Dislocations in charge density wave crystals

S. A. Brazovskiĭ and S. I. Matveenko

L. D. Landau Institute for Theoretical Physics, USSR Academy of Sciences
(Submitted 20 July 1990)
Zh. Eksp. Teor. Fiz. **99**, 1539–1550 (May 1991)

Dislocations and aggregations of solitons in charge-density-wave crystals are studied at low temperatures. The main effects studied involve the Coulomb interactions at low densities of residual carriers. The aggregation energy and distributions of the phase deformations, electric field, and soliton-interaction potential are found. The conditions under which solitons aggregate into growing dislocation loops are discussed. The results provide information on consecutive steps of current conversion in charge-density-wave crystals.

1. INTRODUCTION

In recent years the dislocation mechanism of motion of charge density waves (CDW) has been actively discussed (see Ref. 1 and citations in Ref. 2). A microscopic picture of nucleation of the region of phase slippage in the volume, in terms of closed dislocations, has been suggested in Ref. 3. Later, in connection with elucidation of the role of contact phenomena,[4–7] the formation of phase vortices at the interface, which is equivalent to the motion of the edge dislocation, has been considered.[4,5] A systematic translation of notions of the dislocation theory in a uniaxially deformed crystal into the language of phase deformations of CDW is given in Refs. 8 and 9. A hypothesis of existence of a "comb" of edge dislocations arranged in a consecutive order along a sample surface has been put forward by Gill (see Ref. 1, p. 89, and Ref. 10).

The purely phenomenological approach and direct borrowing of traditional notions of the theory of crystal defects limit the application range of the studies known to the authors in two respects. First, the Coulomb interactions accompanying the deformations of CDW are not taken into account. This confines the application of the theory to the case of high normal-carriers density realized, apparently, only in $NbSe_3$. Allowance for Coulomb interactions is extremely important for the study of effects at low temperatures, which attracts now the greatest attention (see Gruner and Monceau (Ref. 11, p. 137), Monceau (Ref. 1, p. 165), and Nagy (Ref. 11, p. 191).

Second, a microscopic theory of nucleation of phase-slippage centers (PSC) and its juncture with the macroscopic theory of the development of dislocations are urgently needed. In this way one can construct a consistent theory of transformation of the current of normal carriers injected at the contact into the Fröhlich current of CDW. Up to now, consistent microscopic equations were derived[6] for the description of somewhat different "instanton" mechanisms of depinning of the CDW phase from the contact by analogy with nonstationary resistive phenomena in thin superconducting channels (see Gor'kov Ref. 11, p. 403). As in the case of a superconductor, equations of the Gor'kov-Éliashberg type are derived for a gapless regime, i.e., in the vicinity of the transition temperature T_c with strong electron scattering. In the case of CDW with a developed gap $2\Delta_0$ in the electron spectrum, the motion of a plane wall of the amplitude soliton type has been considered.[12] At least for a system of weakly coupled chains ($T_c \ll \Delta_0$), this wall is unstable to disintegration into purely phase solitons of substantially smaller energy (see Refs. 2, 13, and 14).

At present, CDW in essentially quasi-1D compounds are being mainly investigated (see Rouxel and Schlenker,[11] p. 15). In these compounds the gap is developed already near T_c, and at low temperatures there is already a strongly correlated 3D crystal of CDW (see Pouget and Comes,[11] p. 85). As seen from the brief survey above, in these cases it is necessary to reanalyze both the initial microscopic mechanism of the electron conversion in the CDW deformation and the dislocation growth under conditions of a screened Coulomb potential. The first problem has been recently examined in Ref. 2 on the basis of old[13] and recently supplemented[14] concepts expounded in Refs. 13 and 14.

The initial stages of the conversion of normal carriers (e) are almost unambiguously determined in systems with a weak chain coupling characterized by the small ratio of the 3D-ordering temperature T_c to the gap $2\Delta_0$: $T_c \ll \Delta_0$. The process goes via formation of amplitude π-solitons at all T towards formation of 2π-solitons for $T < T_c$,[15,16] and then towards their aggregation into macroscopic PSC. The first stages ($e + \pi$, $\pi + \pi \to 2\pi$) accompanied by energy release are irreversible, and the direction of the process does not depend on the interactions. Nevertheless, the rate of the second process ($\pi + \pi \to 2\pi$), requiring pair collisions, depends on the sign of the interaction: repulsion will replace this process by another one, $e + \pi \to 2\pi$, requiring a high activation energy Δ_0. The third stage ($2\pi + \ldots + 2\pi \to$ PSC) depends, in essence, on the character of interactions. In the case of attraction, PSC will grow without barrier in agreement with new experimental data.[17] In the case of repulsion, the current of 2π-solitons will play the role of the current of normal carriers.

The soliton interaction is realized by deformation and Coulomb forces which, by virtue of the CDW polarizability, are interrelated, and the character of resulting interactions is not clear *a priori*.

In their previous paper[2] the authors have shown that in crystals with CDW the solitons of one sign may be attracted in the direction of the chain axis. The attraction to the common transverse plane $r_\perp = (y,z)$ occurs even for nonscreened interaction dominating in the longitudinal direction x. Therefore it is natural to assume that solitons may aggregate into clusters, the growth of which will lead to the macroscopic slipping of the CDW phase. In the present paper we shall find the deformation, charge, and Coulomb po-

 0038-5646/91/050860-06$03.00

tential distributions in the medium around a soliton cluster, and consider the dependence of the energy of the system on the charge $2N$, where N is the number of 2π-solitons in the cluster. We shall also find the energy $W(N)$ of the cluster and consider the interaction with the gas of microscopic solitons and electrons. The analysis is within the framework of the macroscopic theory of dislocations. In terms of this theory a phase 2π-soliton can be described as a microscopic dislocation loop in the plane perpendicular to the axis of the chain.

2. EQUATIONS OF THE THEORY OF DISLOCATIONS

In the discrete model a 2π-soliton appearing at a jth chain can be taken into account by an additional condition

$$\int \frac{\partial \varphi_n}{\partial x} dx = 2\pi \delta_{n,j}, \tag{1}$$

where φ_n is the phase of CDW on the nth chain, the main contribution to the integral coming from the region of size l of the soliton ($l \sim v/T_c$, where T_c is the temperature of the $3D$-ordering, and v is the Fermi velocity).

