Formation of high-energy beams of charged particles by channeling in crystals

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A general scheme is proposed for describing channeled beams of high-energy charged particles. It is based on studying the "z evolution" of a small subsystem in dynamical contact with a large system. A formally exact equation is obtained for the single-particle distribution function of the particles in the beam at different depths of penetration into a crystal. The first two approximations of this equation are studied. A connection with the continuum potential of Lindhard's theory is established. The asymptotic state of the particle distribution at large depths of penetration into the crystal is studied. The manner in which crystals have a forming influence on beams of high-energy protons and ions is discussed.

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INTRODUCTION

In the last decade, an important direction in theoretical and experimental investigations has been the study of the interaction and behavior of high-energy charged particles moving in crystals at small angles relative to the symmetry axes or planes of the system. There is by now an extensive bibliography on this problem.[1-5] The majority of physical effects encountered here are associated with the appearance of a specific orientation dependence in the observed phenomena, this being due to the interaction of the moving particles with the medium and the anomalously low energy losses of the particles.[6] This is explained by the particular nature of the motion of the particles, which is called *channeling*. It has been shown that this nature of the motion arises as a result of the strongly correlated influence on the moving particle of groups of ions in the crystal situated in symmetry planes or axes of the system. In this connection, it would be interesting to study the possibility of effective formation of beams of high-energy charged particles by channeling in crystals. The approach that we shall use to describe this phenomenon is presented briefly in Ref. 7 and is based on the methods of classical nonequilibrium statistical mechanics and the theory of stochastic processes.[8,9] We shall not dwell here on the justification for the classical description of channeling, since this question is discussed in detail in the literature.[10] We shall merely mention that at the present time there are no serious experimental data that discredit the classical description of channeling for protons and ions, and it is to the description of their motion that we shall apply the proposed scheme.

The existence in the channeling problem of a small effective parameter—the ratio $\varepsilon = |V\varepsilon|/V_z \ll 1$ of the mean transversal component of the particle's velocity to its longitudinal component—makes it possible to develop a perturbation theory with respect to this parameter and study successively the effects that arise in each order in the expansion in ε. The adiabatic approximation,[11,12] in which one ignores processes of energy exchange between the channeled particles and the crystal (the S and Σ systems in the terminology of Refs. 7–9), corresponds to the theory of the $o(\varepsilon)$ approximation. Therefore, it enables one to describe only the "input characteristics" of the channeling. In this approximation, the part played by the crystal reduces to forming effective "walls" of the potential energy, which determine possible directions of channeling of the particles in the channels of the motion. Such a description agrees completely with the description of the motion of the particles by means of the continuum potential of Lindhard's model.[1] An important feature that is not taken into account in the adiabatic approximation is the fact that as the particles move in the channels they are subject to an "irregular" dynamical effect produced by the ions of the crystal; this is responsible for processes in which energy is transferred between the S and Σ subsystems and can lead to a significant change in the state of the S subsystem. The effects associated with allowance for the mutual influence of the S and Σ systems appear in the theory of the $o(\varepsilon^2)$ approximation. One can approach their description in two ways, which correspond to different particularizations of the physical situation.

1) If the perturbing influence of the S system on Σ is such that the change in the state of the Σ system compared with the S system can be ignored and the "irregular" part of this perturbation is small compared with the "regular" part, then the "irregular" perturbation can be approximated by the influence on the S system of certain stochastic perturbing forces, which depend on the time. Specifically for channeling, this means that the average intracrystalline field produced by the ions of the lattice can be regarded as the "regular" effect of the Σ system on S, while the influence of the thermal vibrations of the ions about the equilibrium position can be taken into account by introducing weak stochastic forces. A Hamiltonian approach to the statistical description of the effect of perturbations of this kind is developed in Ref. 8. The equations then obtained for the distribution function of the S system have a Markov Fokker–Planck form, and their coefficients can be expressed in terms of the spectral characteristics of the perturbing forces. The effects associated with the description of channeling by means of equations of this type are described in Refs. 13–18.

2. If the influence of S on Σ cannot be ignored, which corresponds to the channeling of particle beams with

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high density of the "transverse" energy, or the effect of the thermal vibrations is not assumed to be small, it is necessary to treat the problem using a Hamiltonian $H(S)+H(\Sigma)+H_{int}$ that does not depend on the time. The second approach is more general in its formulation and must include the first approach as a special case.

In the present paper, we develop a general scheme for describing channeled beams of charged high-energy particles; the scheme is based on studying the "z evolution" of a small subsystem in dynamical contact with a large system or a thermal reservoir. We obtain a formally exact equation for the single-particle distribution function $f(zS_\perp)$ of the S subsystem, this equation describing the change in the distribution of the particles in the beam with its depth of penetration into the crystal in the plane of the phase variables transversal to the direction of channeling z and V_z. We study the $o(\varepsilon)$ and $o(\varepsilon^2)$ approximations of this equation. We establish the connection between the $o(\varepsilon)$ approximation and Lindhard's theory of the continuum potential. We show further that the z evolution satisfied by the single-particle distribution function $f(zS_\perp)$ of the S subsystem when allowance is made for the mutual influence of the S and Σ systems on each other in the $o(\varepsilon^2)$ approximation is a dynamical stochastic process whose asymptotic state as $z\to\infty$ is completely determined by the thermodynamic state of the crystal and the nature of the interaction between a channeled particle and the ions of the crystal.[1)] Studying the equation of this process and its asymptotic state $f(\infty, S_\perp)$, we discuss the manner in which crystals have a forming influence on beams of high-energy charged particles. Anticipating, we note that there is a qualitative difference between the effects that crystals have on beams of heavy ions and protons. The study of processes of z relaxation is important, since it follows from the data of Refs. 19–21 that an appreciable change in the state of the S system already occurs at relatively small depths of penetration (z) of the particles into the crystal.

1. FORMALLY EXACT EQUATION FOR THE Z EVOLUTION

We begin by giving the basic concepts and assumptions behind the proposed description.

The state of the complete system (the crystal plus the channeled particle) will be described by the total distribution function $D(tS\Sigma)$, where S are the phase variables of the channeled particle, Σ are the phase variables of the crystal, and t is the time. The evolution with respect to t of $D(tS\Sigma)$ is governed by the Liouville equation

$$\frac{\partial}{\partial t} D(tS\Sigma) = \mathcal{J}(S\Sigma)\, D(tS\Sigma), \tag{1}$$

where

$$\mathcal{J}(S\Sigma) = \mathcal{J}(S) + \mathcal{J}(\Sigma) + \mathcal{J}_{int};\ \mathcal{J}(S) = -\mathbf{V}\cdot\nabla_B;$$

$$\mathcal{J}(\Sigma) = -\sum_{j=1}^{N} \mathbf{V}_j \nabla_{r_j} + \sum_{i<j} \nabla_{r_j}\varphi(\mathbf{r}_j-\mathbf{r}_i)\cdot\left(\frac{1}{m_j}\nabla_{V_j} - \frac{1}{m_j}\nabla_{V_j}\right);$$

$$\mathcal{J}_{int} = \sum_{j=1}^{N} \nabla_R U(\mathbf{R}-\mathbf{r}_j)\cdot\left(\frac{1}{M}\nabla_V - \frac{1}{m_i}\nabla_{V_j}\right),\quad S=\{\mathbf{V},\mathbf{R}\};$$

$$\Sigma = \{\ldots, \mathbf{r}_j, \mathbf{V}_i, \ldots\};\ i=1, 2, \ldots, N,$$

M is the mass of the channeled particle, N is the number of sites of the crystal lattice (for simplicity, we shall assume that at each lattice site there is one ion with mass m_j), $U(\mathbf{R})$ is the potential of the interaction between the channeled particle and the lattice ions, $\mathbf{a}\cdot\nabla_b = a_x\nabla_{b_x} + a_y\nabla_{by} + a_z\nabla_{bz}$, and the function $D(tS\Sigma)$ can be assumed normalized to a constant,

$$\int (d\Sigma)\,(dS)\, D(tS\Sigma) = C,$$

which does not depend on the time; C may be unity, the particle number density, etc.

We shall obtain a closed equation for the reduced distribution function $f(zS_\perp)$, this equation describing the z evolution of the channeled particle [or the beam of particles, depending on the normalization of $f(zS_\perp)$] in the "plane" of the phase variables perpendicular to the direction of channeling.

We orient the coordinate system in which we shall describe the motion of the particle to make the z axis coincide with the direction of channeling. Otherwise, the coordinate system can be chosen arbitrarily. Then in the channeling problem there is a one-to-one correspondence between the time of motion and the position of the particle along the z axis; the z coordinate is uniquely related to the time t and vice versa. In view of this one-to-one connection between t and z, it is immaterial which parameter is used to describe the evolution of the system, i.e., the change in its state. For the study of channeling, it is convenient to take the position of the particle along the z axis as the evolution parameter, since the equations can then be formulated in a form convenient for obtaining an expansion with respect to ε. We note that the fact of a one-to-one correspondence between z and t is a consequence of physical observation. As a result, we have

$$\frac{d}{dz} = \frac{\partial}{\partial z} + \left(\frac{\partial t}{\partial z}\right)\frac{\partial}{\partial t}. \tag{2}$$

But $\partial t/\partial z = (V_z)^{-1}$. Finding $\partial/\partial t$ from (2) and substituting it in Eq. (1), we obtain

$$\frac{d}{dz} D'(t(z), V_z, z, S_\perp, \Sigma) = \frac{1}{V_z}\mathcal{J}(S_\perp\Sigma)\, D'(t(z), V_z, S_\perp, z, \Sigma), \tag{3}$$

where

$$\mathcal{J}(S_\perp\Sigma) = \mathcal{J}(S_\perp) + \mathcal{J}(\Sigma) + \mathcal{J}_{int};\ \mathcal{J}(S_\perp) = -\mathbf{V}_\perp\cdot\nabla_{R_\perp};\ S_\perp = \{\mathbf{V}_\perp, \mathbf{R}_\perp\}.$$

In what follows, we set $D'(t(z), V_z, z, S_\perp, \Sigma) = D(z, V_z, S_\perp, \Sigma)$, and then

$$\frac{d}{dz} D'(t(z) V_z, z, S_\perp, \Sigma) = \frac{\partial}{\partial z} D(z, V_z, S_\perp, \Sigma);$$

[1)] We shall not take into account the influence of the subsystem of free conduction electrons in the crystal on S, which can be done by including corresponding additive interaction terms in the treatment.

$$\frac{\partial}{\partial z} D(z, V_z, S_\perp, \Sigma) = \frac{1}{V_z} \mathcal{J}(S_\perp \Sigma) D(z, V_z, S_\perp, \Sigma).$$

Equation (3) cannot yet be regarded as the Liouville equation for the z evolution of the system $S+\Sigma$, since it does not preserve the normalization of the function $D(z, V_z, S_\perp, \Sigma)$, i.e.,

$$\int (dV_z\, dS_\perp\, d\Sigma)\, D(z, V_z, S_\perp, \Sigma) = \varphi(z).$$

This can be seen directly by integrating with respect to V_z, $S_\perp$, and Σ both sides of Eq. (3). Therefore, we carry out a further reduction of the phase space: $V_z, S_\perp, \Sigma \Rightarrow S_\perp, \Sigma$. To this end, we shall assume that the dependence of $D(z, V_z, S_\perp, \Sigma)$ on V_z is completely determined by the deterministic evolution parameter z and the stochastic variables $S_\perp$ and Σ, i.e., V_z is not an independent variable of the description but an observable of the z-evolution process on the $S_\perp$, Σ phase space of events. Hence,

$$\left.\begin{aligned} &\frac{\partial}{\partial z} D(z, V_z(z, S_\perp, \Sigma), S_\perp, \Sigma) \\ &= \frac{d}{dz} D(z, V_z(z, S_\perp, \Sigma), S_\perp, \Sigma) \\ &- \frac{\partial}{\partial V_z} D(z, V_z(z, S_\perp, \Sigma), S_\perp, \Sigma) \frac{\partial V_z(zS_\perp\Sigma)}{\partial z}. \end{aligned}\right\} \quad (4)$$

We substitute (4) in the left-hand side of Eq. (3) and equate the coefficients of the terms of the equation $\partial / \partial V_z\, D(z, V_z, S_\perp, \Sigma)$. We obtain an equation for $V_z(z, S_\perp, \Sigma)$:

$$\frac{\partial}{\partial z} V_z(zS_\perp\Sigma) = -\frac{1}{V_z(z, S_\perp, \Sigma) M} \sum_{j=1}^{N} \frac{\partial}{\partial z} U(\mathbf{R} - \mathbf{r}_j) \quad (5)$$

or

$$V_z(zS_\perp\Sigma) = \sqrt{V_0^2 - \frac{2}{M} \int_0^z \sum_{j=1}^{N} \frac{\partial}{\partial \tau} U_\tau(\mathbf{R} - \mathbf{r}_j)\, d\tau}, \quad (6)$$

where $V_0 = \sqrt{2E_0/M} = V_z(zS_\perp\Sigma)|_{z=0}$ ($z=0$ corresponds to the entry of the particle into the crystal); the subscript τ of U means that the z coordinate of the vector $\mathbf{R}$ is replaced by τ. The above discussion is completely analogous to Bogolyubov's well-known hypothesis about the reduction in the description for renormalization of perturbation theory and the elimination of a "secular" dependence on the time in studies in kinetic theory.[22] From (6), we have

$$\begin{aligned} \frac{1}{V_z(zS_\perp\Sigma)} &= \frac{1}{V_0} \sum_{n=0}^{\infty} \frac{(2n-1)!!}{2^n V_0^{2n}} \left(\frac{2}{M} \int_0^z d\tau \sum_{j=1}^{N} \frac{\partial}{\partial \tau} U_\tau(\mathbf{R} - \mathbf{r}) \right)^n \\ &= \frac{1}{V_0} + F(zS_\perp\Sigma). \end{aligned} \quad (7)$$

After these transformations, Eq. (3) takes the form

$$\frac{\partial}{\partial z} D(zS_\perp\Sigma) = \left[\frac{1}{V_0} + F(zS_\perp\Sigma) \right] \mathcal{J}(S_\perp\Sigma) D(zS_\perp\Sigma), \quad (8)$$

where

$$\frac{\partial}{\partial z} D(z, V_z, (zS_\perp\Sigma), S_\perp\Sigma) = \frac{\partial}{\partial z} D(zS_\perp\Sigma).$$

It is readily seen that the normalization of the function $D(zS_\perp\Sigma)$, which satisfies Eq. (8), is conserved under the z evolution. Note that the transformations made on (3) are identity transformations in the sense that any solution of Eq. (8) is a solution of Eq. (3) and, conversely, any solution of Eq. (3) with the subsidiary condition (5) is a solution of Eq. (8). Thus, our assumption about the nature of the dependence of $D(z, V_z, S_\perp, \Sigma)$ on V_z is equivalent to a restriction of the integral manifold of (3). Equation (8) is the basis of the further investigation. It will be regarded as the Liouville equation describing the z evolution of the S and Σ systems. To obtain an equation for the function $f(zS_\perp)$, we shall follow Ref. 9; the definition of the function $\Delta(zS_\perp\Sigma)$, or, which is the same thing, the choice of the projection operators,[23-25] is uniquely dictated by the boundary conditions of the problem:

$$D(zS_\perp\Sigma)_{z=0} = f(0S_\perp) D_0(\Sigma),$$

where $D_0(\Sigma)$ is the Gibbs distribution for the crystal, and $f(0S_\perp)$ is the initial distribution for the particle.

