Interaction of quasiparticles with coherent crystal boundaries

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The multichannel scattering of quasiparticles by the coherent surface of an ideal crystal is studied. A simple expression is derived for the scattering matrix. This expression reflects the basic features of multichannel reflection from a surface. Analytic anomalies (resonant and threshold in nature) of the scattering matrix are discussed. The conditions for the quantization of the quasiparticle spectrum in parallel-plane crystalline plates and the transmission of quasiparticles across twinning boundaries are examined.

1. INTRODUCTION

Major progress has now been achieved in producing pure, ideal crystals with a long mean free path for quasiparticles. This circumstance and also the considerable interest in the properties of two-dimensional and quasi-two-dimensional systems make it necessary to carry out a systematic study of the interaction of quasiparticles with crystal surfaces.

The interaction of quasiparticles with crystal surfaces is described phenomenologically by a scattering matrix which characterizes how nonspecular the scattering is. This approach makes no distinction between the processes which are caused by surface irregularities (surface defects) and the nonspecular scattering processes which result from the complex nature of the interaction of quasiparticles with an ideal surface.

If we wish to take a systematic approach, we must preface a study of the effect of the various irregularities with a solution of the problem of the scattering of quasiparticles by the ideal surface of a crystal. The interactions of quasiparticles with crystal surfaces have been under study for a fairly long time now (see, for example, Refs. 1–13 and the literature cited there). The scattering of a quasiparticle with a given quasimomentum projection onto the ideal surface is a multichannel process, accompanied by excursions in terms of the surface quasimomentum and differing substantially from specular reflection. The number of channels (when surface states are taken into consideration) depends on the energy spectrum in the interior of the crystal and on the surface structure.

Descriptions of the interactions of quasiparticles with surfaces usually involve the construction and use of a semiclassical boundary condition in some form or other.[9,10] This approach is convenient for crystals with a quadratic quasiparticle dispersion law and also for approximations of the nearly-free-electron type. In several problems, however, it is better to base the description on a purely lattice Hamiltonian, characterized by discrete variables. For phonons, magnons, and bound electrons, for example, it is useful to formulate the boundary condition in terms of the parameters of a lattice Hamiltonian (tunneling frequencies, strength constants, exchange integrals, and so forth), which have values near the surface that differ from the corresponding values in the interior of the crystal.

In general, the boundary condition depends on the properties of the surface and the nature of the quasiparticles. There is accordingly no universal method for describing the interactions of quasiparticles with crystal surfaces. It is nevertheless interesting to attempt to distinguish the general properties of multichannel scattering from the features of specific boundary conditions. This is our purpose in the present paper.

In Sec. 2 we propose a simple expression, (10), for the multichannel scattering matrix, derived on the basis of a lattice Hamiltonian without consideration of the distortion of the parameters of this Hamiltonian near the surface. This expression contains all the features of the multichannel scattering for which the different regions of the energy spectrum of the quasiparticles are formally equivalent. The method proposed here makes it possible in several cases to relate the scattering matrix to the parameters of the Hamiltonian, provided that the latter are distorted only in a narrow surface layer.

When surface distortions are taken into account, the corresponding formal expression casts light on certain general threshold and resonant properties of the scattering matrix describing the scattering of quasiparticles by an ideal surface. These properties are analogous to the anomalies in bulk scattering by impurities near the threshold for a reaction or near a topological transition for constant-energy surfaces.

In the following sections of the paper we examine the quantization conditions for plates and the interaction of quasiparticles with a twinning surface.

2. MULTICHANNEL SCATTERING MATRIX

We consider a triclinic lattice with translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. We number the lattice sites by the vector $\mathbf{n}$, with integer components ($\mathbf{r} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$). The motion of a single-band quasiparticle is described by the tunneling Hamiltonian

$$\hat{H} c_{\mathbf{n}} = \sum_{\mathbf{n}'} t_{\mathbf{n}'} c_{\mathbf{n}+\mathbf{n}'}, \qquad t_{\mathbf{n}} = t_{-\mathbf{n}}. \tag{1}$$

For simplicity we assume that the tunneling frequencies $t_{\mathbf{n}}$ are real; the generalization to the case of complex $t_{\mathbf{n}}$ is obvious. The corresponding energy spectrum in the interior of the crystal is

$$\varepsilon(\mathbf{p}) = \sum_{\mathbf{n}} t_{\mathbf{n}} e^{i\mathbf{n}\mathbf{p}}, \tag{2}$$

where the vector $\mathbf{p}$ is determined by the projections onto the

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vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. In real crystals, information on the Fourier expansion of energy spectrum (2) makes it possible to automatically reconstruct the Hamiltonian (1).