Let us recall (see Ref. 2) that the scale length l is determined by the competition of the energy of the longitudinal phase deformation and the energy of dephasing at neighboring chains $n = j$ and $n \neq j$ under the additional condition (1). When N solitons aggregate into a cluster of chains $\{j\}$, a scale length $\geqslant l$ is conserved only for outer solitons in the cluster, for which the phase difference approximately equals π. For inner chains the phase difference decreases, and the longitudinal scale grows so that the soliton localization length is proportional to N if the Coulomb interaction is taken into account, and to $N^{1/2}$ if this interaction is neglected. Thus, outside the line $\mathscr{D}$ given by the extreme solitons of scale length l, the continual theory is applicable:

$$\varphi_n(x) \to \varphi(\mathbf{r}), \quad \mathbf{r} = (x, \mathbf{r}_\perp).$$

Evidently, the line $\mathscr{D}$ is a dislocation line, so that the conditions (1) take the form

$$\int_L \frac{\partial \varphi}{\partial x_k} dx_k = +2\pi. \tag{2}$$

In general case, when we traverse any closed contour L enclosing the dislocation line $\mathscr{D}$, the CDW phase receives an increment equal to 2π. The direction of passage is related to the chosen direction $\boldsymbol{\tau}$ of the vector tangent to the dislocation line by the right-hand screw rule (see Fig. 24 in Ref. 18). In the framework of the dislocation theory, Eq. (2) corresponds to the case when the displacement vector $\mathbf{u}$ points along the x-axis of the chains, and the Burgers vector $\mathbf{b}$ has the components $\mathbf{b} = (-2\pi, 0, 0) \equiv -2\pi\,\mathbf{n}$, $\mathbf{n} = (1,0,0)$.

We are interested in macroscopic scales $|x - x_j| \gg 1$, $|\mathbf{r}_\perp - \mathbf{r}_{\perp j}| \gg s^{1/2}$ ($x_j, \mathbf{r}_j$ are the soliton coordinates, and s is the cross-section area per chain), on which the condition (1) is equivalent to the differential equation

$$\partial \varphi / \partial x = 2\pi \delta(x - x_j)\, \delta(\mathbf{r}_\perp - \mathbf{r}_{\perp j})\, s. \tag{3}$$

The bypass rule (1) is conveniently written in a differential form

$$[\nabla \mathbf{w}] = 2\pi \boldsymbol{\tau} \delta(\boldsymbol{\xi}), \tag{4}$$

where $w_m = \partial \varphi / \partial x_m$ is an analog of the distortion tensor, and $\boldsymbol{\xi}$ is the two-dimensional radius-vector taken from the axis of the dislocation in the plane perpendicular to the tangent vector $\boldsymbol{\tau}$ at the point considered. Here and below we follow, whenever possible, the notation of Ref. 18.

According to the dislocation theory, the phase φ experiences a discontinuity $\Delta\varphi = \pm 2\pi$ on a certain finite surface $\mathscr{F}$ spanning the contour $\mathscr{D}$ so that at large distances $\varphi \to 0$. On the contrary, in terms of the soliton problem the phase φ is continuous everywhere with respect to x, but receives a finite increment at infinity. This definition corresponds to the transformation of the surface $\mathscr{F}$ into a semi-infinite cylinder spanning the contour $\mathscr{D}$.

In the continual limit one can use a phenomenological model-independent functional of the energy of the system[2]

$$H = \int \frac{d^3 r}{s} \left\{ \frac{v}{4\pi} \left[\left(\frac{\partial \varphi}{\partial x} \right)^2 + \alpha \left(\frac{\partial \varphi}{\partial \mathbf{r}_\perp} \right)^2 \right] + \frac{\Phi}{\pi} \frac{\partial \varphi}{\partial x} - \frac{\varepsilon_\infty (\nabla \Phi)^2}{8\pi e^2} s \right\}, \tag{5}$$

where α is the anisotropy constant ($\alpha \ll 1$), Φ is the electric potential, ε_∞ is the dielectric constant of the medium without the Coulomb effects of the CDW (below we assume that ε_∞ is included in the definition of e^2), and

$$(e/\pi)\, \partial \varphi / \partial x = \rho$$

is the electric charge density.

The Coulomb interaction for CDW has been considered in many studies.[19-22] Note that, contrary to the opinion of some authors, the dielectric constant ε_∞ does not contain a dielectric contribution proportional to ω_p^2/Δ^2 (ω_p is the plasma frequency) and characteristic of the Peierls dielectric without the Fröhlich mode (see Refs. 20, 22).

Varying the functional (5), we obtain the equilibrium condition that may be written in the form

$$\nabla \mathbf{B} = 0, \quad \mathbf{B} = \hat{\nabla} \varphi + 2\Phi \mathbf{n}/v, \tag{6}$$

$$\frac{2}{\varkappa^2} \Delta \Phi + \mathbf{n}\mathbf{w} = 0, \tag{7}$$

where

$$\hat{\nabla} = \left(\frac{\partial}{\partial x}, \alpha \frac{\partial}{\partial \mathbf{r}_\perp} \right), \quad \Delta = \frac{\partial^2}{\partial \mathbf{r}^2}, \quad \varkappa^2 = r_D^{-2} = \frac{8e^2}{vs}$$

and r_D is the Debye screening radius in a metal without CDW.

Let us now derive a differential equation for $\varphi(r)$, allowing for the condition (4). Multiplying Eq. (4) written in vector form by the vector b, we find

$$(\mathbf{n}\nabla)\mathbf{w} - \nabla(\mathbf{n}\mathbf{w}) = 2\pi [\boldsymbol{\tau}\mathbf{n}]\, \delta(\boldsymbol{\xi}). \tag{8}$$

(The square brackets indicate a vector product.)

Substituting Eq. (8) into Eq. (6) differentiated with respect to x, we find finally

$$\hat{\Delta}(\mathbf{n}\nabla)\varphi + \frac{2}{v}(\mathbf{n}\nabla)^2 \Phi = 2\pi \hat{\nabla} [\delta(\boldsymbol{\xi})\, [\mathbf{n}\boldsymbol{\tau}]],$$
$$\hat{\Delta} = \vee \hat{\nabla} = \frac{\partial^2}{\partial x^2} + \alpha \Delta_\perp, \quad \Delta_\perp = \frac{\partial^2}{\partial \mathbf{r}_\perp^2}. \tag{9}$$

The model-independent equations which follow from Eqs. (7)–(9) mean that the field averaged over cross section is not sensitive to the presence and position of solitons and dislocations:

$$\frac{\partial^2}{\partial x^2}\bar{\Phi}(x)-\varkappa^2\bar{\Phi}(x)=\text{const},$$
$$\bar{V}=\bar{\Phi}+\frac{v}{2}\frac{\partial\varphi}{\partial x}=\text{const}, \tag{10}$$

where

$$\bar{f}(x)=\int\frac{d^2r_\perp}{s}f(x,\mathbf{r}_\perp).$$

Note that to proceed from the dislocation to the point-soliton approach[2] we have to redefine the phase

$$\varphi(x,\mathbf{r}_\perp)\to\varphi(x,\mathbf{r}_\perp)+\int^x\rho_s(x',\mathbf{r}_\perp)\,dx',$$

where ρ_s is the soliton density. In the soliton approach[2] the phase φ does not allow for the central chain. In the dislocation approach this means that the chains passing through the loop are not taken into account.