We define the projection operators $\hat{P}_0$ and $\hat{P}$ by

$$\hat{P}_0 = \int (d\Sigma) \ldots; \quad \hat{P} = D_0(\Sigma) \hat{P}_0 \quad (9)$$

and the functions $\Delta(zS_\perp\Sigma)$ and $f(zS_\perp)$ by

$$f(zS_\perp) = \hat{P}_0 D(zS_\perp\Sigma); \quad \Delta(zS_\perp\Sigma) = [1 - \hat{P}] D(zS_\perp\Sigma). \quad (10)$$

Note that

$$\Delta(zS_\perp\Sigma)_{z=0} = 0. \quad (11)$$

Using the definitions (9) and (10), we can obtain from Eq. (8) the following system of equations for the functions $\Delta(zS_\perp\Sigma)$ and $f(zS_\perp)$:

$$\left.\begin{aligned} &\frac{\partial}{\partial z} f(zS_\perp) = \hat{P}_0 \left[\frac{1}{V_0} + F(zS_\perp\Sigma) \right] \mathcal{J}(S_\perp\Sigma) D_0(\Sigma) f(zS_\perp) \\ &+ \hat{P}_0 \left[\frac{1}{V_0} + F(zS_\perp\Sigma) \right] \mathcal{J}(S_\perp\Sigma) \Delta(zS_\perp\Sigma); \\ &\frac{\partial}{\partial z} \Delta(zS_\perp\Sigma) = [1 - \hat{P}] \left[\frac{1}{V_0} + F(zS_\perp\Sigma) \right] \mathcal{J}(S_\perp\Sigma) \Delta(zS_\perp\Sigma) \\ &+ [1 - \hat{P}] \left[\frac{1}{V_0} + F(zS_\perp\Sigma) \right] \mathcal{J}(S_\perp\Sigma) D_0(\Sigma) f(zS_\perp). \end{aligned}\right\} \quad (12)$$

From the system of equations (12), we must eliminate the function $\Delta(zS_\perp\Sigma)$. For this, we consider the equation

$$\frac{\partial}{\partial z} \varphi(zS_\perp\Sigma) = \hat{\mathcal{L}}(z) \varphi(zS_\perp\Sigma), \quad (13)$$

where $\hat{\mathcal{L}}(z) = [1 - \hat{P}][1/V_0 + F(zS_\perp\Sigma)]\mathcal{J}(S_\perp\Sigma)$. The solution of (13) with any initial $\varphi(0, S_\perp, \Sigma)$ can be formally represented in the form

$$\varphi(zS_\perp\Sigma) = T \exp\left[\int_0^z d\tau\, \hat{\mathcal{L}}(\tau) \right] \varphi(0, S_\perp, \Sigma). \quad (14)$$

The symbol T denotes the operation of ordering with respect to the parameter z.

We introduce the operator $\hat{\Gamma}(z)$, which is the left inverse with respect to the operator of the time-ordered exponential of the operator $\hat{\mathcal{L}}(z)$, i.e.,

$$\hat{\Gamma}(z)\, T \exp\left[\int_0^z d\tau\, \hat{\mathcal{L}}(\tau) \right] = 1. \quad (15)$$

After this, in the second equation in (12) we go over from the function $\Delta(zS_\perp\Sigma)$ to the function $\psi(zS_\perp\Sigma)$ in accordance with

$$\Delta(zS_\perp\Sigma) = T\exp\left[\int_0^z d\tau\,\hat{\mathscr{L}}(\tau)\right]\psi(zS_\perp\Sigma). \tag{16}$$

For $\psi(zS_\perp\Sigma)$, we have the equation

$$\frac{\partial}{\partial z}\psi(zS_\perp\Sigma) = \hat{\Gamma}(z)\,[1-\hat{P}]\left[\frac{1}{V_0}+F(zS_\perp\Sigma)\right] \times \mathcal{J}(S_\perp\Sigma)\,D_0(\Sigma)\,f(zS_\perp);\ \psi(zS_\perp\Sigma)_{z=0}=0. \tag{17}$$

Hence, for $\psi(zS_\perp\Sigma)$ we have

$$\psi(zS_\perp\Sigma) = \int_0^z d\tau\,\hat{\Gamma}(\tau)\,[1-\hat{P}]\left[\frac{1}{V_0}+F(\tau S_\perp\Sigma\right]\mathcal{J}_\tau \times (S_\perp\Sigma)\,D_0(\Sigma)\,f(\tau S_\perp), \tag{18}$$

where $\mathcal{J}_\tau(S_\perp\Sigma)$ means that the coordinate z in the expression $\mathcal{J}(S_\perp\Sigma)$ is replaced by τ. Using (16)–(18), we obtain

$$\Delta(zS_\perp\Sigma) = T\exp\left[\int_0^z \hat{\mathscr{L}}(\tau)\,d\tau\right]\int_0^z d\tau\,\hat{\Gamma}(\tau) \times [1-\hat{P}]\left[\frac{1}{V_0}+F(\tau S_\perp\Sigma)\right]\mathcal{J}_\tau(S_\perp\Sigma)\,D_0(\Sigma)\,f(\tau S_\perp). \tag{19}$$

We substitute (19) in the first equation of (12), obtaining a closed and formally exact equation for $f(\tau S_\perp)$:

$$\frac{\partial}{\partial z}f(zS_\perp) = \hat{P}_0\left[\frac{1}{V_0}+F(zS_\perp\Sigma)\right]\mathcal{J}(S_\perp\Sigma)\,D_0(\Sigma)\,f(zS_\perp) + \hat{P}_0\left[\frac{1}{V_0}+F(zS_\perp\Sigma)\right]\mathcal{J}(S_\perp\Sigma)\,T\exp\left[\int_0^z \hat{\mathscr{L}}(\tau)\,d\tau\right] \times\int_0^z d\tau\,\hat{\Gamma}(\tau)\,[1-\hat{P}]\left[\frac{1}{V_0}+F(\tau S_\perp\Sigma)\right]\mathcal{J}_\tau(S_\perp\Sigma)\,D_0(\Sigma)\,f(\tau S_\perp). \tag{20}$$

As we have already emphasized several times above (see also Ref. 7), Eq. (20) has a formal nature. To obtain genuine physical information, we shall develop a perturbation theory for (20). To this end, we ascribe to each physical variable a definite characteristic scale of its measurement, which renders Eq. (20) or the system of equations (12) dimensionless. It is then possible to check the order of magnitude of each term of the equation. Thus, we introduce

$$\left.\begin{aligned} &\mathbf{R}=e\mathbf{R};\ \mathbf{r}_j=e\mathbf{r}_j;\ \mathbf{V}_\perp=v_\perp\mathbf{V}_\perp;\\ &V_z=V_0V_z;\ V_0=\sqrt{2E_0/M};\ U(\mathbf{R})=\Phi_0U(\mathbf{R}).\end{aligned}\right\} \tag{21}$$

For channeling, the following relations between the scales of the quantities (21) are characteristic:

$$\left.\begin{aligned} &v_\perp/V_0=\varepsilon\ll 1;\ \Phi_0/(Mv_\perp^2)\sim 1;\ \Phi_0/(V_0Mv_\perp)\sim\varepsilon;\\ &\Phi_0/E_0=2\Phi_0Mv_\perp^2/(Mv_\perp^2MV_0^2)\sim(v_\perp/V_0)^2\sim(\varepsilon^2);\ l\sim a.\end{aligned}\right\} \tag{22}$$

Note that Φ_0 contains an effective factor related to the number of ions that interact simultaneously with the particle.

2. THE $o(\varepsilon)$ APPROXIMATION

Using (21), we make Eq. (20) dimensionless and retain on its right-hand side quantities of order $o(\varepsilon)$. We obtain the simple equation

$$\frac{\partial}{\partial z}f(zS_\perp) = -\sqrt{\frac{M}{2E_0}}\mathbf{V}_\perp\cdot\nabla_{R_\perp}f(zS_\perp)+\frac{1}{\sqrt{2E_0M}} \times\left\langle\sum_{j=1}^N\nabla_{R_\perp}U(\mathbf{R}-\mathbf{r}_j)\right\rangle_\Sigma\nabla_{V_\perp}f(zS_\perp), \tag{23}$$

where $\langle\ldots\rangle_\Sigma$ denotes averaging of the quantity within the brackets with respect to the Gibbs distribution for the crystal. Equation (23) describes the motion of a particle of mass M in the field of the crystal lattice without allowance for the processes of energy exchange between them. Equation (23) can be obtained directly from (8) by seeking $D(zS_\perp\Sigma)$ in the form $D(zS_\perp\Sigma) = D_0(\Sigma)f(zS_\perp)$, i.e., by completely ignoring the change in the state of the crystal subsystem as a result of the z evolution. It is therefore natural to call (23) the *adiabatic* approximation. The part played by the crystal in this approximation reduces solely to forming the relief of the potential energy surface in the configuration space of the particle and ensuring the possible directions for channeling of the particles. The entire phase space of the states $S_\perp$ of the particle is divided into two parts, which do not intersect in the process of the z evolution; the first corresponds to the trapping of particles into a channel of the motion in the given direction of channeling, while the second corresponds to dechanneling and ensures the spatial distribution of the particles in scattering experiments. It is natural to expect that Eq. (23) describes the picture of the channeling at very small penetration depths and, essentially, is suitable only for calculating the energy characteristics of the capture of particles in channels of the motion and for describing the scattering of particles by crystals in the channeling regime at small penetration depths z.

3. AXIAL CHANNELING OF POSITIVELY CHARGED PARTICLES

We now consider the calculation of $\langle\sum_{j=1}^N U(\mathbf{R}-z_j)\rangle_\Sigma$. For simplicity, we shall assume that the crystal has the symmetry of a cubic lattice and restrict ourselves to the harmonic approximation for it. Then in accordance with Ref. 26,

$$\begin{aligned}\left\langle\sum_{j=1}^N U(\mathbf{R}-\mathbf{z}_j)\right\rangle_\Sigma &= \frac{1}{v}\nu(0)+\frac{2}{v}\sum_{n=1}^\infty \nu(q_0n)\exp[-n^2W_\theta(q_0)] \times\cos(nq_0z)\frac{2}{v}+\frac{2}{v}\sum_{m=1}^\infty \nu(q_0m)\exp[-m^2W_\theta(q_0)]\cos(mq_0x)\\ &+\frac{2}{v}\sum_{l=1}^\infty \nu(q_0l)\exp[-l^2W_\theta(q_0)]\cos(lq_0y)\\ &+\frac{4}{v}\sum_{n,m=1}^\infty \nu\left(q_0\sqrt{n^2+m^2}\right)\exp[-(n^2+m^2)W_\theta(q_0)]\cos(nq_0z) \times\cos(mq_0x)+\frac{4}{v}\sum_{n,l=1}^\infty \nu\left(q_0\sqrt{n^2+l^2}\right)\exp[-(n^2+l^2)W_\theta(q_0)]\\ &\times\cos(lq_0y)\cos(nq_0z)+\frac{4}{v}\sum_{l,m=1}^\infty \nu\left(q_0\sqrt{l^2+m^2}\right) \times\exp[-(l^2+m^2)W_\theta(q_0)]\cos(lq_0y)\cos(mq_0x)\\ &+\frac{8}{v}\sum_{n,m,l=1}^\infty \nu\left(q_0\sqrt{n^2+m^2+l^2}\right) \times\exp[-(n^2+m^2+l^2)W_\theta(q_0)]\cos(lq_0y)\\ &\times\cos(mq_0x)\cos(nq_0z)\ ^{2)},\end{aligned} \tag{24}$$

where $v=\Omega/N$, Ω is the volume of the crystal, n, m, l

are positive integers, N is the number of sites, $q_0 = 2\pi/a$, a is the lattice constant, $v(k)$ is the Fourier transform of the particle–ion interaction potential, and $W_\theta(q_0)$ is the Debye–Waller factor. In the special case under consideration, it is given by the expression[28]

$$W_\theta(q_0) = \frac{v\Theta(q_0^2)}{(2\pi)^3 6m} \sum_{S=1}^{3} \int_0^{q_0} dq \frac{1}{\omega_S^2(q)}. \quad (25)$$

The actual form of (24) for $\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\rangle_\Sigma$ is due to the special choice of the coordinate system in which the motion of the particles is described (Fig. 1). Indeed, in accordance with (24), a maximum of the potential energy corresponds to the particle position $\mathbf{R}_\perp = 0$. [For positively charged particles $U(\mathbf{R}-\mathbf{r}_j) > 0$.] In the case of axial channeling, it is convenient to choose the coordinate system as shown in Fig. 2. The z axis coincides with the "middle" of the channel for the motion of the particles, which corresponds to the minimum of the potential energy of the field of the crystal lattice.

Such a choice of the coordinate system is associated with the following substitution in Eq. (24):

$$\cos[mq_0x] \to (-1)^m \cos[mq_0x]; \quad \cos[lq_0y] \to (-1)^l \cos[lq_0y].$$

Finally, (24) can be represented in the form

$$\begin{aligned}
&\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_\Sigma \\
&= \frac{2}{v} \sum_{n=1}^{\infty} v(q_0 n) \exp[-n^2 W_\Theta(q_0)] \{\cos(q_0 nz) \\
&\quad + (-1)^n \cos(q_0 nx) + (-1)^n \cos(q_0 ny)]\} \\
&\quad + \frac{4}{v} \sum_{n,l=1}^{\infty} v\left(q_0\sqrt{n^2+l^2}\right) \\
&\quad \times \exp[-(n^2+l^2) W_\Theta(q_0)] \{(-1)^l \cos(lq_0x)\cos(nq_0z) \\
&\quad + (-1)^l (-1)^n \cos(lq_0x)\cos(q_0ny) + (-1)^l \cos(lq_0y) \\
&\quad \times \cos(q_0yz)\} + \frac{8}{v} \sum_{n,m,l=1}^{\infty} v\left(q_0\sqrt{n^2+m^2+l^2}\right) \exp[-(n^2+m^2+l^2) \\
&\quad \times W_\Theta(q_0)] \cos(nq_0z)(-1)^l (-1)^m \cos(lq_0y)\cos(mq_0x). \quad (26)
\end{aligned}$$

We now turn to Eq. (23). It has the structure

$$\frac{\partial}{\partial z} f(zS_\perp) = \varepsilon \hat{A}(zS_\perp) f(zS_\perp), \quad (27)$$

where

$$\hat{A}(zS_\perp) = -\sqrt{\frac{M}{2E_0}} \mathbf{v}_\perp \cdot \nabla_{\mathbf{v}_\perp} + \frac{1}{\sqrt{2E_0M}} \left\langle \sum_{j=1}^{N} \nabla_{\mathbf{R}_\perp} U(\mathbf{R}-\mathbf{r}_j)\right\rangle \nabla_{\mathbf{v}_\perp}.$$

Taking into account the expression (26), we see that the coefficient of the small parameter, $\hat{A}(zS_\perp)$, can be represented as a sum of two operators: the operator-valued function $\hat{A}_1(S_\perp)$, which does not depend on z, and the operator-valued function $A_2(zS_\perp)$, which oscillates

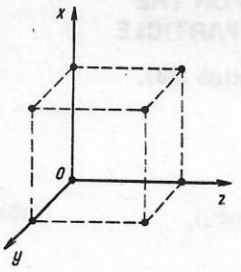

FIG. 1.

rapidly with respect to z. Equations of such type can be solved by the method of averaging[27] developed in nonlinear mechanics. The essence of this method is that Eq. (27) can be approximated to a definite degree of accuracy by an equation of the form

$$\frac{\partial}{\partial z} f(zS_\perp) = \varepsilon \hat{Q}(S_\perp) f(zS_\perp), \quad (28)$$

where

$$\hat{Q}(S_\perp) = \lim_{T\to\infty} \frac{1}{T} \int_0^T d\tau \hat{A}(\tau S_\perp) = \hat{A}_1(S_\perp).$$

In what follows, we shall denote averaging of the operators by a bar. Since the operation $\nabla_{\mathbf{R}_\perp}$ commutes with the averaging, we can average the expression (26) directly:

$$\begin{aligned}
&\overline{\left\langle \sum_j U(\mathbf{R}-\mathbf{r}_j)\right\rangle_\Sigma} \\
&= \frac{1}{v} v(0) + \frac{2}{v} \sum_{m=1}^{\infty} v(q_0 m) \exp[-m^2 W_\Theta(q_0)] \\
&\quad \times [\cos(mq_0x)(-1)^m + \cos(mq_0y)(-1)^m] \\
&\quad + \frac{4}{v} \sum_{n,m=1}^{\infty} v\left(q_0\sqrt{n^2+m^2}\right) \\
&\quad \times \exp[-(n^2+m^2) W_\Theta(q_0)](-1)^m (-1)^n \cos(nq_0x)\cos(mq_0y). \quad (29)
\end{aligned}$$

But the field (29) is none other than the continuum potential model proposed by Lindhard for the classical description of channeling, an additional averaging over the phonon vibrations of the lattice[1] having been made in (29). The central idea of this model is the assumption that the channeled particle does not feel the individual ions of the lattice but interacts directly with rows or planes of strongly correlated ions. Thus, the $o(\varepsilon)$ approximation, or the adiabatic approximation, of Eq. (20) leads to Lindhard's model. The individual influence of the ions can be taken into account by solving (23) perturbatively, the averaged solution being taken as the zeroth approximation.