We assume that the surface of the crystal is defined by the equation $\mathbf{N}\nu\mathbf{n} = 0$, where N_1, N_2, and N_3 are the indices of the surface. To begin the study, we adopt as a boundary condition the condition that the amplitudes $c_\mathbf{n}$ vanish outside the crystal, where we have $\mathbf{N}\nu\mathbf{n} < 0$, and we assume that the parameters $t_\mathbf{n}$ of Hamiltonian (1) are not distorted anywhere up to the surface. We replace n_1 by the new integer coordinate $k = n_1 - (n_2N_2 + n_3N_3)$. We assume $N_1 = 1$, eliminating from consideration the possibility of a surface reconstruction. Inside the crystal we have $-\infty < n_2, n_3 < +\infty, k \geqslant 0$. We take Fourier transforms along the coordinates n_2 and n_3:

$$D_k(\mathbf{q}) = \sum_{n_2,n_3=-\infty}^{+\infty} \exp(iq_2n_2 + iq_3n_3)\, c_{k+N_2n_2+N_3n_3,n_2,n_3}. \tag{3}$$

This step is equivalent to introducing a conserved two-dimensional quasimomentum q ($|q_{2,3}| \leqslant \pi$), which is directed parallel to the surface. The Schrödinger equation for the Hamiltonian (1) is

$$\varepsilon D_k(\mathbf{q}) = \sum_{\mathbf{n}} t_\mathbf{n} e^{-i\mathbf{q}\mathbf{n}} D_{k+\mathbf{N}\mathbf{n}}. \tag{4}$$

It describes a one-dimensional motion of a quasiparticle with a surface quasimomentum $\mathbf{q}$ and an energy ε. Since the integral of motion for a semi-infinite crystal is the vector $\mathbf{q}$, not $\mathbf{p}$, we should express the two components of the vector $\mathbf{p}$ in the spectrum (2) in terms of q: $p = p_1, q_2 = p_2 - p_1N_2$, $q_3 = p_3 - p_1N_3$.

The spectrum (2) is conveniently represented in the form

$$\varepsilon(\mathbf{q}, p) = \sum_{\mathbf{n}} t_\mathbf{n} \exp\{i(\mathbf{q} + p\mathbf{N})\mathbf{n}\} \equiv \sum_{l=-\mathscr{N}}^{\mathscr{N}} t_l(\mathbf{q}) e^{ilp}, \qquad t_l = t_{-l}^{*}. \tag{5}$$

This expression is a definition of $t_l(\mathbf{q})$. Here we have $\mathscr{N} = \mathbf{N}\cdot\mathbf{M}$, and the vector $\mathbf{M}$ characterizes all the coordination spheres which are taken into consideration in (1), (2), and (4): $|n_i| \leqslant M_i$. In terms of the notation in (5), Eq. (4) becomes

$$\varepsilon D_k = \sum_{l=-\mathscr{N}}^{\mathscr{N}} t_l(\mathbf{q}) D_{k+l}. \tag{4'}$$

Inside the crystal, at fixed ε and $\mathbf{q}$, the permissible values of p are determined by the dispersion relation

$$\varepsilon = \varepsilon(\mathbf{q}, p), \tag{6}$$

which is a polynomial of degree $2\mathscr{N}$ in $x = e^{-ip}$. Correspondingly, (6) has $2\mathscr{N}$ roots $p_j = p_j(\varepsilon, \mathbf{q})$; the p_j are either real or pairs of complex conjugates. The real p_j correspond to quasiparticles which are moving in the interior of the crystal, while the complex p_j correspond either to surface waves ($\operatorname{Im} p_j < 0$) or solutions which grow exponentially with distance into the interior of the crystal ($\operatorname{Im} p_j > 0$). All the $2\mathscr{N}$ solutions p_j can be classified as $\mathscr{N}$ waves p_j^{+} which are arriving at the surface and $\mathscr{N}$ outgoing waves p_j^{-}. For real p_j, the classification in terms of p_j^{+} and p_j^{-} is carried out on the basis of the sign of $v_j = \partial\varepsilon(\mathbf{q}, p)/\partial p|_{p=p_j}$, while for complex p_j we have $\operatorname{Im} p_j^{+} > 0$.

A general solution of Eq. (4) is the sum of waves and

$$D_k = \sum_{j=1}^{\mathscr{N}} A_j^{+} e^{-ikp_j^{+}} + \sum_{j=1}^{\mathscr{N}} A_j^{-} e^{-ikp_j^{-}}, \tag{7}$$

the multichannel scattering matrix S, which relates the amplitudes of the reflected waves (A_j^{-}) with those of the incident waves (A_j^{+}),

$$\mathbf{A}^{-} = \hat{S}\mathbf{A}^{+} \tag{8}$$

($\mathbf{A}^{\pm} = \{A_1^{\pm}, \ldots, A_{\mathscr{N}}^{\pm}\}$), is determined from the boundary condition $D_k = 0$ for $k < 0$. Equating (7) to zero at the nonequivalent points $k = -1, -2, \ldots, -\mathscr{N}$, we find

$$\hat{X}_{-}\mathbf{A}^{-} = -\hat{X}_{+}\mathbf{A}^{+}, \qquad (X_{\pm})_{ik} = (x_i^{\pm})^{-k}. \tag{9}$$