Eliminating φ from Eq. (7), we find the equation for the field Φ:

$$K\Phi=-\pi\varkappa^2v\hat{\nabla}(\delta(\xi)[\mathbf{n}\boldsymbol{\tau}]), \tag{11}$$

where

$$K=\hat{\Delta}\Delta-\varkappa^2(\mathbf{n}\nabla)^2. \tag{12}$$

The equations for the fields $\partial\varphi/\partial x$ and $V=\Phi+(v/2)(\partial\varphi/\partial x)$ are obtained from Eq. (11) with the help of Eq. (7):

$$v\frac{\partial\varphi}{\partial x}=-2\frac{\Delta}{\varkappa^2}\Phi,\quad V=\left(1-\frac{\Delta}{\varkappa^2}\right)\Phi. \tag{13}$$

It follows from (11) and (13) that the fields Φ, φ, and V have singularities on the dislocation line.

Let us introduce now for the operator K the Green function $D(\mathbf{r})$ related to the single-soliton solutions Φ_s and φ_s studied earlier:[2]

$$KD(\mathbf{r})=s\delta(\mathbf{r}).$$

Then

$$-\pi\alpha v\varkappa^2\Delta_\perp D(\mathbf{r})=2\Phi_s(\mathbf{r}), \tag{14}$$
$$2\pi(\varkappa^2-\Delta^2)\frac{\partial}{\partial x}D(\mathbf{r})=2\varphi_s. \tag{15}$$

It is easy to derive from (11) an expression for Φ in the form of an integral over the dislocation line $\mathscr{D}$, and then over the surface $\mathscr{F}$ arbitrarily spanning $\mathscr{D}$:

$$\Phi=\pi\alpha\varkappa^2\int_{\mathscr{D}}[\mathbf{n}\nabla]\,dlD(\mathbf{r}-\mathbf{r}'). \tag{16}$$

Using Eq. (14), we find hence

$$\Phi=\frac{2}{s}\int_{\mathscr{F}}d\mathbf{f}'\,\mathbf{n}\Phi_s(\mathbf{r}-\mathbf{r}')+\pi\alpha\varkappa^2G,$$
$$G=\frac{1}{s}\int_{\mathscr{F}}d\mathbf{f}'(\nabla-(\mathbf{n}\nabla)\mathbf{n})(\mathbf{n}\nabla)D(\mathbf{r}-\mathbf{r}'). \tag{17}$$

The first term in Eq. (17) has a simple physical meaning of a superposition of the fields of point fictitious solitons filling the projection of the dislocation surface normal to n. The second term vanishes for a loop lying in the transverse plane.

The fields $\partial\varphi/\partial x$ and V are obtained from (16) with the help of relations (13). Using Eqs. (11), (13), and (15) we find

$$\frac{\partial}{\partial x}V=-\frac{\alpha v}{s}\oint_{\mathscr{D}}d\mathbf{l}[\nabla\varphi_s(\mathbf{r}-\mathbf{r}')\mathbf{n}]$$
$$=-\frac{\alpha v}{s}\int_{\mathscr{F}}d\mathbf{f}'(\mathbf{n}\nabla-(\mathbf{n}\nabla)\nabla)\varphi_s(\mathbf{r}-\mathbf{r}'). \tag{18}$$

Integrating (18) over x, we have

$$V=-\frac{\alpha}{s}\int_{\mathscr{F}_c}df_c\,\nabla\varphi_s(\mathbf{r}-\mathbf{r}')=-\frac{\alpha}{s}\int_{V_c}d^3r'\,\Delta_\perp\varphi_s(\mathbf{r}-\mathbf{r}'). \tag{19}$$

Here $\mathscr{F}_c$ and V_c are the surface and volume of a semi-infinite cylinder spanning the contour $\mathscr{D}$ with generators parallel to n, and $df_c=[dl\times n]dx$ is the element of the cylinder surface.

Similar to (19), we find from (13) and (16) the following expression for the phase

$$\varphi(\mathbf{r})=\frac{1}{s}\int_{\mathscr{F}_c}d\mathbf{f}_c'\,\nabla\Delta D(\mathbf{r}-\mathbf{r}'). \tag{20}$$

Let us find, at last, a convenient expression of the type of Eq. (17) for the phase φ in the form of the superposition of the fields of soliton sources

$$\varphi^*(\mathbf{r})=\frac{2}{s}\int_{\mathscr{F}}d\mathbf{f}'\,\mathbf{n}\varphi_s(\mathbf{r}-\mathbf{r}'). \tag{21}$$

For this purpose we use an easily verified identity

$$\mathbf{n}K=(\mathbf{n}\nabla)^2(\Delta-\varkappa^2)\mathbf{n}+\alpha\Delta(\Delta\mathbf{n}-(\mathbf{n}\nabla)\nabla)$$
$$+\alpha\Delta(\mathbf{n}\nabla)(\nabla-(\mathbf{n}\nabla)\mathbf{n}). \tag{22}$$

Applying the operator (22) term-by-term to the function $D(r-r')$, we integrate over $\mathscr{F}$. The left-hand side of (22) gives a δ-function singularity on $\mathscr{F}$; the first, second, and third terms on the right-hand side give $\partial\varphi^*/\partial x$, $\partial\varphi/\partial x$, and $\alpha\Delta\partial G/\partial x$, respectively [cf. (15), (21), and (17)]. The result is

$$\varphi(\mathbf{r})=\varphi^*(\mathbf{r})+2\pi\theta_r\{\mathscr{F}\}-\alpha\Delta G,$$

where φ^* and G are defined by (21) and (17), and $\theta_r\{\mathscr{F}\}$ is the unit discontinuity function on the surface $\mathscr{F}$:

$$\frac{\partial\theta_r\{\mathscr{F}\}}{\partial x}=\int_{\mathscr{F}}\frac{df'}{s}\mathbf{n}\delta(\mathbf{r}-\mathbf{r}').$$

If we choose the cylinder $\mathscr{F}_c$ as the surface $\mathscr{F}$, the first and the second terms on the right-hand side of Eq. (22) vanish as well as the second term in the definition of G [see (17)]. As a result, we find the formula (20). For a plane loop we choose a plane surface $\mathscr{F}$ so that $G=0$. In this case φ and φ^* differ only in the definition of the discontinuity. At large distances

from a loop enclosing N chains (a cluster with a charge $2Ne$),

$$\varphi^*(\mathbf{r}) \approx 2N\varphi_s(\mathbf{r}), \quad \varphi^*(\mathbf{r}) \to 0, \quad x \to \infty.$$

The function $\varphi^*(\mathbf{r})$ has a discontinuity $\delta\varphi^*|_F = -2\pi$; therefore, by virtue of Eq. (22), the function $\varphi(\mathbf{r})$ does not have a discontinuity, i.e., it varies monotonicly from 0 to 2π along the x axis, if we cross the surface $\mathscr{F}$:

$$\varphi(-\infty, \mathbf{r}_\perp) = 0, \quad \varphi(\infty, \mathbf{r}_\perp) = 2\pi.$$

Thus, the definition of the phase φ^* corresponds to the concept of discontinuity of displacements in the theory of dislocations, and the definition of the phase φ corresponds to the physical picture of aggregation of 2π-solitons. The continuity of the phase $\varphi(\mathbf{r})$ with respect to x and its invariance under the choice of the surface $\mathscr{F}$ follows from its definition

$$\varphi(x, \mathbf{r}_\perp) = -\frac{2}{\pi}\int_{-\infty}^{x} dy\, \Delta\Phi(y, \mathbf{r}_\perp),$$

since the charge density $-\Delta\Phi/4\pi$ has no singularities on any surface.