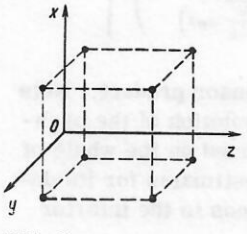

FIG. 2.

[2)] For some forms of long-range potentials, $v(0)$ does not exist. However, the value of the potential energy (24) can always be redefined by this component.

4. HARMONIC APPROXIMATION FOR THE TRAJECTORY OF A CHANNELED PARTICLE

The solution of the averaged equation (23),

$$\frac{\partial}{\partial z} f(zS_\perp) = -\sqrt{\frac{M}{2E_0}}\, \mathbf{V}_\perp \cdot \nabla_{\mathbf{R}_\perp} f(zS_\perp) + \frac{1}{\sqrt{2E_0 M}} \times \overline{\left\langle \sum_{j=1}^{N} \nabla_{\mathbf{R}_\perp} U(\mathbf{R}-\mathbf{r}_j) \right\rangle_\Sigma} \nabla_{\mathbf{v}_\perp} f(zS_\perp), \tag{30}$$

can be represented in the form

$$f(zS_\perp) = g(T_{-z} S_\perp), \tag{31}$$

where $g(S_\perp)$ is the initial distribution function and the operator T_z is defined on $S_\perp$ by the equations

$$\left.\begin{aligned} &\frac{\partial x}{\partial t} = V_x; \\ &\frac{\partial y}{\partial t} = V_y; \qquad t = \sqrt{\frac{M}{2E_0}}\, z; \\ &\frac{\partial}{\partial t} V_x = -\frac{\partial}{\partial x} \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle_\Sigma} \frac{1}{M}; \\ &\frac{\partial}{\partial t} V_y = -\frac{\partial}{\partial y} \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle_\Sigma} \frac{1}{M}. \end{aligned}\right\} \tag{32}$$

In (29), we restrict ourselves to the first term. Such an approximation can be justified in the case when $U(\mathbf{R})$ has a long-range nature, which actually corresponds to the channeling of heavy ions.[2] Then the main contribution in the sum (29) corresponds to small values of (n,m). From (32), we finally obtain

$$\left.\begin{aligned} &\frac{\partial^2 x}{\partial t^2} = -\frac{2q_0}{Mv}\, \nu(q_0) \sin(q_0 x) \exp[-W_\Theta(q_0)]; \\ &\frac{\partial^2}{\partial t^2} y = -\frac{2q_0}{Mv}\, \nu(q_0) \sin(q_0 y) \exp(-W_\Theta(q_0)]. \end{aligned}\right\} \tag{33}$$

The system of equations (32) with the known restrictions on the initial conditions (small values of V_0^x and V_0^y) describes oscillations about the position of equilibrium, which can be calculated in the harmonic approximation:

$$\left.\begin{aligned} &q_0 x \ll \pi/2;\ q_0 y \ll \pi/2; \\ &\frac{\partial^2}{\partial t^2} x = -\Re(\Theta q_0)\, x;\ \frac{\partial^2}{\partial t^2} y = -\Re(\Theta q_0)\, y; \\ &\Re(\Theta q_0) = \omega^2(\Theta) = \frac{2q_0^2}{Mv}\, \nu(q_0) \exp[-W_\Theta(q_0)]. \end{aligned}\right\} \tag{34}$$

The operator T_z corresponding to the harmonic approximation is

$$\left.\begin{aligned} &T_z \begin{pmatrix} x \\ V_x \end{pmatrix} \otimes \begin{pmatrix} y \\ V_y \end{pmatrix} = T_z \begin{pmatrix} x \\ V_x \end{pmatrix} \otimes T_z \begin{pmatrix} y \\ V_y \end{pmatrix}; \\ &T_z = \begin{pmatrix} \cos\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right) & \frac{1}{\omega_\Theta} \sin\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right) \\ -\omega_\Theta \sin\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right) & \cos\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right) \end{pmatrix}. \end{aligned}\right\} \tag{35}$$

Here, the symbol $\otimes$ denotes the tensor product. Note that by virtue of the approximate solution of the problem (32) the operator T_z is not defined on the whole of the phase space. One can obtain estimates for its domain of definition. This corresponds to the interior points of the ellipse[11]

$$x^2\omega_\Theta^2 + V_x^2 = (\omega_\Theta a/12)^2; \qquad y^2\omega_\Theta^2 + V_y^2 = (\omega_\Theta a/12)^2. \tag{36}$$

The trajectory of the particle in the harmonic approximation has the form

$$\begin{bmatrix} x(z) \\ y(z) \end{bmatrix} = \begin{bmatrix} x_0 \\ y_0 \end{bmatrix} \cos\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right) + \frac{1}{\omega_\Theta} \begin{bmatrix} V_x^0 \\ V_y^0 \end{bmatrix} \sin\left(\sqrt{\frac{M}{2E_0}}\, \omega_\Theta z\right), \tag{37}$$

where $\begin{bmatrix} x_0 \\ y_0 \end{bmatrix}$ and $\begin{bmatrix} V_0^x \\ y_0 \end{bmatrix}$ are the initial position and velocity of the particle at the point $z = 0$.

Further, we use perturbation theory to take into account the terms of Eq. (23) neglected in the averaging and obtain the corrections to the harmonic approximation of the trajectory (37) in the case of channeling. With allowance for the terms of rapidly oscillating nature with the largest magnitude, the equation of motion for $f(zS_\perp)$ in the harmonic approximation has the form

$$\frac{\partial}{\partial z} f(zS_\perp) = -\sqrt{\frac{M}{2E_0}}\, \mathbf{V}_\perp \cdot \nabla_{\mathbf{R}_\perp} f(zS_\perp) + \sqrt{\frac{M}{2E_0}} [R(\Theta q_0) + h(\Theta q_0 z)] \left[x \frac{\partial}{\partial V_y} + y \frac{\partial}{\partial V_y}\right] f(zS_\perp), \tag{38}$$

where

$$h(\Theta q_0 z) = \frac{4q_0^2}{Mv}\, \nu(q_0\sqrt{2}) \exp[-2W_\Theta(q_0)] \cos(q_0 z) - \frac{8q_0^2}{Mv}\, \nu(q_0\sqrt{3}) \exp[-3W_\Theta(q_0)] \cos(q_0 z).$$

Using the expression (37) as the zeroth approximation for the trajectory of the channeled particle, we obtain for the trajectory of the particle in the harmonic approximation in the first order of perturbation theory the expression

$$\begin{bmatrix} x(z) \\ y(z) \end{bmatrix} = \begin{bmatrix} A_x(z) \\ A_y(z) \end{bmatrix} \cos\left(\omega_\Theta \sqrt{\frac{M}{2E_0}}\, z\right) + \begin{bmatrix} B_x(z) \\ B_y(z) \end{bmatrix} \sin\left(\omega_\Theta \sqrt{\frac{M}{2E_0}}\, z\right), \tag{39}$$

where

$$A_{\binom{x}{y}}(z) = \binom{x_0}{y_0} + \int_0^z d\tau \sqrt{\frac{M}{2E_0}}\, h(\Theta q_0 \tau) \left\{ \frac{1}{\omega_\Theta} \binom{x_0}{y_0} \times \sin\left(2\omega_\Theta \sqrt{\frac{M}{2E_0}}\, \tau\right) - \frac{1}{\omega_\Theta^2} \binom{V_0^x}{V_0^y} \sin^2\left(\omega_\Theta \sqrt{\frac{M}{2E_0}}\, \tau\right) \right\};$$

$$B_{\binom{x}{y}}(z) = \frac{1}{\omega_\Theta} \binom{V_0^x}{V_0^y} + \sqrt{\frac{M}{2E_0}} \int_0^z d\tau h(\Theta q_0 \tau) \left\{ \frac{1}{2\omega_\Theta^2} \begin{bmatrix} V_0^x \\ V_0^y \end{bmatrix} \times \sin\left(2\omega_\Theta \sqrt{\frac{M}{2E_0}}\, \tau\right) - \frac{1}{\omega_\Theta} \binom{x_0}{y_0} \sin^2\left(\omega_\Theta \sqrt{\frac{M}{2E_0}}\, \tau\right) \right\}.$$

Allowance for the oscillating terms in Eq. (23) leads to a modulation in the amplitude of the channeled particle, this being determined by the individual influence of the ions of the crystal.

Using the expression (29), we can estimate the critical angle of entry of the particles into the crystal governing the capture of particles into the channeling regime. For axial channeling in a cubic crystal,

$$\frac{M(V_0 \sin\alpha_c)^2}{2} = \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle}^{*}_{\substack{\Sigma x=a/2 \\ y=0}} = \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle}^{*}_{\substack{\Sigma x=0 \\ y=a/2}};$$

$$\overline{\left\langle \sum_j U(\mathbf{R}-\mathbf{r}_j) \right\rangle}^{*}_{\Sigma} = \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle_\Sigma} - \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) \right\rangle}_{\substack{\Sigma x=0 \\ y=0}}. \tag{40}$$

Then, since $\sin\alpha_c \sim \alpha_c$ at small α_c, we have

$$\alpha_c = \left(\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle}^{*}_{\substack{x=a/2\\ y=0}}/E_0\right)^{1/2}. \tag{41}$$

5. PLANAR CHANNELING OF POSITIVELY CHARGED PARTICLES

We now consider the situation when the direction of the channel of the motion of the particles makes an arbitrary angle with a crystallographic axis. Again, we shall assume that the crystal has cubic symmetry and the harmonic approximation applies. By virtue of the translational symmetry of the lattice, definite selection rules with respect to $\mathbf{k}$ exist for averages of the form $\langle\sum_{j=1}^{N}\exp(-i\mathbf{k}\cdot\mathbf{r})\rangle_\Sigma$. However, if our coordinate system in the case of planar channeling is arranged in such a way that the symmetry axes of the crystal are not parallel to the axes of the coordinate system, the selection rules with respect to $\mathbf{k}$ will differ somewhat from those earlier. We denote by o, x, y, z the coordinate system in which we consider the motion of the particles. We direct the z axis along the channel of the motion of a particle. We choose the coordinate system o, x, x', y', z' to make its axes ox', oy', oz' coincide with the directions of the principal crystallographic axes of the cubic crystal. Thus, as can be seen in Fig. 3, the channeling direction oz makes the angle α with the direction of the crystallographic axis oz'. The axis ox coincides with the axis ox'. Equation (23) is written down in the coordinate system o, x, y, z'. The selection rules for the correlation averages with respect to the crystal subsystem can be established very readily in the coordinate system o, x', y', z', since in it the principal symmetry axes of the group of translations of the crystal coincide with the directions of the coordinate axes. Expressing the value of $\mathbf{k}\cdot\mathbf{r}_j$ in the coordinate system o, x', y', z', we have

$$\left.\begin{aligned} &\mathbf{k}\cdot\mathbf{r}_j = k_x x_{\prime\prime} + k_z z_j + k_y y_j;\\ &x_j = x'_j,\\ &y_j = y'_j\cos\alpha - z'_j\sin\alpha;\\ &z_j = z'_j\cos\alpha + y'_j\sin\alpha, \end{aligned}\right\} \tag{42}$$

whence

$$\mathbf{k}\cdot\mathbf{r}_j = k_x x'_j + y'_j(k_y\cos\alpha + k_z\sin\alpha) + z'_j(k_z\cos\alpha - k_y\sin\alpha) \tag{43}$$

and

$$\left\langle\sum_{j=1}^{N}\exp(-i\mathbf{k}\cdot\mathbf{r}_j)\right\rangle_\Sigma = \left\langle\sum_{j=1}^{N}\exp[-ik_x x'_j - iy'_j(k_z\sin\alpha + k_y\cos\alpha) - iz'_j(k_z\cos\alpha - k_y\sin\alpha)]\right\rangle_\Sigma. \tag{44}$$

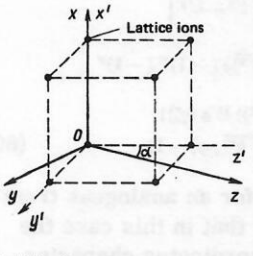

FIG. 3.

Since the axes ox, oy', oz' coincide with the principal axes of the translational symmetry of the crystal, the average (44) must not be changed by a translation in the directions ox', oy', oz' by an amount that is a multiple of the lattice constant. Hence, for k_x, k_y, k_z we have

$$\begin{aligned} k_z &= q_0(n\cos\alpha + l\sin\alpha);\\ k_y &= q_0(l\cos\alpha - n\sin\alpha);\\ k_x &= q_0 m, \end{aligned} \tag{45}$$

where $q_0 = 2\pi/a$; n, m, l are positive integers between $-\infty$ and $+\infty$.

Under rotations of the coordinate axes, the square of a vector is invariant, and therefore $(\mathbf{k}')^2 = (\mathbf{k})^2$. Using this, and also the explicit form of the expression for the Debye–Waller factor,[28] we obtain

$$\begin{aligned} &\frac{1}{v}\sum_{\mathbf{k}} v(k)\exp(i\mathbf{k}\cdot\mathbf{R})\frac{1}{N}\left\langle\sum_{j=1}^{N}\exp(-i\mathbf{k}\cdot\mathbf{r}_j)\right\rangle_\Sigma\\ &= \frac{1}{v}\sum_{n,m,l} v(q_0\sqrt{n^2+m^2+l^2})\exp[(-n^2-l^2-m^2)W_\Theta(q_0)]\\ &\times\exp[iq_0 mx]\exp[iq_0 n(z\cos\alpha - y\sin\alpha)]\exp[iq_0 l(z\sin\alpha + y\cos\alpha)]. \end{aligned} \tag{46}$$

In what follows, to describe the channeling effect, it will be convenient to displace the coordinate system o, x, y, z by a vector $\mathbf{b}$ to make the channeling axis oz coincide with the line of the minimum of the potential energy on the energy surface corresponding to the given direction α:

$$\mathbf{b} = (b_x, b_y, b_z) = (b_1, b_2\cos\alpha - b_3\sin\alpha, b_3\cos\alpha + b_2\sin\alpha). \tag{47}$$

