how the introduced operators $T\exp\left[-\int_0^z \hat{\mathcal{L}}(\tau)d\tau\right]$, $\hat{\Gamma}(\tau)$ operate upon functions. Thus it is very important to know the small parameters which occur in this problem. They allow us to develop an expansion for equation (17) or for the system of equations (9).

The first small parameter is the effective parameter connected with the weakness of interaction between the fast particles and ions of the lattice. This can be explained taking into account that in classical mechanics the near-forward scattering is usually connected with the weakness of interaction between scatterer and scattered systems. This small parameter is denoted by ε . The second small parameter in this case is the angle between the direction of motion

of incident particle and the crystal axis or crystal plane. These small parameters are the same for light or heavy particles.

$\psi \sim \hbar \ll 1$: $\hbar$ is the effective parameter of smallness.

The initial energy of the incident particle in the channeling is high. Thus $E_0 \sim \varepsilon^{-1} \gg 1$, i.e., the initial energy of the incident particle is proportional to a large parameter.

For light particles the product $\varepsilon^{-1}\hbar$ can reasonably be supposed of the order of unity. In this case v_c is a large quantity and the terms with coefficients like $\sqrt{\frac{M}{2E_0}} = \frac{1}{v_c}$ are proportional to another small parameter δ. For light particles

$$v_c^{-1} \sim \delta \ll 1 \ ; \qquad \varepsilon^{-1}\hbar \sim 1 .$$

In the case of heavy particles the channeling parameter proportional to $\sqrt{\frac{M}{2E_0}}$ can be not small enough and the terms with coefficients proportional to $\sqrt{\frac{M}{2E_0}}$ become important. In this case we propose the following relations

$$\delta^{-1}\hbar \sim 1 \ ; \qquad P^{-1} \sim \tilde{\delta} \ll 1 ,$$

where P is the incident particle momentum.

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