3. ENERGY

Let us consider now the energy of the system in the presence of an arbitrary dislocation loop. Using Eq. (7), we transform the last term in the energy functional (5). As a result, the energy takes on the form

$$H = \frac{v}{4\pi s}\int d^3r\, \mathbf{wB}, \tag{23}$$

where $\mathbf{B}$ is defined in (6). Eqs. (4)–(6) and (23) show that our system is equivalent to a certain magnetic medium with the "magnetic induction" $\mathbf{B}$ and "field" $2\mathbf{w}$ in the presence of a unit current in the contour $\mathscr{D}$. Equation (7) plays the role of the linear anisotropy and nonlocal susceptibility.

Introducing the vector-potential $\mathbf{A}$ according to $\mathbf{B} = [\nabla \times \mathbf{A}]$, we obtain from (23) after standard transformations

$$H = \frac{v}{2s}\int_{\mathscr{D}} \mathbf{A}\, d\mathbf{l} = \frac{v}{2s}\int_{\mathscr{F}} \mathbf{B}\, d\mathbf{f}. \tag{24}$$

Having chosen the cylinder surface $\mathscr{F}_c$ as the surface $\mathscr{F}$, we have

$$H = \frac{\alpha}{2}\frac{v}{s}\int_{\mathscr{F}_c} d\mathbf{f}_c\, \nabla\varphi. \tag{25}$$

For a plane loop

$$H = \frac{1}{c}\int_{\mathscr{F}} V df, \tag{26}$$

i.e., the energy is integrated as a sum of potentials of point solitons in the plane of the dislocation loop. Evidently, the field φ in Eqs. (24)–(26) cannot have a discontinuity on the same surface.

4. PLANE RING DISLOCATION

It is natural to expect that at a given N the configuration with a minimum energy is the one with axial symmetry characterized by a ring dislocation of radius R_0 ($\pi R_0^2 = N$) in the transverse plane. To find the fields Φ, φ, and V we use Eqs. (17), (21), and (19). Single soliton solutions φ_s and Φ_s in these formulae have been recently investigated in Ref. 2. Let us recall that all the fields decrease exponentially over a microscopic scale length d in the transverse sector:

$$\begin{gathered} d \ll \alpha^{1/2}|x| < r_\perp, \\ \Phi_s,\ \varphi_s \propto \exp(-r/d), \quad d = 2\alpha^{1/2}/\varkappa, \end{gathered} \tag{27}$$

and have a peculiar mixed exponential dependence in the longitudinal sector:

$$\begin{gathered} \alpha^{1/2}|x| > r_\perp \gg d, \\ \Phi_s = \frac{e^2\varkappa}{4}|f(\mathbf{r})|, \quad \varphi = -\frac{\varkappa^2 s}{16}g(r), \\ g(\mathbf{r}) \approx \frac{1}{\tilde{x}}\exp\left(-\frac{\tilde{r}_\perp^{\,2}}{2|\tilde{x}|}\right), \quad f(\mathbf{r}) \approx |g(\mathbf{r})|, \end{gathered} \tag{28}$$

where $\tilde{\mathbf{r}} = (\tilde{x}, \tilde{\mathbf{r}}_\perp) = \varkappa r/2$, $\tilde{r} = |\tilde{\mathbf{r}}|$.

We shall use exact solutions[2] of Eqs. (14), (15) for $\alpha = 1$ valid at all $\mathbf{r}$:

$$f(\mathbf{r}) = \left(\operatorname{ch}\tilde{x} - \operatorname{sh}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right)h(\mathbf{r}), \tag{29}$$

$$g(\mathbf{r}) = \left(\operatorname{sh}\tilde{x} - \operatorname{ch}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right)h(\mathbf{r}), \tag{30}$$

where $h(r) = \exp(-\tilde{r})/\tilde{r}$.

In the important case $\alpha \ll 1$ the solutions (27) and (28) are obtained from (28)–(30) by a scale transformation

$$\begin{aligned} &\Phi_s(x, \mathbf{r}_\perp) \to \alpha^{1/2}\Phi_s(x\alpha^{1/2}, \mathbf{r}_\perp), \\ &\varphi_s(x, \mathbf{r}_\perp) \to \varphi_s(x\alpha^{1/2}, \mathbf{r}_\perp). \end{aligned} \tag{31}$$

Substituting (28)–(30) into (17) and (21), we find

$$\Phi(\mathbf{r}) = \frac{v}{8}\left(\operatorname{ch}\tilde{x} - \operatorname{sh}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right)I(\tilde{\mathbf{r}}), \tag{32}$$

$$\varphi^*(\mathbf{r}) = -\frac{1}{4}\left(\operatorname{sh}\tilde{x} - \operatorname{ch}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right)I(\mathbf{r}), \tag{33}$$

$$V = \frac{v\varkappa}{16}\left[\operatorname{ch}\tilde{x}\left(1 + \frac{\partial^2}{\partial\tilde{x}^2}\right) - 2\operatorname{sh}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right]I(\tilde{r}), \tag{34}$$

where

$$I = 2\int_{|\tilde{r}_\perp'| < \varkappa R_0/2} d^2\tilde{\mathbf{r}}_\perp' \frac{\exp\{-[\tilde{x}^2 + (\tilde{\mathbf{r}}_\perp - \tilde{\mathbf{r}}_\perp')^2]^{1/2}\}}{[\tilde{x}^2 + (\tilde{\mathbf{r}}_\perp - \tilde{\mathbf{r}}_\perp')^2]^{1/2}}. \tag{35}$$