As a result, (46) can be rewritten in the form

$$\begin{aligned} &\left\langle\sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r})\right\rangle_\Sigma = \frac{1}{v}v(0) + \frac{2}{v}\sum_{n=1}^{\infty} v(q_0 n)\\ &\times\exp[-n^2 W_\Theta(q_0)]\{\cos[nq_0(z\cos\alpha - y\sin\alpha) + nq_0 b_3]\\ &+\cos(nq_0 x + nq_0 b_1) + \cos[nq_0(z\sin\alpha + y\cos\alpha) + nq_0 b_2]\}\\ &+\frac{4}{v}\sum_{n,m=1}^{\infty} v(q_0\sqrt{n^2+m^2})\exp[-(n^2+m^2)W_\Theta(q_0)]\\ &\times\{\cos(mq_0 x + mq_0 b_1)\cos[nq_0(z\cos\alpha - y\sin\alpha) + nq_0 b_3]\\ &+\cos(mq_0 x + mq_0 b_1)\cos[nq_0(y\cos\alpha + z\sin\alpha) + nq_0 b_2]\}\\ &+\frac{2}{v}\sum_{n,l=1}^{\infty} v(q_0\sqrt{n^2+l^2})\exp[-(n^2+l^2)W_\Theta(q_0)]\\ &\times\{\cos(nq_0 z\cos\alpha - nq_0\sin\alpha y + lq_0 y\cos\alpha\\ &+lq_0 z\sin\alpha + nq_0 b_3 + b_2 q_0 l)\\ &+\cos(lq_0 z\sin\alpha + nq_0 y\sin\alpha + lq_0 z\sin\alpha + nq_0 b_3 + b_2 q_0 l)\\ &+\cos(lq_0 z\sin\alpha + nq_0 y\sin\alpha + lq_0 y\cos\alpha - nq_0 z\cos\alpha\\ &-nq_0 b_3 + b_2 q_0 l)\} + \frac{4}{v}\sum_{n,m,l=1}^{\infty} v(q_0\sqrt{n^2+m^2+l^2})\\ &\times\exp[-(n^2+m^2+l^2)W_\Theta(q_0)]\cos(mq_0 x + mq_0 b_1)\\ &\times\{\cos(nq_0 z\cos\alpha - nq_0 y\sin\alpha + lq_0 y\cos\alpha\\ &+lq_0 z\sin\alpha + nq_0 b_3 + lq_0 b_2) + \cos(lq_0 z\sin\alpha\\ &+nq_0 y\sin\alpha + lq_0 y\cos\alpha - nq_0 z\cos\alpha - nq_0 b_3 + lq_0 b_2)\}. \end{aligned} \tag{48}$$

The expression (48) must be used to find the coefficients in Eq. (23). The case $\alpha = 0$ corresponds to axial channeling. We shall again solve Eq. (23) by the method of averaging, which will correspond to its solution up to

terms of order $o(\varepsilon)$:

$$\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} = \lim_{T\to\infty}\frac{1}{T}\int_0^T \left\langle d\tau \sum_{j=1}^{N} U_\tau(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}. \tag{49}$$

The subscript τ in U_τ indicates that the z component of $\mathbf{R}$ is replaced by τ. As a result, for $\overline{\langle\sum_j^N U(\mathbf{R}-\mathbf{r}_j)\rangle_\Sigma}$ we have

$$\begin{aligned}
\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} &= \frac{1}{v}\nu(0)+\frac{2}{v}\sum_{m=1}^{\infty}\nu(q_0 m)\\
&\times \exp[-m^2 W_\Theta(q_0)]\cos(mq_0 x + mq_0 b_1)\\
+\frac{2}{v}\sum_{l,\,n=1}^{\infty}&\nu\left(q_0\sqrt{n^2+l^2}\right)\exp[-(l^2+n^2)W_\Theta(q_0)]\\
\times\cos[(nq_0\sin\alpha+lq_0\cos\alpha)y+b_2 lq_0-b_3 nq_0]&\,\Delta(lq_0\sin\alpha-nq_0\cos\alpha)\\
+\frac{4}{v}\sum_{n,\,m,\,l}&\nu\left(q_0\sqrt{n^2+m^2+l^2}\right)\exp[-(n^2+m^2+l^2)W_\Theta(q_0)]\\
\times\cos(mq_0 x+mq_0 b_\perp)\cos[(nq_0\sin\alpha+lq_0\cos\alpha)y+b_2 lq_0-b_3 nq_0]&\\
\times\Delta(lq_0\sin\alpha-nq_0\cos\alpha).&
\end{aligned} \tag{50}$$

In (50), $\alpha\neq 0$, and $\Delta(x)$ is the Kronecker delta:

$$\Delta(x)=\begin{cases}1, & x=0;\\ 0, & x\neq 0.\end{cases}$$

In (50), the directions of the axis of the channel of the motion of the particle are distinguished when the following equation is satisfied:

$$l\sin\alpha - n\cos\alpha = 0;\quad \alpha=\tan^{-1}\, n/l. \tag{51}$$

We call these directions *channels of the motion of the particles*. We relate the indices n and l, which determine the direction of channeling, to the Miller indices.[29] For this, we consider Fig. 4, in which α determines the direction of channeling, $ox'y'z'$ is associated with the principal axes of the translational symmetry of the crystal, and $ox'dz$ is the plane along which the channeling occurs. Note that, like the Miller indices, the direction α is specified by the smallest numbers. Thus, we express n and l in terms of the Miller indices of the plane along which the channeling of the particles takes place. Let the Miller indices be (o, k', l'). Note that k' is always negative; this is due to our choice of the coordinate system. The oz axis is directed along the channel of the motion of the particles. Then

$$\alpha = -\mathrm{arctg}\,(l'/k'); \tag{52}$$

$$\Delta(lq_0\sin\alpha - nq_0\cos\alpha) = \Delta(l+k'n/l'). \tag{53}$$

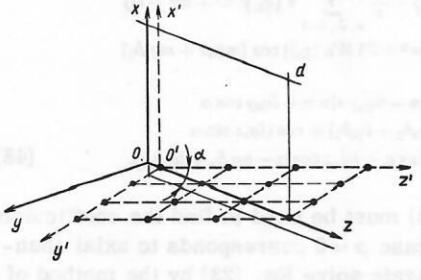

FIG. 4.

In (53), l and n are always integers strictly greater than zero. It follows that $k'n/l'$ must also always be an integer. Therefore, the sum in (50) must always begin with the term l and the following assertion is true: The nonvanishing terms in the sum (50) are those which satisfy the condition

$$n = l'p;\quad l=-k'p;\quad p=1,\,2,\,3,\,\ldots. \tag{54}$$

We now consider the determination of the coordinates of the vector $\mathbf{b}$. It is readily seen that the previously formulated conditions on $\mathbf{b}$ give

$$b_1 = a/2; \tag{55}$$

$$b_2 lq_0 - b_3 nq_0 = \pi p. \tag{56}$$

Equation (56) for b_2 and b_3 must be sought for the smallest possible non-negative b_2 and b_3. This follows from the definition of $\mathbf{b}$, whence

$$b_3 = 0;\quad b_2 = -(a\pi/2)\,l'/k'. \tag{57}$$

Using (53) and (54), we can readily represent the expression $nq_0\sin\alpha + lq_0\cos\alpha$ in the form

$$nq_0\sin\alpha + lq_0\cos\alpha = pq_0\sqrt{l'^2+k'^2}. \tag{58}$$

Using (52), (53), (57), and (58) and going over in (50) from summation over n and l to summation over p, we have

$$\begin{aligned}
\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} &= \frac{1}{v}\nu(0)+\frac{2}{v}\sum_{m=1}^{\infty}\nu(q_0 m)\exp[-m^2 W_\Theta(q_0)]\\
&\times(-1)^m\cos(mq_0 x)+\frac{2}{v}\sum_{p=1}^{\infty}\nu(q_0 p\sqrt{l'^2+k'^2})\\
\times\exp[-(l'^2+k'^2)p^2 W_\Theta(q_0)]&\,(-1)^p\cos[q_0\sqrt{l'^2+k'^2}\,py]\\
+\frac{4}{v}\sum_{m,\,p=1}^{\infty}&\nu\left(q_0\sqrt{m^2+p^2(k'^2+l'^2)}\right)(-1)^m(-1)^p\\
&\times\exp\{-[m^2+p^2(l'^2+k'^2)]W_\Theta(q_0)\}\\
&\times\cos(mq_0 x)\cos(q_0 py\sqrt{l'^2+k'^2}).
\end{aligned} \tag{59}$$

Finally, as in (40), we redefine the field (59) by a constant, so as to make the channel axis of the motion of the particles correspond to the zero of the potential energy:

$$\begin{aligned}
\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} &\Rightarrow \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}^{*}}\\
=\frac{4}{v}\sum_{m=1}^{\infty}&\nu(q_0 m)\exp[-m^2 W_\Theta(q_0)](-1)^{m+1}\sin^2(mq_0 x/2)\\
+\frac{4}{v}\sum_{p=1}^{\infty}&\nu(q_0 p)\sqrt{l'^2+k'^2}\exp[-p^2(l'^2+k'^2)W_\Theta(q_0)]\\
&\times(-1)^{p+1}\sin^2\left[\frac{q_0 yp}{2}\sqrt{l'^2+k'^2}\right]\\
+\frac{4}{v}\sum_{p,\,m=1}^{\infty}&\nu\left(q_0\sqrt{m^2+p^2(k'^2+l'^2)}\right)(-1)^m(-1)^p\\
&\times\exp[-(m^2+p^2(k'^2+l'^2))W_\Theta(q_0)]\\
&\times[\cos(mq_0 x)\cos(q_0\sqrt{l'^2+k'^2}\,py)-1].
\end{aligned} \tag{60}$$

The expression (60) can be used for an analogous treatment of planar channeling. Note that in this case the symmetry between the x and y coordinates character-

istic of axial channeling is lost:

$$\max_{x\,(y=0)} \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}^{*}} \neq \max_{y(x=0)} \overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}^{*}}.$$

Therefore, there exist two critical angles $\alpha_c^{(x)}$ and $\alpha_c^{(y)}$ of entrance:

$$\left.\begin{aligned} \alpha_c^{(x)} &= \left(\frac{\max\limits_{x\,(y=0)} \overline{\left\langle \sum\limits_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}^{*}}}{E_0}\right)^{1/2}; \\ \alpha_c^{(y)} &= \left(\frac{\max\limits_{y\,(x=0)} \overline{\left\langle \sum\limits_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}^{*}}}{E_0}\right)^{1/2}, \end{aligned}\right\} \tag{61}$$

where $\alpha_c^{(x)}$ is the angle between the axis of the channel of motion of the particles and the x component of the velocity, and $\alpha_c^{(y)}$ is the corresponding angle with the y component. Similarly, the frequencies of the oscillation of the trajectory of the channeled particle in the x and y directions are different. In the framework of the approximation considered earlier, we have

$$\begin{aligned} (\omega_{\Theta}^{x})^2 &\approx \frac{2q_0^2}{Mv}\, \nu(q_0) \exp[-W_{\Theta}(q_0)]; \\ (\omega_{\Theta}^{y})^2 &\approx \frac{2(l'^2+k'^2)}{Mv}\, \nu\left(q_0\sqrt{l'^2+k'^2}\right) \exp[-(l'^2+k'^2)\, W_{\Theta}(q_0)] \\ &- \frac{4(l'^2+k'^2)}{Mv}\, \nu\left(q_0\sqrt{1+l'^2+k'^2}\right) \exp[-(1+l'^2+k'^2)\, W_{\Theta}(q_0)]. \end{aligned} \tag{62}$$

If the direction of channeling is such that the relations (51) are not satisfied, i.e., the direction of channeling does not coincide with the channel of the motion or the channel of the motion corresponds to large Miller indices, then for $\langle\sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\rangle_{\Sigma}$ we have

$$\begin{aligned} &\overline{\left\langle \sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} \approx \frac{4}{v} \sum_{n=1}^{\infty} \nu(q_0 n) \\ &\times \exp[-n^2 W_{\Theta}(q_0)]\,(-1)^{n+1} \sin^2\left(\frac{q_0 n x}{2}\right). \end{aligned} \tag{63}$$

This will correspond to motion of the particles in one plane, and the problem (23) reduces to a one-dimensional problem.

6. THE $o(\varepsilon^2)$ APPROXIMATION

We consider the following order of the expanded equation (20); to be able to ignore the effects associated with the noncollectivized influence of the ions of the crystal on S, which lead to a rapidly oscillating dependence, we shall average directly the system of equations (12). We introduce a Fourier representation of the interaction potential in accordance with

$$\sum_{j=1}^{N} U(\mathbf{R}-\mathbf{r}_j) = \frac{1}{\Omega} \sum_{k} \nu(k) \exp[i\mathbf{k}\mathbf{R}] \sum_{j=1}^{N} \exp[-i\mathbf{k}\mathbf{r}_j],$$

where Ω is the volume of the crystal, and $\nu(k)$ is the Fourier transform of the function $U(\mathbf{R})$. Then after averaging with respect to z, we obtain for $\overline{\mathcal{J}I_{\text{int}}^{\perp}}$

$$\left.\begin{aligned} \overline{\mathcal{J}I_{\text{int}}^{\perp}} &= \frac{1}{\Omega} \sum_{k_\perp} i\mathbf{k}_\perp \nu(k_\perp) \exp[i\mathbf{k}_\perp \mathbf{R}_\perp] \sum_{j=1}^{N} \exp(-i\mathbf{k}_\perp \mathbf{r}_j) \\ &\quad \times \left[\frac{1}{M}\nabla_{\mathbf{v}_\perp} - \frac{1}{m}\nabla_{\mathbf{v}_j^{\perp}}\right]; \\ \langle \overline{\mathcal{J}I_{\text{int}}^{\perp}}\rangle_{\Sigma} &= \overline{\langle \mathcal{J}I_{\text{int}}^{\perp}\rangle_{\Sigma}};\quad \nu(k_\perp) = \nu(k)_{k_z=0}. \end{aligned}\right\} \tag{64}$$

As a result of our transformations, the system of equations (12) is reduced to the following form in the $o(\varepsilon^2)$ approximation:

$$\left.\begin{aligned} \frac{\partial}{\partial z} f(zS_\perp) &= \frac{1}{V_0}\mathcal{J}I(S_\perp\Sigma) f(zS_\perp) + \overline{\left\langle \sum_{j=1}^{N} \nabla_{\mathbf{R}_\perp} U(\mathbf{R}-\mathbf{r}_j)\right\rangle_{\Sigma}} \\ &\times \int (d\Sigma) \sum_{j=1}^{N} \nabla_{\mathbf{R}_\perp} \overline{U(\mathbf{R}-\mathbf{r}_j)}\, \frac{1}{MV_0} \nabla_{\mathbf{v}_\perp} \Delta(zS_\perp\Sigma); \\ \frac{\partial}{\partial z}\Delta(zS_\perp\Sigma) &= \frac{1}{V_0}\overline{\mathcal{J}I(S_\perp\Sigma)}\,\Delta(zS_\perp\Sigma) \\ &+ \frac{1}{V_0}[\overline{\mathcal{J}I_{\text{int}}^{\perp}} - \overline{\langle \mathcal{J}I_{\text{int}}^{\perp}\rangle_{\Sigma}} D_0(\Sigma) f(zS_\perp) \\ &- \frac{1}{V_0} D_0(\Sigma)\hat{P}_0 \overline{\mathcal{J}I_{\text{int}}^{\perp}}\Delta(zS_\perp\Sigma);\quad \mathcal{J}I(S_\perp\Sigma) = \mathcal{J}I(S\Sigma)\,|_{\mathcal{J}I(S_\perp)}. \end{aligned}\right\} \tag{65}$$

From Eqs. (65) we eliminate the function $\Delta(zS_\perp\Sigma)$, $(\Delta(zS_\perp\Sigma)_{z=0}=0)$ and retain on the right-hand side of the resulting equation terms of order up to $o(\varepsilon^3)$:

$$\begin{aligned} \frac{\partial}{\partial z} f(zS_\perp) &= \frac{1}{V_0}\Big[-\mathbf{V}_\perp\nabla_{\mathbf{R}_\perp} \\ &+ \Big\langle \sum_j \nabla_{\mathbf{R}_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_{\Sigma} \frac{1}{M}\nabla_{\mathbf{v}_\perp}\Big] f(zS_\perp) \\ &+ \frac{1}{MV_0^2\Omega^2} \int_0^z d\tau \nabla_{\mathbf{v}_\perp} \sum_{k_\perp,\,k'_\perp} i\mathbf{k}_\perp \nu(\mathbf{k}_\perp)\,\nu(k'_\perp) \exp[i\,(\mathbf{k}_\perp+\mathbf{k}'_\perp)\,\mathbf{R}_\perp] \\ &\times \Big[\Phi_{kk'}(T)\frac{i\mathbf{k}'_\perp}{M}\nabla_{\mathbf{v}_\perp} + \frac{1}{\Theta}\frac{\partial}{\partial T}\Phi_{kk'}(T)\Big] f(\tau S_\perp).\quad T = \frac{z-\tau}{V_0}, \end{aligned} \tag{66}$$

where $\vartheta = k_B T^0$, in which k_B is Boltzmann's constant and T^0 is the absolute temperature;

$$\begin{aligned} \Phi_{kk'}(T) &= \Big\langle \sum_j \exp[-i\mathbf{k}_\perp \mathbf{r}_j^{\perp}] \exp[T\mathcal{J}I(\Sigma)] \sum_j \exp[-i\mathbf{k}'_\perp \mathbf{r}_j^{\perp}]\Big\rangle_{\Sigma} \\ &- \Big\langle \sum_j \exp[-i\mathbf{k}_\perp \mathbf{r}_j^{\perp}]\Big\rangle_{\Sigma} \Big\langle \sum_j \exp[-i\mathbf{k}'_\perp \mathbf{r}_j^{\perp}]\Big\rangle_{\Sigma}. \end{aligned}$$