To analyze Eqs. (32)–(35), we should take into account that the function $I(\mathbf{r})$ is proportional to the effective "electron potential" of a charged disk in an isotropic medium with a unit screening length. Near the plane $x = 0$ we have

$$\varphi \approx \pi\theta(R_0 - r_\perp), \quad V \approx \Phi \approx \frac{\pi}{2}v\varkappa\theta(R_0 - r_\perp) \tag{36}$$

with exponentially small corrections. For example, we find on the dislocation axis the exact values

$$I(x,0)=4\pi[\exp(-|\tilde{x}|)-\exp[-(\tilde{x}^2+\tilde{R}_0^2)^{1/2}]].$$

Let us now study the field distribution near the dislocation line

$$|x|\ll R_0, \quad |y|\ll R_0, \quad y=R_0-r_\perp.$$

Considering the interior part of the loop as an infinite half-plane $y>0$, we get from (35)

$$I(\tilde{x},\tilde{y})=4\pi\theta(\tilde{y})\exp(-|\tilde{x}|)-4\operatorname{sgn}\tilde{y}\int_{|\tilde{y}|}^{\infty}K_0((\tilde{x}^2+\tilde{y}^2)^{1/2})\,dz$$
$$=2\pi\exp(-|\tilde{x}|)+4\int_0^{\tilde{y}}K_0((\tilde{x}^2+z^2)^{1/2})\,dz, \quad (37)$$

where $K_0(t)$ is a modified Bessel's function and $\tilde{y}=\varkappa y/2$.

In addition to (36), we find that on the cylinder $y=0$ the function φ, as well as Φ, takes on half the values (36) at $r<R_0$.

The derivatives of Φ and φ and, consequently the field V, have diverging singularities on the line $\mathscr{D}$. This is easily seen for the transverse components $E_\perp$ and $F_\perp$ of the field and force, respectively:

$$E_\perp=\frac{\partial\Phi}{\partial y}=\frac{v\varkappa^2}{2}\left[\operatorname{ch}\tilde{x}-\operatorname{sh}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right]K_0(\tilde{\rho}), \quad (38)$$

$$F_\perp=\frac{\partial V}{\partial y}=\frac{v\varkappa^2}{4}\left[\operatorname{ch}\tilde{x}\left(1+\frac{\partial^2}{\partial\tilde{x}^2}\right)-2\operatorname{sh}\tilde{x}\frac{\partial}{\partial\tilde{x}}\right]K_0(\tilde{\rho}), \quad (39)$$

where $\tilde{\rho}^2=\tilde{x}^2+\tilde{y}^2$.

At minimum distances $\tilde{\rho}\ll 1$ we have

$$I\approx 2\pi-4[\tilde{y}\ln\rho+\tilde{x}\operatorname{arctg}(y/x)],$$
$$E_\perp\approx\frac{v\varkappa^2}{4}\frac{\tilde{x}^2}{\tilde{\rho}^2}, \quad F_\perp\approx\frac{v\varkappa^2}{8}\frac{\tilde{x}^2-\tilde{y}^2}{\tilde{\rho}^4}, \quad (40)$$
$$V\approx\frac{v\varkappa}{8}\frac{\tilde{y}}{\tilde{\rho}^2}+\frac{\pi}{4}v\varkappa.$$

The formulae (40) show that the attraction to the dislocation cylinder takes place on the outside in the sector $|x|<-y$. The potential energy is negative on the outside, and the electric field is always directed outside.

In Eq. (40) $F_\perp$ and the first term in the expression for V evidently correspond, as they ought to at $r<r_D$, to the free phase for a standard vortex filament. The quantity $E_\perp$ and the second term in the expression for V are the corrections due to the Coulomb interaction. Note that the region $\varkappa r\ll 1$ is attainable only if the minimum longitudinal width l of the dislocation filament is smaller than the Coulomb length d. For arbitrary $\alpha<1$ this means that

$$l^2\ll d^2, \quad l^2\sim s/\alpha, \quad d^2\sim\alpha/\varkappa^2,$$

hence

$$\gamma^2=e^2/\hbar v\varepsilon_\infty<\alpha^2. \quad (41)$$

Thus, the singularity range and, accordingly, strong attraction of the solitons to the dislocation line are attainable for the systems with a sufficiently weak Coulomb interaction and a relatively strong interchain coupling.

At large distances $\varkappa R_0\gg\rho\gg 1$ the functions E and F decrease rapidly in the horizontal sector:

$$E_\perp\sim F_\perp\propto e^{-\rho}, \quad \varkappa R_0\gg|\tilde{y}|>\tilde{x}\gg 1.$$

In the vertical sector we have a mixed law

$$E_\perp\approx F_\perp\approx\frac{v}{2}\varkappa^2\left(\frac{\pi}{2|x|}\right)^{1/2}\exp\left(-\frac{\tilde{y}^2}{2\tilde{x}}\right), \quad (42)$$
$$\varkappa R_0\gg|\tilde{x}|>|\tilde{y}|\gg 1,$$

which is a two-dimensional analog of the three-dimensional soliton solutions.[2] We see that in the region (42) the Coulomb interactions dominate, the forces are directed outward and from the line $\mathscr{D}$, and the energy is positive.

Let us recall that the transition from the special case $\alpha=1$ to the general one $\alpha<1$ is carried out with the help of the scale transformation (31).

5. WEAK SCREENING

The effect of screening by residual carriers (electrons or solitons) on the inner structure of a dislocation becomes important when the screening length λ^{-1} is smaller than the loop size ($\lambda^{-1}\ll R_0$). According to Ref. 2, we can allow for screening by the substitution $\Delta\to\Delta-\lambda^2$ in Eqs. (12), (13), and (15) at invariant $\hat{\Delta}$ and $\Delta_\perp$. As a result, at large distances we must use single-soliton solutions of the form obtained in Ref. 2:

$$\varphi_s(\mathbf{r})=\frac{s}{4\alpha^*}\frac{\partial}{\partial x}\frac{1}{(x^2+r_\perp^2/\alpha^*)^{1/2}},$$
$$\Phi_s(\mathbf{r})=\frac{v}{2}\frac{\alpha}{\alpha^*}\frac{\partial}{\partial x}\varphi_s, \quad (43)$$

where $\alpha^*=\alpha\lambda^2/\varkappa^2\ll\alpha$.

Thus, the phase distribution is determined by the effective problem for a dislocation without the Coulomb field, but with an enhanced anisotropy α^*. From (21) we find the evident result

$$\varphi^*(\mathbf{r}^*)=\Omega/2, \quad \mathbf{r}^*(x,\mathbf{r}_\perp/(\alpha^*)^{1/2}),$$
$$\lambda|\mathbf{r}_\perp|\gg 1, \quad |r^*|\gg d/\alpha^*,$$

where Ω is the solid angle in reduced coordinates r^*, at which the dislocation loop $\mathscr{D}$ is seen from the observation point. As seen from Eq. (43), the main contribution to the interaction V, in terms of the parameter $\varkappa^2/\lambda^2\gg 1$, is given by the electron potential Φ. This potential has a quadrupole character, i.e., there are sectors of negative $[x<r_\perp/(\alpha^*)^{1/2}]$ and positive $[x>r/(\alpha^*)^{1/2}]$ energy. Thus, we find the fields $2N\varphi_s$, $2N\Phi_s$, and $2NV_s$ far from the loop $|r|\gg R_0$.