We shall call the integro-differential part of Eq. (66) the *collision integral*. An equation of the type (66) was obtained for the first time in Ref. 9 in a study of the evolution of small subsystems in weak dynamical contact with a thermal reservoir. It was also shown in Ref. 9 that this equation describes a stochastic process which, under the assumption that the system is nearly spatially homogeneous, converges as $t \to \infty$ to a Maxwell distribution with respect to the momenta (Σ is a spatially homogeneous system). We investigate the asymptotic behavior of Eq. (8) as $z \to \infty$ without assuming that the dynamical contact between the systems S and Σ is weak and in the case when Σ is a harmonic crystal.[29]

7. ASYMPTOTIC BEHAVIOR OF EQUATION (10) AS $z \to \infty$

We transform the collision integral of Eq. (66) to Fokker–Planck form. By this we shall mean that it has a representation in which we separate explicitly an operator construction $\hat{C}$ which vanishes on the Maxwell velocity distribution, i.e., $\hat{C}\Phi_0(\mathbf{V}_\perp)$, where $\Phi_0(\mathbf{V}_\perp)$ is the Maxwell distribution. For this, it is sufficient to transform the part of the collision integral of the form

$$\begin{aligned} Q_1 &= \frac{1}{V_0^2 M\Omega^2\Theta}\nabla_{\mathbf{v}_\perp} \int_0^z d\tau \sum_{k_\perp,\,k'_\perp} i\mathbf{k}_\perp \nu(k_\perp)\,\nu(k'_\perp) \\ &\times \exp[i\,(k_\perp+k'_\perp)\,\mathbf{R}_\perp] \frac{\partial}{\partial T}\Phi_{kk'}(T) f(\tau S_\perp). \end{aligned} \tag{67}$$

We propose the following method of transformation. Integrating by parts, we transfer the derivative with respect to τ in (67) from the function $\Phi_{kk'}(T)$ to $f(\tau S_\perp)$. For $\partial f(\tau S_\perp)/\partial\tau$, we use the equation itself, i.e., we make one iteration and substitute in the obtained expression the quantities that contribute to the collision integral of Eqs. (66) to order not higher than $o(\varepsilon^2)$. However, it is convenient to formulate Eq. (66) from the beginning in such a way that when this procedure of transferring the derivative is carried out we obtain instead of $\partial f(\tau S_\perp)/\partial\tau$ a small quantity of order higher than $o(\varepsilon)$, so that it can be ignored directly. For this, we consider the system of equations (65).

We introduce the notation

$$\left.\begin{aligned}
&\mathcal{L}\equiv \mathcal{J}(S_\perp)+\langle\overline{\mathcal{J}}^{\perp}_{\text{int}}\rangle_\Sigma+\mathcal{J}(\Sigma);\quad A\equiv\mathcal{J}(S_\perp)+\langle\overline{\mathcal{J}}^{\perp}_{\text{int}}\rangle_\Sigma;\\
&\Psi\equiv\overline{\mathcal{J}}^{\perp}_{\text{int}}-\langle\overline{\mathcal{J}}^{\perp}_{\text{int}}\rangle_\Sigma+\frac{1}{\Omega}\sum_{k_\perp}\mathbf{i}k_\perp v(k_\perp)\times\\
&\quad\times\exp[\mathbf{i}k_\perp\cdot\mathbf{R}_\perp]\sum_j\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}^\perp]\cdot\frac{1}{m_j}\nabla_{V_j^\perp};\\
&G(z)=\exp\left[\frac{z}{V_0}\mathcal{L}\right];\quad \Psi^*=\mathcal{J}(S_\perp)+\Psi;\\
&J(z)=\exp\left[\frac{z}{V_0}A\right];\quad R(z)=\exp\left[\frac{z}{V_0}\mathcal{J}(\Sigma)\right].
\end{aligned}\right\}\tag{68}$$

Since the operators A and $\mathcal{J}(\Sigma)$ act on different variables of the functions $S_\perp$ and Σ, they commute, i.e., $[A,\mathcal{J}(\Sigma)]_{(-)}=0$. Hence,

$$G(z)=J(z)\,R(z)=R(z)\,J(z),\tag{69}$$

and we shall use this equation frequently in what follows. For $\Delta(zS_\perp\Sigma)$ in the notation of (69) we obtain from the second equation of the system of equations (65) with allowance for the initial condition

$$\begin{aligned}
\Delta(zS_\perp\Sigma)=&\frac{1}{V_0}\int_0^z d\tau G(z-\tau)\Big[\Psi-\sum_{j=1}^{N}\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\\
&\times\frac{1}{m_j}\nabla_{V_\perp^j}\Big]D_0(\Sigma)f(\tau S_\perp)+\\
+\sum_{n=1}^{\infty}\frac{1}{V_0}\int_0^z d\tau_n G(z-\tau_n)\Big[&\Psi^*-\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_\perp^j}\\
&-D_0(\Sigma)\hat{P}_0\overline{\mathcal{J}}^{\perp}_{\text{int}}\Big]\cdots\frac{1}{V_0}\int_0^{\tau_2}d\tau_1 G(\tau_2-\tau_1)\\
&\times\Big[\Psi^*-\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}-D_0(\Sigma)\hat{P}_0\overline{\mathcal{J}}^{\perp}_{\text{int}}\Big]\\
\times\int_0^{\tau_1}d\tau G(\tau_1-\tau)\Big[\Psi-\sum_j\nabla_{R_\perp}&\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}\Big]D_0(\Sigma)f(\tau S_\perp).
\end{aligned}\tag{70}$$

The series (70) is none other than a formal Neumann series[30] for one of the integral representations of Eq. (65). If it is substituted in place of $\Delta(zS_\perp\Sigma)$ in Eq. (65), we obtain a formal closed equation for the function $f(zS_\perp)$. Now we need the equation of the $o(\varepsilon^2)$ approximation. Therefore, in (70) we must separate the terms that have order not higher than $o(\varepsilon)$, and we can ignore the remainder. We consider

$$\begin{aligned}
\Delta_1=&\frac{1}{V_0}\int_0^z d\tau G(z-\tau)\Big[\Psi-\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}\Big]\\
&\times D_0(\Sigma)f(\tau S_\perp);\quad \Delta_1=\Delta_1^{(1)}+\Delta_1^{(2)}.
\end{aligned}\tag{71}$$

The first term is

$$\begin{aligned}
\Delta_1^{(1)}=&\frac{1}{V_0}\int_0^z d\tau G(z-\tau)\Big[\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\\
&-\Big\langle\sum_j\nabla_{R_\perp}U(\mathbf{R}-\mathbf{r}_j)\Big\rangle_\Sigma\Big]\frac{1}{M}\nabla_{V_\perp}f(\tau S_\perp)D_0(\Sigma).
\end{aligned}\tag{72}$$

We transform the second term $\Delta_1^{(2)}$. We follow the chain of equations

$$\begin{aligned}
\Delta_1^{(2)}=&-\frac{1}{V_0}\int_0^z d\tau G(z-\tau)\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}D_0(\Sigma)f(\tau S_\perp)\\
=&\frac{G(z)}{V_0}\int_0^z d\tau G(-\tau)\frac{1}{\Omega}\sum_{k_\perp}\mathbf{i}k_\perp v(k_\perp)\exp[\mathbf{i}k_\perp\cdot\mathbf{R}_\perp]\\
&\times\sum_j\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp]\Big[\frac{\mathbf{V}_j^\perp}{\Theta}D_0(\Sigma)f(\tau S_\perp)\\
=&-\frac{G(z)}{\Theta}\int_0^z d\tau\frac{1}{\Omega}\sum_{k_\perp}v(k_\perp)\exp[\mathbf{i}k_\perp\cdot\mathbf{R}(\tau)]\\
&\times\frac{\partial}{\partial\tau}\Big(\sum_j{}'\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp(\tau)]\Big)D_0(\Sigma)G(-\tau)f(\tau S_\perp)\\
=&-\frac{G(z)}{\Theta}\int_0^z d\tau\frac{\partial}{\partial\tau}\Big\{\frac{1}{\Omega}\sum_{k_\perp}v(k_\perp)\\
&\times\exp[\mathbf{i}k_\perp\cdot\mathbf{R}_\perp(\tau)]\sum_j{}'\exp[-\mathbf{i}k_\perp\mathbf{r}_j^\perp(\tau)]G(-\tau)D_0(\Sigma)f(\tau S_\perp)\Big\}\\
+\int_0^z d\tau\frac{1}{\Omega}\sum_{k_\perp}v(k_\perp)&\Big[\frac{\partial}{\partial\tau}\exp(\mathbf{i}k_\perp\cdot\mathbf{R}_\perp(\tau))\Big]\sum_j{}'\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp(\tau)]\\
\times G(-\tau)D_0(\Sigma)f(\tau S_\perp)+&\int_0^z d\tau\frac{1}{\Omega}\sum_{k_\perp}v(k_\perp)\exp[\mathbf{i}k_\perp\mathbf{R}_\perp(\tau)]\\
&\times\sum_j{}'\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp(\tau)]\frac{\partial}{\partial\tau}[G(-\tau)D_0(\Sigma)f(\tau S_\perp)].
\end{aligned}$$

In the transformations, we have used the equations

$$\begin{aligned}
&\frac{1}{m_j}\nabla_{V_j^\perp}D_0(\Sigma)=-\frac{\mathbf{V}_j^\perp}{\Theta}D_0(\Sigma);\ G(z-\tau)=G(z)G(-\tau);\\
&G(-\tau)\varphi(\mathbf{R}_1,\mathbf{V}_1,\ldots\mathbf{r}_j^\perp\mathbf{V}_j^\perp\ldots)\\
&=\varphi(\mathbf{R}(\tau)_\perp,\mathbf{V}(\tau)_\perp,\ldots\mathbf{r}_j(\tau)^\perp,\mathbf{V}_j(\tau)^\perp\ldots);\\
&G(-\tau)\varphi(\ldots)\Psi(\ldots)=G(-\tau)\varphi(\ldots)G(-\tau)\Psi(\ldots);\\
&\frac{\partial}{\partial\tau}[G(-\tau)\mathbf{r}_j^\perp]=\mathbf{V}_j^\perp(\tau)
\end{aligned}$$

and introduced the notation

$$\sum_j{}'\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp(\tau)]=\sum_j\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^-(\tau)]-\chi,$$

where χ is a function that does not depend on τ. This arbitrariness in the transformation of $\Delta_1^{(2)}$ is due to the circumstance that any function which does not depend on τ can be taken into the expression to which $\partial/\partial t$ is applied. This arbitrariness can be eliminated by requiring that $\langle\Delta_1^{(2)}\rangle_\Sigma=0$. This property held before the transformation of $\Delta_1^{(2)}$. Hence,

$$\chi=\langle\sum_j\exp[-\mathbf{i}k_\perp\cdot\mathbf{r}_j^\perp]\rangle_\Sigma.$$

Now $\partial/\partial\tau[G(-\tau)D_0(\Sigma)f(\tau S_\perp)]$ has an order of magnitude higher than $o(\varepsilon)$. Indeed,

$$\frac{\partial}{\partial\tau}[G(-\tau)D_0(\Sigma)f(\tau S_\perp)]=D_0(\Sigma)\frac{\partial}{\partial\tau}[J(-\tau)f(\tau S_\perp)].$$

In (65) we make a change of variables, replacing $o(\varepsilon)$ by $g(\tau S_\perp)=J(-\tau)f(S_\perp\tau)$. As a result, we obtain for $g(\tau S_\perp)$ the equation

$$\frac{\partial}{\partial\tau}g(\tau S_\perp)=J(\tau)\hat{P}_0^{\Sigma}\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{MV_0}\nabla_{v_\perp}\Delta(zS_\perp\Sigma),$$

from which it can be seen that $\partial g(zS_\perp)/\partial z\sim o(\varepsilon)$, since $\Delta(zS_\perp\Sigma)$ itself is $\sim o(\varepsilon)$. Finally, we obtain for Δ_1 up to order $o(\varepsilon^2)$

$$\Delta_1=\frac{1}{V_0}\int_0^z d\tau G(z-\tau)\Big[\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_{j=1}^N\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big]$$
$$\times D_0(\Sigma)\Big[\frac{1}{M}\nabla_{v_\perp}+\frac{\mathbf{V}_\perp}{\Theta}\Big]f(\tau S_\perp)-\frac{1}{\Theta}\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}$$
$$-\Big\langle\sum_j U(\mathbf{R}-\mathbf{r}_j)\Big\rangle_\Sigma\Big]D_0(\Sigma)f(zS_\perp)+\frac{1}{\Theta}G(z)$$
$$\times\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]D_0(\Sigma)f(oS_\perp).\qquad(73)$$

In (73), we separate the terms of order $o(1)$:

$$\Delta_1\approx-\frac{1}{\Theta}\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]D_0(\Sigma)f(zS_\perp)$$
$$+\frac{G(z)}{\Theta}\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]D_0(\Sigma)f(0S_\perp).\qquad(74)$$

It can be seen from (73) that when the derivative is transferred we obtain terms that renormalize in the equation for $f(S_\perp z)$ the term which describes the influence of the crystal field, and also terms with memory that are "proportional" to $f(0S_\perp)$. Such terms occur in all orders of the series (70). They owe their appearance to the terms of the series (70) that contain a number of operators $\nabla_{V_j^\perp}$ equal to their order in $1/V_0$: we separate them:

$$\Delta^*(zS_\perp\Sigma)=\sum_n{}'\Delta_n^*(zS_\perp\Sigma);$$
$$\Delta_n^*(zS_\perp\Sigma)=\frac{(-1)^n}{V_0^n}\int_0^z d\tau_1G(z-\tau_\perp)$$
$$\times\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}\cdots\int_0^{\tau_{n-1}}d\tau_nG(\tau_{n-1}-\tau_n)$$
$$\times\sum_j{}'\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}D_0(\Sigma)f(\tau_nS_\perp).\qquad(75)$$