The fields near the line $\mathscr{D}$ can be found in the simplest way by solving directly Eq. (11). After the substitution $\Delta\to\Delta-\lambda^2$ Eq. (11) acquires the form of the equation for a dipole filament:

$$\left(\frac{\partial^2}{\partial x^2}+\alpha^*\frac{\partial^2}{\partial y^2}\right)\Phi=-\pi\alpha v\frac{\partial}{\partial y}\delta(x)\delta(y), \quad y=R_0-|r_\perp|. \quad (44)$$

Eqs. (44) and (13) yield

$$V \approx \Phi \approx \frac{v}{2}\frac{\varkappa^2}{\lambda^2}\frac{\partial\varphi}{\partial x} = \frac{v\alpha}{2(\alpha^*)^{1/2}}\frac{\varkappa}{\lambda}\frac{y}{y^2+x^2\alpha^*}. \quad (45)$$

At the boundary of the validity range, $\lambda |r^*| \sim 1$, the interaction reaches the following value in the dislocation plane:

$$V_{max} \approx \alpha^{1/2} v\varkappa.$$

This result is of the type given by Eq. (40), but with a drastically narrowed vertical sector, $|x| > |y|/(\alpha^*)^{1/2}$. In the remaining region the solitons are attracted to the loop $\mathscr{D}$ on the outside.

6. ENERGY

The energy of a plane ring loop is calculated with the help of Eq. (26), using the results of the exact solution (34) and (35) with the scale transformation (31). As follows from Eqs. (36) and (40), the quantity V is constant everywhere inside the plane of the loop, except for a narrow ring $\tilde{y} \ll 1$, $y = R_0 - r_\perp$. Substituting the obtained solutions into Eq. (26), we find

$$H = {}^1/_2 \pi \alpha^{1/2} v\varkappa N + C \ln N, \quad N = \pi R_0^2/s. \quad (46)$$

The last term in this formula corresponds to the self-energy of the dislocation line. The coefficient $C \sim 1$ should be replaced by $C \sim \ln(\alpha/\gamma)$, if the condition (41) holds.

If the size of the loop is larger than the screening length, then V decreases according to Eq. (45) on moving away from $\mathscr{D}$. The main contribution is again made by the Coulomb field, which is distributed on $\mathscr{F}$ similar to the phase gradient [see (45)]. To logarithmic accuracy, the resulting energy differs from the standard vortex energy by a large factor of order $\varkappa/\lambda$:

$$H = \frac{\pi v}{s(\alpha^*)^{1/2}} R_0 \ln(R_0\lambda) \propto \frac{\varkappa}{\lambda} E_s N^{1/2} \ln N. \quad (47)$$

The soliton aggregation into a dislocation loop is advantageous, from the point of view of energy, if

$$\mu = \partial H/\partial N < E_s \propto v(\alpha/s)^{1/2}. \quad (48)$$

We see that for loops of limited radius $\lambda R_0 < 1$ we have

$$\mu/E_s \propto \gamma,$$

i.e., for large N the aggregation is always advantageous irrespective of the anisotropy parameter α. Let us recall that under the additional condition (41) the joining of a soliton occurs without a barrier. If large loops ($\lambda R_0 > 1$) are screened, aggregation at large N is always advantageous.

7. CONCLUSION

We have studied loop dislocations in a CDW crystal arising due to the soliton aggregation. The main results are due to the Coulomb interaction effects. We have found and solved equilibrium equations for the Coulomb potential and the CDW order parameter. Far from the dislocation loop the fields φ and Φ are multiples of the soliton fields: $\varphi \approx 2N\varphi_s$, $\Phi \approx 2N\Phi_s$. In the plane of the loop the fields Φ and φ, apart from exponentially small terms, are constant (36), except for a narrow vicinity of the dislocation line, where the behavior of φ corresponds to a standard vortex filament (40). In this vicinity, taking place under the condition (41), solitons are attracted to the dislocation line on the outside, in the sector $|x| < -y$.

In the presence of residual carriers (electrons, solitons) screening effects become essential, the phase distribution at large distances being similar to that without the Coulomb interaction, but with an enhanced anisotropy (43). Near the dislocation loop the distribution of the fields V, ϕ, and φ is similar to that without screening, but with a sharply narrowed vertical sector of repulsion (45).

We have calculated the energy of a plane ring loop. Contrary to the standard case of a vortex filament, the energy has a term proportional to the area of the dislocation loop, or to the number of solitons (46). We have shown that for systems with a weak Coulomb interaction the soliton aggregation into a dislocation is advantageous irrespective of the anisotropy parameter. If the size of the loop is larger than the screening length, the energy has a standard form (47), and the soliton aggregation is advantageous at least for large N.

[1] Physica **21**, Suppl. 3 (1989) (Proc. of the Third Eur. Conf. on Low Dimensional Conductors and Superconductors, Dubrovnik, 1989).
[2] S. A. Brazovskiĭ and S. I. Matveenko, Zh. Eksp. Teor. Fiz. **99**, 887 (1991) [JETP **72**, 492 (1991)].
[3] P. A. Lee and T. M. Rice, Phys. Rev. B **19**, 3970 (1979).
[4] N. P. Ong, G. Verma, and K. Maki, Phys. Rev. Lett. **52**, 663 (1984).
[5] N. P. Ong and K. Maki, Phys. Rev. B **32**, 6682 (1985).
[6] L. P. Gor'kov, Pisma Zh. Eksp. Teor. Fiz. **38**, 76 (1983) [JETP Lett. **38**, 87 (1983)].
[7] I. Batistic, A. Bjelis, and L. Gor'kov, J. de Phys. **45**, 1659 (1984).
[8] J. Dumas and D. Feinberg, Europhys. Lett. **2**, 555 (1986).
[9] D. Feinberg and J. Friedel, J. de Phys. **49**, 485 (1988).
[10] Synthetic Metals 1991 (Proc. of the Int. Conf. on Science and Technology of Synthetic Metals. Tubingen, 1990).
[11] Modern Problems in *Condensed Matter Science,* Amsterdam, Elsevier Sci. Publ., V. 25, 1989.
[12] S. N. Artyomenko, A. F. Volkov, and A. N. Kruglov, Zh. Eksp. Teor. Fiz. **91**, 1536 (1986) [JETP **64**, 906 (1986)].
[13] S. Brazovskiĭ and N. Kirova, Soviet Scientific Reviews, sec. A: Physics Reviews V. 6, ed. by I. M. Khalatnikov. Chur-London-Paris-N.Y.-Melbourne, Harwood Acad. Publ. 1984, p. 99.
[14] S. Brazovskiĭ, see Ref. 11, p. 425.
[15] S. Brazovskiĭ, N. Kirova, and V. Yakovenko, J. de Phys. **44**, C3-1525 (1983).
[16] B. Horovits and J. A. Krumhansl, Phys. Rev. Lett. **38**, 778 (1977).
[17] V. C. Saint-Lager, P. Monseau, and M. Renard, Europhys. Lett. **9**, 585 (1989).
[18] L. D. Landau and E. M. Lifshitz, *Hydrodynamics* [in Russian], Nauka, Moscow, 1988 [transl. in press].
[19] P. A. Lee and H. Fukuyama, Phys. Rev. B **17**, 542 (1987).
[20] S. A. Brazovskiĭ, Zh. Eksp. Teor. Fiz. **78**, 677 (1980) [JETP **51**, 342 (1980)].
[21] S. Barisic, Low-Dimensional Conductors and Superconductors, Ed. by D. Jerome and L. G. Caron. NATO ASI Ser. B **155**, 395 (1987). Mol. Cryst. Liq. Cryst. **119**, 413 (1985).
[22] I. V. Krive, A. S. Rozhavskiĭ, and I. O. Kulik, Fiz. Nizk. Temp. **12**, 1123 (1986) [Sov. J. Low Temp. Phys. **12**, 635 (1986)].