To prove the proposition formulated below, we also study the function Δ_2^* (in the brackets, we shall indicate instead of the arguments the order of the considered quantity):

$$\Delta_2^*(o(1))=-\frac{1}{V_0}\int_0^z d\tau_1G(z-\tau_\perp)\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}$$
$$\times\Delta_1^*(\tau_1o(1))=\frac{1}{V_0\Theta}\int_0^z d\tau_\perp G(z-\tau_\perp)\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}$$
$$\times\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]D_0(\Sigma)f(\tau_1S_\perp)$$
$$-\frac{1}{V_0\Theta}G(z)\int_0^z d\tau_\perp G(-\tau)\sum_j\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}G(\tau_1)$$
$$\times\Big[\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_j\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]D_0(\Sigma)f(oS_\perp)$$
$$\approx\frac{1}{\Theta^2}G(z)\int_0^z d\tau_1\frac{\partial}{\partial\tau_1}\Big[G(-\tau_1)\frac{1}{\Omega^2}\sum_{k_\perp,k'_\perp}v(k_\perp)$$
$$\times v(k'_\perp)\exp[i\mathbf{k}_\perp\mathbf{R}_\perp+i\mathbf{k}'_\perp\mathbf{R}_\perp]\frac{1}{2!}D_2(k_\perp k'_\perp)D_0(\Sigma)f(\tau_1S_\perp)\Big]$$
$$-\frac{1}{V_0\Theta}\int_0^z d\tau_1G(z-\tau_\perp)\sum_{j=1}^N\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\frac{1}{m_j}\nabla_{V_j^\perp}G(\tau_1)$$
$$\times\sum_{j=1}^N{}'\overline{U(\mathbf{R}-\mathbf{r}_j)}D_0(\Sigma)f(oS_\perp)=\frac{1}{\Theta^2}\frac{1}{\Omega^2}\sum_{k_\perp k'_\perp}v(k_\perp)v(k'_\perp)$$
$$\times\exp[i(\mathbf{k}_\perp+\mathbf{k}'_\perp)\cdot\mathbf{R}_\perp]\frac{1}{2!}D_2(k_\perp,k'_\perp)D_0(\Sigma)f(zS_\perp)$$
$$-\frac{1}{\Theta^2\Omega^2}G(z)\sum_{k_\perp k'_\perp}v(k_\perp)v(k'_\perp)\exp[i(\mathbf{k}_\perp+\mathbf{k}'_\perp)\mathbf{R}_\perp]\frac{1}{2!}D_2(k_\perp,k'_\perp)$$
$$\times D_0(\Sigma)f(oS_\perp)-\frac{1}{V_0\Theta}\int_0^z d\tau_1G(z-\tau_1)\sum_{j=1}^N\nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}$$
$$\times\frac{1}{m_j}\nabla_{V_j^\perp}G(\tau_1)\Big[\sum_{j=1}^N\overline{U(\mathbf{R}-\mathbf{r}_j)}-\Big\langle\sum_{j=1}^N\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big\rangle_\Sigma\Big]$$
$$\times D_0(\Sigma)f(\tau_1S_\perp).$$

In these transformations, we have used the equation $\nabla_{V_j^\perp}D_0(\Sigma)=-\nabla_j^\perp D_0(\Sigma)/\vartheta$ and arguments from Proposition 2 in Appendix 1; in the Appendix, we also introduce the functions $D_n(k_\perp^{(1)},\ldots,k_\perp^{(n)})$ and study some of their properties. Thus, the function $\Delta_2^*(o(1))$ can be represented in the form

$$\Delta_2^*(o(1))=\frac{1}{\Theta^2}\frac{1}{\Omega^2}\sum_{k_\perp k'_\perp}v(k_\perp)v(k'_\perp)\exp[i(\mathbf{k}_\perp+\mathbf{k}'_\perp)\cdot\mathbf{R}_\perp]$$
$$\times\frac{1}{2!}D_2(k_\perp,k'_\perp)D_0(\Sigma)f(zS_\perp)+G(z)\Psi_2D_0(\Sigma)f(oS_\perp),\qquad(76)$$

where Ψ_2 can be readily established by comparison with the previous expression. For Ψ_2, we have the property

$$\langle\Psi_2\rangle_\Sigma=0.\qquad(77)$$

Proceeding further in exactly the same way, we can show that for $\Delta_n^*(o(1))$ we have the representation

$$\Delta_n^*(o(1))=\frac{(-1)^n}{\Theta^n\Omega^nn!}\sum_{k_\perp^{(1)},\ldots,k_\perp^{(n)}}v(k_\perp^{(1)})\ldots v(k_\perp^{(n)})$$
$$\times\exp[i(\mathbf{k}_\perp^{(1)}+\ldots+\mathbf{k}_\perp^{(n)})\cdot\mathbf{R}_\perp]D_n(k_\perp^{(1)},\ldots,k_\perp^{(n)})D_0(\Sigma)f(zS_\perp)$$
$$+G(z)\Psi_nf(oS_\perp)D_0(\Sigma),\qquad(78)$$

where

$$\Psi_n=\frac{(-1)^{n+1}}{\Omega^n\Theta^n}\sum_{k_\perp^{(1)}\ldots k_\perp^{(n)}}v(k_\perp^{(1)})\ldots v(k_\perp^{(n)})$$
$$\times\exp[i(\mathbf{k}_\perp^{(1)}+\mathbf{k}_\perp^{(2)}+\mathbf{k}_\perp^{n})\cdot\mathbf{R}_\perp]\frac{1}{n!}D_n(k_\perp^{(1)},\ldots,k_\perp^{(n)})$$
$$+\int_0^z d\tau G(-\tau)\tilde{\varphi}_n(\tau);$$

$\tilde{\varphi}_n(\tau)$ is a function which satisfies the equation $\langle\tilde{\varphi}_n(\tau)\rangle_\Sigma=0$. If necessary, the form of $\tilde{\varphi}_n$ can be found for each n, but the general expression for it is not very complicated. By means of Eq. (78) and Eq. (A.2) in Appendix 1 we can readily find the "renormalization" of the crystal field under the assumptions we have made:

$$\frac{1}{V_0}\hat{P}_0\overline{J}_{\text{int}}^\perp\Delta(zS_\perp\Sigma)=\frac{1}{V_0}\sum_{n=1}^\infty\hat{P}_0\frac{(-1)^n}{\Theta^n\Omega^n}\overline{J_{\text{int}}^\perp}$$
$$\times\sum_{k_\perp^{(1)},\ldots,k_\perp^{(n)}}v(k_\perp^{(1)})\ldots v(k_\perp^{(n)})\exp[i(\mathbf{k}_\perp^{(1)}+\ldots+\mathbf{k}_\perp^{(n)})\cdot\mathbf{R}_\perp]$$
$$\times\frac{1}{n!}D_n(k_\perp^{(1)},\ldots,k_\perp^{(n)})D_0(\Sigma)f(zS_\perp)$$
$$+\frac{1}{V_0}\sum_{n=1}^\infty\hat{P}_0\overline{J_{\text{int}}^\perp}G(z)\Psi_nD_0(\Sigma)f(oS_\perp)$$
$$=\frac{1}{V_0}\Big\langle\overline{J_{\text{int}}^\perp}\frac{\exp\Big[-\frac{1}{\Theta}\sum_{j=1}^N\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big]}{\Big\langle\exp\Big[-\frac{1}{\Theta}\sum_{j=1}^N\overline{U(\mathbf{R}-\mathbf{r}_j)}\Big)\Big\rangle_\Sigma}\Big\rangle_\Sigma f(zS_\perp)$$
$$-\frac{1}{V_0}\langle\overline{J_{\text{int}}^\perp}\rangle_\Sigma f(zS_\perp)+\frac{1}{V_0}\sum_{n=1}^\infty\langle\overline{J_{\text{int}}^\perp}G(z)\Psi_n\rangle_\Sigma f(oS_\perp).\qquad(79)$$

Equation (79) contains terms associated with the memory of the system, i.e., terms that contain the function $f(oS_\perp)$. We show that such terms become unimportant when $z \to \infty$, i.e., for large z:

$$\langle \overline{J_{\text{int}}^{\perp}} G(z) \Psi_n \rangle_\Sigma = \left\langle \overline{J_{\text{int}}^{\perp}} G(z) \frac{(-1)^{n+1}}{n!\,\Theta^n \Omega^n} \sum_{k_\perp^{(1)}, \ldots, k_\perp^{(n)}} v(k_\perp^{(1)}) \ldots v(k_\perp^{(n)}) \times \exp\left[i\left(\mathbf{k}_\perp^{(1)} + \ldots \mathbf{k}_\perp^{(n)}\right)\cdot \mathbf{R}_\perp\right] D_n(k_\perp^{(1)}, \ldots, k_\perp^{(n)}) \right\rangle_\Sigma + \left\langle \overline{J_{\text{int}}^{\perp}} G(z) \int_0^z G(-\tau)\, \tilde{\varphi}(\tau)\, d\tau \right\rangle_\Sigma .$$

In accordance with the principle of correlation weakening for the structure moments (Appendix 2), we have

$$\left\langle \overline{J_{\text{int}}^{\perp}} G(z) \sum_{k_\perp^{(1)}, \ldots, k_\perp^{(n)}} v(k_\perp^{(1)}) \ldots v(k_\perp^{(n)}) \times \exp\left[i\left(\mathbf{k}_\perp^{(1)} + \ldots + \mathbf{k}_\perp^{(n)}\right)\cdot \mathbf{R}_\perp\right] D_n(k_\perp^{(1)}, \ldots, k_\perp^{(n)}) \right\rangle_{\Sigma_{z\to\infty}} = \left\langle \overline{J_{\text{int}}^{\perp}} \right\rangle_\Sigma \sum_{k_\perp^{(1)}, \ldots, k_\perp^{(n)}} v(k_\perp^{(1)}) \ldots v(k_\perp^{(n)}) \times \exp\left[i\left(\mathbf{k}_\perp^{(1)} + \ldots + \mathbf{k}_\perp^{(n)}\right)\cdot \mathbf{R}_\perp\right] \langle D_n(\mathbf{k}_\perp^{(1)}, \ldots, k_\perp^{(n)})\rangle_\Sigma = 0$$

by virtue of Proposition 1. Further,

$$\left\langle \overline{J_{\text{int}}^{\perp}} G(z) \int_0^z G(-\tau)\, \tilde{\varphi}_n(\tau)\, d\tau \right\rangle_\Sigma = \left\langle \overline{J_{\text{int}}^{\perp}} G(z) \int_0^\infty d\tau G(-\tau)\, \tilde{\varphi}_n(\tau) \right\rangle_\Sigma - \int_0^\infty d\tau \left\langle \overline{J_{\text{int}}^{\perp}} G(z-\tau)\, \tilde{\varphi}_n(\tau) \right\rangle_\Sigma .$$

The quantity $\int_z^\infty d\tau \langle \mathbf{J}\mathbf{I}_{\text{int}}^{\perp} G(z-\tau)\tilde{\varphi}_n(\tau)\rangle_\Sigma$ tends in the limit $z \to \infty$ to zero; $\int_0^\infty G(-\tau)\tilde{\varphi}_n(\tau)d\tau$ is some operator function. When it is applied to the function $D_0(\Sigma)$, we always obtain an expression of the type

$$\int_0^\infty G(-\tau)\, \tilde{\varphi}_n(\tau)\, D_0(\Sigma)\, d\tau = \int_0^\infty d\tau G(-\tau)\, \tilde{\Psi}_n(\tau)\, D_0(\Sigma),$$

where $\tilde{\Psi}_n(\tau)$ has operator structure only with respect to the variables $S_\perp$, so that with respect to the variables of Σ the quantity $\int_0^\infty d\tau G(-\tau)\Psi_n(\tau)$ is simply a function of the state of the crystal, and therefore an expansion in normal oscillations holds for it and in the limit $z \to \infty$ the principle of correlation weakening is valid, i.e.,

$$\left\langle \overline{J_{\text{int}}^{\perp}} G(z) \int_0^\infty G(-\tau)\, \tilde{\Psi}_n(\tau)\, d\tau \right\rangle_{\Sigma_{z\to\infty}} = \left\langle \overline{J_{\text{int}}^{\perp}} \right\rangle_\Sigma J(z) \times \int_0^\infty G(-\tau) \langle \tilde{\Psi}_n(\tau)\rangle_\Sigma\, d\tau = 0.$$

Thus, we see that for large z the terms of the transformed crystal field containing a memory become unimportant; the memory is "erased" by the z evolution. Thus, at large z we have the following substitution under transformations of the indicated type:

$$\frac{1}{V_0} \overline{\langle J_{\text{int}}^{\perp} \rangle_\Sigma} \Rightarrow \frac{1}{V_0} \left\langle \frac{\exp\left[-\frac{1}{\Theta}\sum_{j=1}^N \overline{U(\mathbf{R}-\mathbf{r}_j)}\right]}{\left\langle \exp\left[-\frac{1}{\Theta}\sum_{j=1}^N \overline{U(\mathbf{R}-\mathbf{r}_j)}\right]\right\rangle_\Sigma} \overline{J_{\text{int}}^{\perp}} \right\rangle_\Sigma = -\frac{\Theta}{V_0} \nabla_{R_\perp} \ln \left\langle \exp\left(-\frac{1}{\Theta}\sum_{j=1}^N \overline{U(\mathbf{R}-\mathbf{r}_j)}\right)\right\rangle_\Sigma \frac{1}{M}\nabla_{V_\perp}. \qquad (80)$$

To obtain the renormalization of the collision integral under these transformations, it is necessary to separate all the terms in the expansion (70) for $\Delta(zS_\perp\Sigma)$ that contribute to the order $o(\varepsilon)$. The direct realization of this program entails in this case very cumbersome calculations. However, one can proceed differently. We note that the asymptotic formula (80) uniquely recovers the form of the projection operator, which is associated, in its turn, with the obtaining of a well-defined type of equation from the Liouville equation for the complete system.[25] Therefore, knowing the projection operator, we can obtain the asymptotic form of the "collision operator" in a shorter manner by beginning with Eq. (8). Equation (66) was obtained with the following initial conditions, which are obvious for the channeling problem:

$$D(zS_\perp\Sigma)_{z=0} = D_0(\Sigma)\, f(zS_\perp)_{z=0},$$

which corresponded to the pair of projection operators

$$\hat{P}_0 = \int (d\Sigma)\ldots; \quad \hat{P} = D_0(\Sigma)\,\hat{P}_0.$$

The asymptotic formula (80) dictates the following pair of operators:

$$\hat{P}_0 = \int (d\Sigma)\ldots; \quad \hat{P} = P(S_\perp\Sigma)\,\hat{P}_0, \qquad (81)$$

where

$$P(S_\perp\Sigma) = \frac{D_0(S_\perp\Sigma)}{\hat{P}_0 D_0(S_\perp\Sigma)} = \frac{\exp\left[-\frac{1}{\Theta}\sum_{j=1}^N \overline{U(\mathbf{R}-\mathbf{r}_j)}\right] D_0(\Sigma)}{\left\langle \exp\left[-\frac{1}{\Theta}\sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)}\right]\right\rangle_\Sigma};$$

$D_0(S_\perp\Sigma)$ is the Gibbs distribution for the system $S_\perp + \Sigma$. Note that the system $S_\perp$ is two-dimensional both with respect to $\mathbf{R}_\perp$ and $V_\perp$, and the interaction between $S_\perp$ and Σ has the form $\overline{U(\mathbf{R}-\mathbf{r}_j)}$. Proceeding as in the derivation of Eq. (66) once more, but with the pair of operators (81), we obtain in the $o(\varepsilon^2)$ approximation the following equation for $f(zS_\perp)$ to describe the z evolution of the system S at large z:

$$\left.\begin{aligned} &\frac{\partial}{\partial z} f(zS_\perp) \\ &= \frac{1}{V_0}\left[-\mathbf{V}_\perp \nabla_{\mathbf{R}_\perp} + \hat{P}_0 P(S_\perp\Sigma)\,\overline{J_{\text{int}}^{\perp}}\right] f(zS_\perp) + Q(f(\tau S_\perp)); \\ &Q(f(\tau S_\perp)) \\ &= \frac{1}{MV_0^2}\int_0^z d\tau \nabla_{V_\perp} \langle \mathbf{F}; \mathbf{F}(T)\rangle \left[\frac{1}{M}\nabla_{V_\perp} + \frac{1}{\Theta}\mathbf{V}_\perp\right] f(\tau S_\perp); \\ &\langle \mathbf{F}; \mathbf{F}(T)\rangle = \hat{P}_0 \sum_{j=1}^N \nabla_{R_\perp} U(\mathbf{R}-\mathbf{r}_j)\, R(T)\, P(S_\perp\Sigma) \\ &\times \left[\sum_{j=1}^N \nabla_{R_\perp} U(\mathbf{R}-\mathbf{r}_j) - \hat{P}_0 P(S_\perp\Sigma) \sum_{j=1}^N \nabla_{R_\perp} U(\mathbf{R}-\mathbf{r}_j)\right]. \end{aligned}\right| \qquad (82)$$

In the high-temperature limit, or for weak interaction between S and Σ, when $\Theta^{-1}\sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)} \ll 1 \sim \delta$ in 0 (1 with respect to δ), the approximation (80) takes the form of the equation obtained in Ref. 27. It follows from the operator structure of the "collision integral" that the Maxwellian momentum distribution function makes it vanish. Thus, we have shown that irrespective of the initial distribution $f(0S_\perp')$ of the beam of particles channeled through the crystal $f(zS_\perp)$ tends at sufficiently great depths of penetration z into the crystal to some stationary distribution with Maxwellian distribution with respect to $\mathbf{V}_\perp$. The z evolution of the func-

tion $f(zS_\perp)$ is described by a typical equation of Fokker–Planck type but of non-Markov form.

To conclude this section, we give some qualitative arguments for estimating the order of magnitude of z at which thermalization of the beam arises as a result of the z evolution of the system. In the thermalized state $f_0(S_\perp)$, the state of the S system is completely determined by the thermodynamic state of the crystal and the nature of its interaction with the crystal and does not depend on the initial state $f(0S_\perp)$ of the beam at entrance into the crystal. Therefore, to estimate the order of magnitude of z_e we shall assume that thermalization is determined by the time of complete loss of "memory" of the S system, i.e., when one can ignore the terms in the expansion (79) associated with the memory of the system, which provides the justification for going over in the description from Eq. (66) to its asymptotic variant (82). The randomization process of the system in the z evolution is itself determined by the terms of order $o(\varepsilon^2)$, and in the derivation of Eqs. (66) and (82) we must take them into account in all the series which arise in the expansions. At large z, the correlation functions which occur in the coefficient of $f(0S_\perp)$ in Eq. (79) are damped as V_0/z, i.e.,

$$\sum_n \frac{1}{\Gamma_0}\langle \overline{J_{\text{int}}^{+}} G(z)\,\Psi_n\rangle_{z\to\infty} \sim \varepsilon B/z.$$

We can ignore the memory of the system if $\varepsilon B/z$ has order $o(\varepsilon^3)$. In analyzing the order of magnitude of the terms in Eqs. (66) and (82), we proceeded as follows. For each physical quantity we introduced its characteristic scale (21) and made the equation dimensionless. The dimensionless parameter then obtained for each term of the equation indicated its order of magnitude: $\varepsilon z_M B/z \sim [1] z_M/z \sim \varepsilon^2$, where [1] denotes a dimensionless quantity of order 1.

For channeling, the characteristic scale of the lengths is a distance of the order of the distances between the ions in the crystals: $z_M \sim 1$ Å, $\varepsilon^2 = E_\perp^c/E_0$. For protons $E_\perp^c \approx 5$ eV (Ref. 1), and we take E_0 to be, for example, of order 0.5 MeV; $\varepsilon^2 \sim 10^{-5}$–$10^{-6}$, so that $z_e \approx 10^5$–10^6 Å. For heavy ions $E_\perp^c \approx 10^2$ eV (Ref. 2), and for the same values of E_0 we have $z_e \approx 10^6$–10^7 Å.

8. STATIONARY STATE

The limiting state is found from the condition of stationarity with respect to z, i.e., $\partial f(zS_\perp)/\partial z = 0$, and the condition that the "collision integral" vanish. The second condition leads to the Maxwellian momentum distribution, and to determine the dependence of the distribution in the $\mathbf{R}_\perp$ plane we have the equation

$$-\mathbf{v}_\perp \nabla_{R_\perp} f_0(S_\perp) + \left\langle \frac{\exp\left[-\frac{1}{\Theta}\sum_{j=1}^{N}\overline{U(\mathbf{R}-\mathbf{r}_j)}\right]}{\left\langle \exp\left[-\frac{1}{\Theta}\sum_{j=1}^{N}\overline{U(\mathbf{R}-\mathbf{r}_j)}\right]\right\rangle_\Sigma} \times \sum_j \nabla_{R_\perp}\overline{U(\mathbf{R}-\mathbf{r}_j)}\right\rangle_\Sigma \frac{1}{M}\nabla_{v_\perp} f_0(S_\perp) = 0. \tag{83}$$

Up to a normalization constant, the solution of (83) is

$$f_0(S_\perp) = \exp\left[-\frac{MV_\perp^2}{2\Theta}\right]\left\langle \exp\left[-\frac{1}{\Theta}\sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)}\right]\right\rangle_\Sigma, \tag{84}$$

where

$$\sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)} = \frac{1}{\Omega}\sum_{k_\perp\neq 0} v(k_\perp)\exp[i\mathbf{k}_\perp\mathbf{R}_\perp]\sum_{j=1}^{N}\exp[-i\mathbf{k}_\perp\mathbf{r}_j^\perp] - \Theta U_0. \tag{85}$$

The part of the interaction corresponding to $k_\perp = 0$ in the sum (85) is included in the constant ΘU_0. The constant U_0 is chosen on the basis of the condition that the potential energy of the particle vanish in the field of the crystal lattice at the center of the channel of the motion. Equation (83) admits the introduction of such a constant:

$$U_0 = \ln\left\langle \exp\left(-\frac{1}{\Theta}\sum_{k_\perp\neq 0} v(k_\perp)\frac{1}{\Omega}\sum_j \exp[-i\mathbf{k}_\perp\mathbf{r}_j^\perp]\right)\right\rangle_\Sigma. \tag{86}$$

We now discuss some effects of the formation of a beam of high-energy particles by crystals. To be specific, we investigate the case of axial channeling through a crystal with cubic Bravais lattice (Fig. 5).[29] In Fig. 5, the numbers 1, 2, 3, ... denote the ions of the crystal; the z axis coincides with the channeling direction; a is the lattice constant; the ions 1, 6, 5, 3 lie in a plane perpendicular to the channeling direction.

We consider

$$\Phi(\mathbf{R}_\perp) = \frac{1}{\Omega}\sum_{k_\perp\neq 0} v(k_\perp)\exp[i\mathbf{k}_\perp\mathbf{R}_\perp]\sum_j \exp(-i\mathbf{k}_\perp\mathbf{r}_j^\perp). \tag{87}$$

In (87), the summation is over all positions of the ions of the lattice. We introduce the indices l, m_l, where l labels the close-packed chain of ions of the crystal parallel to the channeling direction, and m_l marks the position of the ions in chain l; then $j = \{l, m_l\}$. Because $\Phi(\mathbf{R})$ is independent of the coordinate z, we have

$$\Phi(\mathbf{R}_\perp) = \sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)} = \overline{\sum_j U(\mathbf{R}-\mathbf{r}_j-\mathbf{z})} = \Phi(\mathbf{R}-\mathbf{z}), \tag{88}$$

where $\mathbf{z}$ is any vector with the coordinates $(0, 0, z)$. In (87), we separate the summation over l and m_l and for each fixed l we sum over m_l:

$$\Phi(\mathbf{R}_\perp) = \frac{1}{a}\frac{1}{\Lambda^2}\sum_{k_\perp} v(k_\perp) \times \exp[i\mathbf{k}_\perp\mathbf{R}_\perp]\sum_j \exp[-i\mathbf{k}_\perp\mathbf{r}_j^\perp] = \sum_l \frac{1}{a}\int_{-\infty}^{+\infty} dz\, U\left(\sqrt{z^2+(\mathbf{R}_\perp-\mathbf{r}_\perp^l)^2}\right), \tag{89}$$

where $\Lambda^3 = \Omega$ and $\mathbf{r}_\perp^l$ are the coordinates of the intersection of the chain l of ions of the crystal cell with the

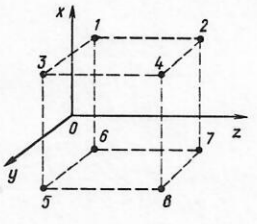

FIG. 5.

plane *oxy*. In what follows, by the unit cell of the crystal we shall understand a two-dimensional structure in the *oxy* plane formed by l chains of lattice ions.

When the function $f(zS_\perp)$ is normalized to unity, it describes the probability distribution for the state of the particle over all possible realizations of its states. It includes not only states corresponding to energy capture of the particle in the channel (we shall call such states *below-barrier* states) but also dechanneling states, i.e., *above-barrier* states. When $f(zS_\perp)$ is normalized to the transversal density of the particles, it will describe accordingly the fraction of the particles that are in the channel of the motion and the fraction of dechanneled particles. Let us make more precise these concepts of below- and above-barrier states. To each energy state of a particle there corresponds a definite accessible region of the unit cell of the crystal.[1] We consider the simplest case of a square lattice formed by chains of atoms (Fig. 6). The points in Fig. 5 indicate the positions of the chains of atoms parallel to the channeling, and the hatched region corresponds to the accessible part of the unit cell corresponding to energy $E_\perp$. As $E_\perp$ increases, the region A increases and it can be assumed that it is joined to the similar regions of the neighboring unit cells, as is shown in Fig. 7. Then the particle cannot be localized within one unit cell and will go over to its neighbors. We denote the critical value of the energy $E_\perp$ at which this begins to happen by E_c. Channeling is characterized by the relation $E_c \gg \Theta$.[1,2] The critical value of E_c in the considered case of a lattice of cubic symmetry (Fig. 5) is determined by the minimax principle

$$E_c = \min_x \max_y \left\langle \sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)} \right\rangle_\Sigma = \max_x \min_y \left\langle \sum_j \overline{U(\mathbf{R}-\mathbf{r}_j)} \right\rangle_\Sigma. \quad (90)$$

Further, we classify the states of the particle (or beam of particles, depending on the method of normalization) as follows. We say that the state $\varphi(S_\perp)$ of the particle S is a below-barrier state if

$$\langle E_\perp \rangle_\varphi = \int (dS_\perp)\, \varphi(S_\perp)\, E_\perp < E_c, \quad (91)$$

where

$$E_\perp = \frac{M\mathbf{V}_\perp^2}{2} + \overline{\left\langle \sum_j U(\mathbf{R}-\mathbf{r}_j) \right\rangle_\Sigma}.$$

We say that states for which the opposite relation to (91) holds are above-barrier states. The physical meaning of these assertions is clear. When the state opposite to (91) is realized, an energy greater than the energy corresponding to capture of the particles is

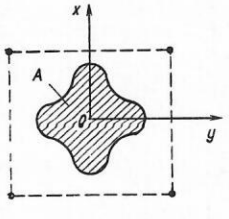

FIG. 6.

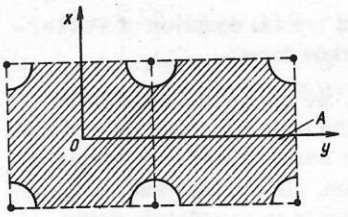

FIG. 7.

"concentrated" in the channel, and it is natural to assume that in this case the particles can leave the channel. Let $\varphi'(S_\perp)$ be some initial distribution of the particles in the beam at the entrance to the crystal for which (91) holds, and suppose there exists a certain dispersion with respect to $\mathbf{V}_\perp$ in the distribution of the particles:

$$\langle \mathbf{V}_\perp^2 \rangle_{\varphi'} = \int dS \mathbf{V}_\perp^2 \varphi'(S_\perp).$$

We shall assume that the beam is directed parallel to a crystal axis. In accordance with (84), its dispersion at sufficiently large penetration depths will be

$$\langle \mathbf{V}_\perp^2 \rangle_f = 2\Theta/M. \quad (92)$$

Therefore, if

$$\langle \mathbf{V}_\perp^2 \rangle_{\varphi'} > 2\Theta/M \quad (93)$$

we shall observe an improvement of the dispersion characteristics of the channeled beam of particles. But if

$$\langle \mathbf{V}_\perp^2 \rangle_{\varphi'} < 2\Theta/M, \quad (94)$$

then we shall observe a deterioration. The improvement of the dispersion characteristics of the beam of particles will also occur for above-barrier initial states. However, in this case it is natural to expect delocalization of the beam in the $\mathbf{R}_\perp$ plane due to transitions of the particles to neighboring channels of the motion (to neighboring unit cells). (We shall here assume that by virtue of the inequality $E_c \gg \vartheta$ the final stationary state of the beam of the particles is a below-barrier state.) Let us consider this in more detail. Suppose the initial distribution $f(0S_\perp)$ is an above-barrier distribution. (We again assume that the beam is directed parallel to a crystal axis. We shall still regard $\sqrt{\langle \mathbf{V}_0^2 \rangle}$ as sufficiently small compared with V_0, so that we can meaningfully speak of channeling, $\varepsilon \ll 1$.) Then besides the cooling of the beam of particles as a result of the z evolution, i.e., the decrease of $\sqrt{\langle \mathbf{V}_\perp^2 \rangle}$ with increasing z, delocalization of the beam due to transitions of particles to neighboring unit cells in the $\mathbf{R}_\perp$ plane will be observed. Two competing processes will be observed: a) heat transfer between the beam of particles and the crystal, leading to a forming influence of the crystal on the beam; b) delocalization of the beam of particles. If the heat-transfer processes predominate over the dechanneling processes, then, after a certain z', the delocalization must cease, and thereafter the beam must be subject to only the forming in-

fluence of the crystal. The mechanisms of these processes require more detailed study.

We consider briefly some distinctive aspects of the forming influence of crystals on beams of light and heavy channeled ions.

Protons. A feature of the interaction of protons with rows and planes of ions is the short-range nature of the forces,[6] so that almost everywhere in the plane of the unit cell a proton can be regarded as a free particle, and it is only when the crystallographic rows or planes are approached to very short distances $|\mathbf{R}_\perp| \sim a/2$ that the repulsive forces occasionally increase. This makes it possible to approximate the interaction of the proton with the ions by a set of rectangular wells (Fig. 8).

For a proton, U_0 is of order 5 eV, $U_0/\Theta \gg 1$, and therefore the probability of finding a proton in a region of $\mathbf{R}_\perp$ corresponding to such a potential energy is negligibly small and the stationary distribution can be approximately represented in the form

$$f_0(S_\perp) = \frac{2\Theta}{\pi M} \exp\left[-\frac{MV_\perp^2}{2\Theta}\right] \frac{1}{(a-b)^2}, \quad a \gg b. \tag{95}$$

Thus, the proton can be assumed to be distributed with almost equal probability in the plane $\mathbf{R}_\perp$ of the unit cell.

Ions. Ions are characterized by a long-range interaction with the rows or planes of lattice ions. For example, for channeling of copper ions through a copper crystal between the rows (1, 1, 0) the interaction function has the form shown in Fig. 9. The position $\mathbf{R}_y = 0$ in Fig. 9 corresponds to the position of the ion at the center of the channel of the motion. This nature of the interaction has the consequence that the probability of finding the ion at the center of the unit cell of the channel will be many times greater than it is at the periphery, and the probability will decrease rapidly as the periphery is approached. All this justifies one in saying that the crystal tends to "focus" a beam of heavy ions toward the center of the channel.

Of course, this description indicates only the qualitative difference of the forming influence of the crystals on beams of high-energy particles corresponding to the nature of the interaction between them and the ions of the crystal. In deriving Eqs. (66) and (82), we ignored, as we have already said, the electron subsystem of the crystal, whose influence on the system S cannot be taken into account by the function $U(\mathbf{R})$. As a justification for this approximation one can argue that the investigated forming influences of the crystal on a beam of particles are determined by processes of heat transfer

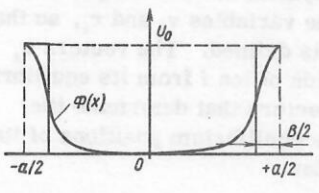

FIG. 8.