Translated by E. Khmelnitski

Multiwave resonance in fast-electron diffraction in thin crystals

S. L. Dudarev

Moscow Engineering-Physics Institute
(Submitted 7 September 1990)
Zh. Eksp. Teor. Fiz. **99**, 1551–1564 (May 1991)

The problems of the diffraction and inelastic scattering of nonrelativistic fast electrons in crystals are solved for the case in which the angle (ϑ) between the momentum vector of the particle and a crystallographic axis is many times the Lindhard angle. The solutions are analyzed. At certain values of ϑ, a resonant coupling may arise between states of quasifree motion of the particle and Bloch states from the low-lying narrow band in the energy spectrum of an electron in the $2D$ transverse periodic potential of the crystal. The onset of a resonance of this type in the final state of the inelastic-scattering problem may be responsible for the anomalies which have recently been seen in experiments on the transmission and reflection of electrons from crystalline targets.

INTRODUCTION

In research on the motion of fast electrons in crystals it is generally assumed that the periodic potential has a strong effect on the shape of the trajectory only if the angle between the particle momentum **p** and the atomic plane or axis is less than or equal to the Lindhard angle:

$$\vartheta \lesssim \vartheta_L = (\overline{U}/\varepsilon_p)^{1/2}, \tag{1}$$

where $\overline{U}$ is on the order of the internal crystal potential, and ε_p is the energy of the particle.[1] In a quantum-mechanical formulation of the scattering problem, inequality (1) is the condition of a pronounced restructuring of a plane wave incident on a crystal, accompanied by simultaneous excitation of a large number of Bragg diffraction reflections.[2–6] In particular, when condition (1) holds, the whole set of the coefficients in the expansion of the electron wave function in a perturbation-theory series in Fourier components of the periodic crystal potential, which correspond to a certain plane of the reciprocal-lattice vectors orthogonal to the particle momentum **p** become anomalously large (Ref. 2). From the geometric standpoint, condition (1) is equivalent to the configuration in Fig. 1a, in which the Ewald sphere[7] $\mathbf{p}^2 = 2m\varepsilon_p$ is tangent to this plane of reciprocal-lattice vectors.

However, it is not difficult to show that the relative positions of the Ewald sphere and the three-dimensional system of reciprocal-lattice sites in Fig. 1a do not account for all the cases which might correspond to a pronounced dynamic restructuring of the wave function of the particles incident on the crystal. In particular, the configuration in Fig. 1b also corresponds to the case of the simultaneous excitation of many diffraction reflections—a number of reflections comparable in order of magnitude to the number of features in case 1a. We denote by g the distance between successive planes of reciprocal-lattice vectors. It is a straightforward matter to derive the angle ϑ_r, between the momentum vector of the electron and the crystal axis, for the case corresponding to Fig. 1b:

$$\vartheta_r = 2 \arcsin [(g/2p)^{1/2}]. \tag{2}$$

The probability for the excitation of Bragg reflections in case 1b can be estimated in the following way. The angle (2) through which the electron is deflected in the course of the scattering corresponds to a momentum transfer on the order of $\Delta p \sim (2pg)^{1/2}$. Since the matrix element of the periodic crystal potential corresponding to a diffractive reflection by a certain reciprocal-lattice vector **G** contains a Debye-Waller factor[2] $\exp(-1/2\langle(\mathbf{Gu})^2\rangle)$, all processes with a momentum transfer $\Delta p \gtrsim (\langle u^2\rangle)^{-1/2}$ are suppressed (here and below, we are using a system of units with $\hbar = 1$). Comparison of the latter inequality with (2) leads to an upper limit on the energy of the electrons:

$$\varepsilon_p \lesssim 1/mg^2(\langle u^2\rangle)^2. \tag{3}$$

Under ordinary conditions the right side of (3) would be some tens of kiloelectron volts, suggesting that a special motion of the fast electrons in the crystal might arise at nonrelativistic energies in the scattering geometry in Fig. 1b.

As we will see below, for a motion of this type a multiwave resonant coupling typically arises between (on the one hand) free semiclassical states of the particle which correspond to relatively large angles between **p** and the lat-

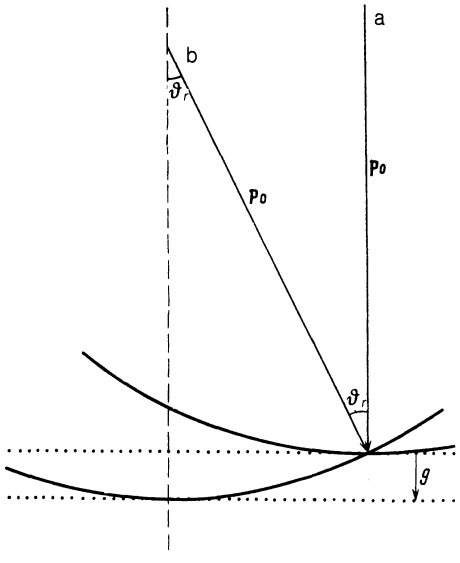

FIG. 1. Relative positions of the Ewald sphere and the system of reciprocal-lattice sites of the crystal. a—The electrons are incident approximately normally on the crystal surface, and inequality (1) holds; b—a multiwave resonance arises in the solution of the diffraction problem.