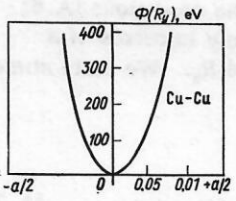

FIG. 9.

between the S system and the crystal. But in these processes the electrons of the Fermi fluid in the crystal play a small part at ordinary crystal temperatures compared with the ions of the crystal, since only a small fraction of the electrons in the immediate vicinity of the Fermi surface participates in the heat-transfer processes.[29]

APPENDIX 1

Structure expansion for $P_0^*(S\Sigma)$

$$P_0^*(S\Sigma) = \exp\left[-\frac{1}{\Theta}\sum_j^N U(\mathbf{R}-\mathbf{r}_j)\right] \Big/ \left\langle \exp\left[-\frac{1}{\Theta}\sum_j^N U(\mathbf{R}-\mathbf{r}_j)\right]\right\rangle_\Sigma. \tag{A.1}$$

In $P_0^*(S\Sigma)$, we omit the subscript $\perp$ of S. For the present treatment, this is unimportant. We call the following expansion of $P_0^*(S\Sigma)$ the structure expansion, and the functions $D_n(k_1, \ldots, k_n)$ structure functions:

$$P_0^*(S\Sigma) = 1 + \sum_{n=1}^{\infty} (-1)^n \frac{1}{\Theta^n \Omega^n n!} \prod_{j=1}^{n} v(k_j) \exp[i\mathbf{k}_j\mathbf{R}]\, D_n(k_1, \ldots, k_n). \tag{A.2}$$

We obtain an equation for determining $D_n(k_1, \ldots, k_n)$. By virtue of the definition, the structure function is even with respect to all permutations of its arguments $\mathbf{k}_i$.

$$\exp\left[-\frac{1}{\Theta}\sum_j U(\mathbf{R}-\mathbf{r}_j)\right] = P_0^*(S\Sigma)\left\langle \exp\left[-\frac{1}{\Theta}\sum_j U(\mathbf{R}-\mathbf{r}_j)\right]\right\rangle_\Sigma. \tag{A.3}$$

We write the exponentials in (A.3) in terms of series and use the Fourier representation for the interaction potential. After this, we equate the functions in (A.3) on the two sides of the equation that have equal powers of the Fourier representation of the interaction. We obtain

$$R_n(k_1, \ldots, k_n) = \sum_{m=0}^{n} \frac{n!}{m!\,(n-m)!} D_m(k_1, \ldots, k_m) M_{n-m}(k_{m+1}, \ldots, k_n). \tag{A.4}$$

In (A.4), we have introduced the notation

$$R_n(k_1, \ldots, k_n) = \prod_{j=1}^{n} \Big[\sum_{e=1}^{N} \exp(-i\mathbf{k}_j^{(e)}\mathbf{r}_e)\Big];$$
$$M_n(k_1, \ldots, k_n) = \langle R_n(k_1, \ldots, k_n)\rangle_\Sigma.$$

In what follows, we shall call the function $M_n(k_1, \ldots, k_n)$ the n-th structure moment. Equation (A.4) can be regarded as a recursion relation for determining D_m in terms of R_m and M_m:

$$D_n(k_1, \ldots, k_n) = R_n(k_1, \ldots, k_n) - \sum_{m=0}^{n-1} \frac{n!}{m!\,(n-m)!} D_m(\ldots) M_{n-m}(\ldots); \tag{A.5}$$

$$D_0 = 0, \quad D_1(k) = R_1(k) - M_1(k), \quad M_0 = 1. \tag{A.6}$$

The recursion relation (A.5) and the conditions (A.6) make it possible to express D_n solely in terms of a combination of the functions M_n and R_n. We state some of the propositions which we use.

Proposition 1.

$$\langle D_n(k_1, \ldots, k_n)\rangle_\Sigma = 0. \tag{A.7}$$

Equation (A.7) follows directly from the property $\langle P_0^*(S\Sigma)\rangle_\Sigma = 1$. Let $\Psi(k_1, \ldots, k_n)$ be any function summable with $D_n(k_1, \ldots, k_n)$ and symmetric with respect to all permutations of its arguments k_i. In $D_n(k_1, \ldots, k_n)$, we introduce a time dependence:

$$D_n^t(k, \ldots, k_n) = R(t)\, D_n(k_1, \ldots, k_n). \tag{A.8}$$

We define the following operator $\hat{\Gamma}_n$, which acts on $D_n^t(k_1, \ldots, k_n)$:

$$\hat{\Gamma}_n D_n^t(k_1, \ldots, k_n) = \sum_{k_1, \ldots, kn} \Psi(k_1, \ldots, k_n)\, D_n^t(k_1, \ldots, k_n). \tag{A.9}$$

Proposition 2. Under the sign of the operator $\hat{\Gamma}$,

$$-\frac{\partial}{\partial\tau} D_n^\tau = n \sum_{j=1}^{N} \exp[-i\mathbf{k}\mathbf{V}_j(-\tau)]\, i\mathbf{k}\mathbf{V}_j(-\tau)\, D_{n-1}^\tau. \tag{A.10}$$

Proof. Note that under the sign of the operator $\hat{\Gamma}_n$

$$\hat{\Gamma}_n \sum_{i=1}^{m} \Psi(k_l)\, D_n^t(k_1, \ldots, k_n) = m\hat{\Gamma}_n \Psi(k)\, D_n^t(k_1, \ldots, k_n); \tag{A.11}$$

we have omitted the index i of $\Psi(k)$ on the right-hand side of (A.11), since it is unimportant under the sign of $\hat{\Gamma}_n$. Using (A.11), we can readily prove (A.10) by induction. Indeed,

$$\begin{aligned}
-\hat{\Gamma}_n \frac{\partial}{\partial\tau} D_n^\tau(k_1, \ldots, k_n) &= \hat{\Gamma}_n \Big\{ n \sum_{j=1}^{N} \exp[-i\mathbf{k}\mathbf{r}_j(-\tau)]\, \mathbf{k}\mathbf{V}_j(-\tau)\, R_{n-1}^\tau \\
&\quad + \sum_{m=0}^{n-1} \frac{n!}{m!\,(n-m)!} \frac{\partial}{\partial\tau} D_m^\tau(k_1, \ldots, k_m)\, M_{n-m} \Big\} \\
&= \hat{\Gamma}_n \Big[\sum_{j=1}^{N} [i\mathbf{k}\mathbf{V}_j(-\tau)] \exp[-i\mathbf{k}\mathbf{r}_j(-\tau)]\, nR_{n-1}^\tau \\
&\quad - n \sum_{j=1}^{N} \exp[-i\mathbf{k}\mathbf{r}_j(-\tau)]\, [i\mathbf{k}\mathbf{V}_j(-\tau)] \sum_{m=1}^{n-1} \frac{(n-1)!}{(m-1)!\,(n-m)!} D_{m-1}^\tau M_{n-m} \Big] \\
&= \hat{\Gamma}_n n \sum_{j=1}^{N} \exp[-i\mathbf{k}\mathbf{r}_j(-\tau)]\, [i\mathbf{k}\mathbf{V}_j(-\tau)]\, D_{n-1}^\tau,
\end{aligned}$$

i.e., it follows from the assumption (A.10) for $n \leq n_0$ that (A.10) holds for $n = n_0 + 1$:

$$\begin{aligned}
R_n^t(k_1, \ldots, k_n) &= R(t)\, R_n(k_1, \ldots, k_n); \\
M_n^t(k_1, \ldots, k_n) &= R(t)\, M_n(k_1, \ldots, k_n) = M_n(k_1, \ldots, k_n).
\end{aligned}$$

APPENDIX 2

Principle of correlation weakening for the structure moments

We prove the following property of the structure moments for a harmonic crystal:

$$\begin{aligned}
&M_t^m(1, \ldots, n) \\
&= \Big\langle \prod_{j=1}^{m} \Big[\sum_{l_j=1}^{N} \exp(-i\mathbf{k}_j \cdot \mathbf{r}_{l_j}) \Big]\, R(t) \prod_{j=m+1}^{n} \Big[\sum_{l_j=1}^{N} \exp[-i\mathbf{k}_j \cdot \mathbf{r}_{l_j}] \Big] \Big\rangle_{\Sigma t \to \infty} \\
&= \Big\langle \prod_{j=1}^{m} \Big[\sum_{l_j=1}^{N} \exp(-i\mathbf{k}_j \cdot \mathbf{r}_{l_j}) \Big] \Big\rangle_\Sigma \Big\langle \prod_{j=m+1}^{m} \Big[\sum_{l_j=1}^{N} \exp[-i\mathbf{k}_j \cdot \mathbf{r}_{l_j}] \Big] \Big\rangle_\Sigma \\
&= M_m(1, \ldots, m)\, M_{n-m}(1+m, \ldots, n).
\end{aligned} \tag{A.12}$$

For $\mathbf{r}_j(t)$, we can use an expansion with respect to the normal vibrations of a harmonic crystal.[28] We introduce the notation

$$\left.\begin{aligned}
&\mathbf{r}_j(t) = \mathbf{R}_j^0 + \sum_{\lambda=1}^{3N} \mathbf{u}_j^\lambda(t); \\
&\mathbf{u}_j^\lambda(t) = \mathbf{S}_j^\lambda a \exp[-i\omega_\lambda t] + \mathbf{S}_j^{\lambda *} a^+ \exp[i\omega_\lambda t]; \\
&\mathbf{S}_j^\lambda = i\hbar^{1/2} (2M_j N\omega_\lambda)^{-1/2}\, \mathbf{e}_j^\lambda \exp[i\mathbf{q}\cdot\mathbf{R}_j^0]; \\
&[a^+, a]_{(-)} = -1, \quad j = \{\mathbf{R}_j^0, S'\}, \quad \lambda = \{q, S\}; \\
&\mu_j^\nu(t) = \mathbf{k}_l \cdot \mathbf{S}_j^\nu \exp(-i\omega_\lambda t),
\end{aligned}\right\} \tag{A.13}$$

where $\mathbf{R}_j^0$ is the equilibrium position of site j of the crystal lattice, S' is the number of ions per lattice site, $\mathbf{q}$ is the wave vector, and S labels the branch of elementary excitations of the harmonic crystal. Using repeatedly the equations

$$\begin{aligned}
&\exp\hat{A} \exp\hat{B} = \exp\{(1/2)[\hat{A}, \hat{B}]\} \exp[\hat{A} + \hat{B}]; \\
&\mu_j^\nu(t)\, \mu_j^{\nu *}(t) = \mu_j^\nu(0)\, \mu_j^{\nu *}(0),
\end{aligned} \tag{A.14}$$

and making fairly lengthy transformations in the spirit of the calculations of Ref. 28, we obtain

$$\begin{aligned}
M_t^m(1, \ldots, n) &= \prod_{j=1}^{n} \Big[\sum_{R_j^0} \exp[i\mathbf{k}_j \mathbf{R}_j^0] \Big] \\
&\times \prod_{\nu}^{3N} \exp\Big[-\frac{1}{2} \sum_{l=1}^{m-1} \mu_{j_l}^\nu \sum_{k=l+1}^{m} \mu_{j_k}^{*\nu} + \text{h. c.} \Big] \\
&\times \exp\Big[-\frac{1}{2} \Big| \sum_{l=1}^{m} \mu_{j_l}^\nu \Big|^2 \Big] \exp\Big[-\frac{z^\nu}{1-z^\nu} \Big| \sum_{l=1}^{m} \mu_{j_l}^\nu \Big|^2 \Big] \\
&\times \prod_{\nu}^{3N} \exp\Big[-\frac{1}{2} \sum_{l=m+1}^{n-1} \mu_{j_l}^\nu \sum_{k=l+1}^{n} \mu_{j_k}^{*\nu} + \text{h. c.} \Big] \\
&\times \exp\Big[-\frac{1}{2} \Big| \sum_{l=m+1}^{n} \mu_{j_l}^\nu \Big|^2 \Big] \exp\Big[-\frac{z^\nu}{1-z^\nu} \Big| \sum_{l=m+1}^{n} \mu_{j_l}^\nu \Big|^2 \Big] \\
&\times \exp\Big\{ -\frac{z^\nu}{1-z^\nu} \Big(\sum_{l=1}^{m} \mu_{j_l}^\nu \sum_{l=m+1}^{n} \mu_{j_l}^{*\nu}(x) + \text{h. c.} \Big) \Big\},
\end{aligned} \tag{A.15}$$

where $z^\nu = \exp[-\hbar\omega^\nu/\theta]$, h.c. is the complex-conjugate expression, and R_j^0 under the summation sign denotes summation over the equilibrium positions of the ions. As $t \to \infty$,

$$\prod_{\nu}^{3N} \exp\Big\{ -\frac{z^\nu}{1-z^\nu} \Big(\sum_{l=1}^{m} \mu_{j_l}^\nu \sum_{l=m+1}^{n} \mu_{j_l}^{*\nu} + \text{h. c.} \Big) \Big\}_{t\to\infty} \to 1. \tag{A.16}$$

Hence, for (A.15), we have the limiting relation (A.12). [Equation (A.14) holds only for operators whose commutator is a c number.]

Now suppose $\varphi(S_\perp, \ldots, \mathbf{v}_i, \mathbf{r}_i, \ldots)$ is a function defined on the phase space of the system $S + \Sigma$ and square-integrable with respect to the variables $\mathbf{v}_i$ and $\mathbf{r}_i$, so that a Fourier transform of it is defined. The vectors $\mathbf{v}_\perp$ and $\mathbf{r}_i$ describe the deviation of ion i from its equilibrium position. It is these vectors that determine the state space of Σ, since the equilibrium positions of its ions are fixed. We consider

$$\langle J_{\text{int}}^\perp G(t)\, \varphi(S_\perp, \ldots, \mathbf{v}_i, \mathbf{r}_i, \ldots)\rangle_\Sigma. \tag{A.17}$$

For this quantity we can formulate the following proposition.

Proposition 3.

$$\langle \mathcal{J}_{\text{int}}^{\perp} G(t)\, \varphi(S_{\perp}, \ldots, \mathbf{v}_l, \mathbf{r}_l, \ldots)\rangle_{\Sigma_{t\to\infty}} = \overline{\langle \mathcal{J}_{\text{int}}^{\perp}\rangle_{\Sigma}}\, \langle \varphi(S_{\perp}, \ldots, \mathbf{v}_l, \mathbf{r}_l, \ldots)\rangle_{\Sigma}. \tag{A.18}$$

The validity of (A.18) can be proved as follows. For (A.17), we introduce the Fourier representation:

$$\begin{aligned}
&\langle \mathcal{J}_{\text{int}}^{\perp} R(t)\, \varphi(S_{\perp}, \ldots, \mathbf{v}_l, \mathbf{r}_l, \ldots)\rangle_{\Sigma} \\
&= \frac{1}{\Omega^{N+1}} \frac{1}{L^N} \sum_{\substack{k_1, \ldots, k_{N+1} \\ l_1, \ldots, l_N}} \exp[i\mathbf{k}_1\mathbf{R}]\, \nu(k_1)\, \varphi(S, k_2, \ldots, k_{N+1}, l_{\perp}, \ldots, l_N) \\
&\times \Big\langle \sum_{j=1}^{N} \exp[-i\mathbf{k}_{\perp}\cdot\mathbf{r}_j]\, G(t) \exp[i\mathbf{k}_2\cdot\mathbf{r}_1 + \ldots + i\mathbf{k}_{N+1}\cdot\mathbf{r}_N] \\
&\times \exp[i\mathbf{l}_1\cdot\mathbf{v}_1 + \ldots + i\mathbf{l}_N\mathbf{v}_N]\Big\rangle_{\Sigma},
\end{aligned}$$

where $\varphi(S, k_2, \ldots, k_{N+1}, l_n, \ldots, l_N)$ is the Fourier transform of the function φ; L is some sufficiently large volume in the v_l space, so that in the limit $L \to \infty$ the sums over l can be replaced by integrals; $\mathbf{R}_j = \mathbf{r}_j^n + \mathbf{n}_j$, where $\mathbf{n}_j$ is the equilibrium position of ion j and $\mathbf{r}_j^n$ in its thermal deviation from $\mathbf{n}_j$. The introduction of a "box" in the velocity space is of an auxiliary nature, and need not be done. Further, for $\mathbf{r}_j^n$ we use the representation (A.14) and note that $\mathbf{v}^n(t) = \mathbf{d}/dt\, \mathbf{r}^n(t)$. Then an expression for the expansion in normal vibrations can also be readily obtained for the vectors $\mathbf{v}_j^n$. After this, (A.18) follows from the principle of correlation weakening for the structure moments.

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