 0038-5646/91/050866-08$03.00

tice axes and (on the other) "bound" Bloch states corresponding to narrow bands of transverse motion in the $2D$ periodic potential of the crystal. In particular, under the conditions of this multiwave resonance there may be a complete "capture" of a nonrelativistic electron from a plane wave into a bound state of transverse motion, localized near atomic axes of the crystal (by way of comparison, the probability for the filling of bound states in the case in which electrons are incident normally on a target is no greater than $\sim 50\%$; Ref. 8).

Special motivation for analyzing multiwave resonant scattering comes from some anomalies recently seen experimentally in the angular distributions of electrons scattered inelastically through relatively large angles with respect to the lattice axes of a crystal.[9-13] Some nearly regular intensity rings were observed in Refs. 9–13 in addition to the customary angular distribution of the scattered particles (a pattern of intersecting lines and bands[3,4]). These rings appeared both in experiments on the passage of fast electrons through thin crystals[11] and in experiments on reflection[9,12] and backscattering[13] from bulk samples. The expression derived below for the differential cross section for inelastic collisions of fast electrons in a thin crystal makes it possible to work from ideas concerning a multiwave resonance to explain the experimental results of Refs. 9–13. In several cases, it becomes possible to find a good quantitative agreement between the theoretical intensity profiles and the observed angular distributions of inelastically scattered particles.

1. WAVE FUNCTION IN THE ELASTIC-SCATTERING PROBLEM

The motion of a fast electron in matter can be represented as a diagram sequence of events of elastic scattering by a periodic crystal potential averaged over thermodynamic equilibrium,

$$U_0(\mathbf{r})=\frac{1}{\mathscr{Z}}\sum_n e^{-E_n/T}\langle n|U(\mathbf{r})|n\rangle, \tag{4}$$

and of inelastic collisions in exciting internal degrees of freedom of the target.[2] The summation in (4) is over the eigenstates of the electron and phonon subsystems of the crystal, $|n\rangle$, with energies E_n; T is the absolute temperature; and $\mathscr{Z}=\Sigma_n \exp(-E_n/T)$. In accordance with the usual experimental situation,[10,11] we restrict the analysis below to the case in which electrons pass through a relatively thin crystal, whose dimension (L) along the direction of motion of the particles does not exceed the mean free path (l) of the electrons with respect to inelastic interactions (at $\varepsilon_p \sim 10^5$ eV, for example, the mean free path of the electrons with respect to the excitation of the phonon subsystem of the crystal is[14] 10^3 Å).

The wave function of the problem of elastic scattering in a thin crystal is the solution of the equation

$$-\frac{1}{2m}\frac{\partial^2}{\partial \mathbf{r}^2}\Psi+U_0(\mathbf{r})\Psi=\varepsilon_p\Psi \tag{5}$$

with a boundary condition for the incident wave,

$$\psi_{inc}(\mathbf{r})=e^{i\mathbf{pr}}. \tag{5a}$$

We assume that the crystal occupies the spatial region $0<z<L$ and that the vector $\mathbf{p}$ makes a small angle ϑ with the z axis. Under condition (1) for fast particles, with

$$pg/m \gg |\overline{U}|, \tag{6}$$

in solving Eq. (5) we can restrict the Fourier expansion of potential (4) to reciprocal-lattice vectors $\{\mathbf{G}_h\}$ which lie in the xy plane.[2] We seek the wave function of the fast electron in (5), (5a) as a superposition of transmitted and diffracted waves with slowly varying amplitudes:

$$\Psi(\mathbf{r})=\sum_h \varphi_h(z)\exp[i(\mathbf{p}+\mathbf{G}_h)\mathbf{r}]. \tag{7}$$

Substituting (7) into (5), we find a system of coupled differential equations for the amplitudes $\varphi_h(z)$:

$$v\cos\vartheta\frac{\partial}{\partial z}\varphi_h+i(\varepsilon_h-\varepsilon_0)\varphi_h+i\sum_s \Lambda_{hs}\varphi_s=0, \tag{8}$$

where v is the velocity of the electron, $\varepsilon_h=(\mathbf{p}+\mathbf{G}_h)^2/2m$, and the quantities Λ_{hs} are the Fourier components of the periodic crystal potential,

$$\Lambda_{hs}=\Lambda(\mathbf{G}_h-\mathbf{G}_s)=\frac{1}{\Omega_0}\int_{\Omega_0} d^3r U_0(\mathbf{r})\exp[-i(\mathbf{G}_h-\mathbf{G}_s)\mathbf{r}], \tag{9}$$

where Ω_0 is the volume of the unit cell.

The condition $\varepsilon_p \gg |\overline{U}|$ allows us to ignore the reflected waves in formulating the boundary conditions on (8), so we can write[15]

$$\varphi_h(0)=\delta_{h0}. \tag{10}$$

We can solve Eqs. (9) by transforming the set of functions $\{\varphi_h(z)\}$ to the new representation

$$\varphi_j(z)=\sum_h (C^+(\mathbf{q}))_{jh}\varphi_h(z), \tag{11}$$

where the unitary matrix $C_{hj}(\mathbf{q})$ is fixed by the condition

$$\sum_{s,h}(C^+(\mathbf{p}))_{js}\left\{\frac{(\mathbf{q}+\mathbf{G}_h)^2}{2m}\delta_{sh}+\Lambda_{sh}\right\}C_{hj'}(\mathbf{p})=E_j\delta_{jj'}=E_j(\mathbf{q})\delta_{jj'}. \tag{12}$$

A direct comparison of (11) and (12) with Eqs. (3.8) and (3.9) of Ref. 2 easily reveals that the matrix $C_{hj}(\mathbf{q})$, which depends on only the projection $\mathbf{q}$ of the momentum $\mathbf{p}$ onto the xy plane, determines a basis of Bloch functions of the transverse motion in the $2D$ potential $U_0(x,y)$:

$$b_j(\mathbf{q},\boldsymbol{\rho})=\sum_h C_{hj}(\mathbf{q})\exp[i(\mathbf{q}+\mathbf{G}_h)\boldsymbol{\rho}], \tag{13}$$

where $\boldsymbol{\rho}$ is a $2D$ vector with the components x, y. In representation (11) and (12), the solution (10) becomes

$$\varphi_j(z)=C_{0j}^*(\mathbf{q})\exp\left[\frac{iz}{v\cos\vartheta}\left(\frac{\mathbf{q}^2}{2m}-E_j\right)\right]. \tag{14}$$

The value of $\varphi_j(z)$ at $z=0$ is the same as the known result from the sudden-perturbation theory:[1,2]

$$\varphi_j(0)=C_{0j}^*(\mathbf{q})=\frac{1}{S_0}\int_{S_0} d^2\rho\, b_j^*(\mathbf{q},\boldsymbol{\rho})e^{i\mathbf{q}\boldsymbol{\rho}}, \tag{15}$$

where S_0 is the area of the $2D$ unit cell of the crystal in the xy plane.