If follows from (9) that the scattering matrix (8), $\hat{S} = -\hat{X}_{-}^{-1}\hat{X}_{+}$, consists of elements $S_{ik} = -D_{ik}/D$, where $D = \det \hat{X}_{-}$, D_{ik} is the determinant of the same matrix, except that the powers x_k^{+} replace x_i^{-} in column i; and D and D_{ik} are Vandermond determinants, which converge to the product of all possible differences $x_l - x_m$. Terms which do not contain x_i^{-} and x_k^{+}, drop out of the ratio D_{ik}/D, and as a result we find

$$S_{ik}^{(0)} = -\frac{x_i^{-}}{x_k^{+}} \prod_{j\neq i}^{(\mathscr{N}-1)} \frac{1 - x_j^{-}/x_k^{+}}{1 - x_j^{-}/x_i^{-}}. \tag{10}$$

How are the wave-conversion amplitudes related to the reflection coefficients? To answer this question, we need to find an expression for the flux J_k which appears in the continuity equation

$$\frac{\partial}{\partial t}|D_k|^2 + J_{k+1} - J_k = 0.$$

The time derivative is calculated with the help of the Schrödinger equation (4′). We find

$$J_k = -\frac{i}{2} \sum_{l=-\mathscr{N}}^{\mathscr{N}} \operatorname{sign} l \sum_{m=1}^{|l|} [t_l(\mathbf{q}) D_{k-m}^{*} D_{k-m+l} - t_l^{*}(\mathbf{q}) D_{k-m} D_{k-m+l}^{*}].$$

For a wave $D_k = A_{je}{}^{-ikpj}$ the flux

$$J_k = |D_k|^2 v_j \tag{11}$$

is proportional to the quasiparticle velocity $v_j = \partial\varepsilon(q, p_j)/\partial p_j$.

Inside the crystal, for a wave with real p_j, we have $J_k = |A_j|^2 v_j$, while for complex p_j the flux is $J_k = |A_j|^2 v_j \exp\{2k \operatorname{Im} p_j\}$. For internal waves the ratio of the particle flux in the reflected wave to the flux in the incident wave is

$$P_{ik}^{(0)} = \frac{v_i^{-}}{v_k^{+}} |S_{ik}^{(0)}|^2$$

$$= -\left|\frac{x_i^{-}}{x_k^{+}}\right|^2 \prod_{l\neq k} \frac{1 - x_i^{-}/x_l^{+}}{1 - x_k^{+}/x_l^{+}} \prod_{l\neq i} \frac{1 - x_l^{-*}/x_k^{+*}}{1 - x_l^{-*}/x_i^{-*}}. \tag{12}$$

The products in (12) formally contain all the roots $x_j^{\pm}$ of the dispersion relation (6). For complex p_l, however, by virtue of the relation $x_l^{\pm *} = 1/x_l^{\pm}$ (for real p_l, we have $x_l^{\pm *} = 1/x_l^{\pm}$), the corresponding terms in the products (12) cancel each other out, so that the only factors which actually figure in (12) are those which correspond to purely internal waves.

The probabilities for transitions between channels, $R_{ik} = |S_{ik}|^2$, enter the boundary condition on the kinetic equation (Ref. 12, for example). In contrast with (12), we should incorporate in R_{ik} all channels, including those which correspond to complex p_j. It can be seen from (10) that surface waves with large $|\mathrm{Im}\, p_j|$ make an exponentially small contribution. The convergence of the products (10) and (12) with increasing $\mathcal{N}$ is equivalent to the convergence of the Fourier series for the spectrum (2). If we ignore the distortions of the crystal in the surface layer, we find that the multichannel scattering matrix is expressed exclusively in terms of the roots of the dispersion relation (6) in the interior of the crystal.

For surface scattering, we can distinguish between two sources of multichannel behavior. The first is associated with the fact that the symmetry of the surface is lower than that of the interior of the crystal. The second is the complex nature of the interior energy spectrum, (2), for which even for the surface of highest symmetry (100), the dispersion relation (6) has many roots. The number of these roots is determined by the number of coordination spheres considered in the Fourier expansion (2). It can be shown that incorporating one more coordination sphere in (2) introduces additional real roots p_j only if the corresponding coefficient t_n is not small. If, on the other hand, all the t_n beyond a certain point decrease rapidly, the incorporation of more remote coordination spheres simply adds complex p_j with a large imaginary part. Such components make an exponentially small contribution to (10), and they drop out entirely from the product (12). The existing real p_j shift negligibly in the process.

A solution which has been found can formally be generalized to incorporate distortions of the Hamiltonian near the surface. If the distortions span the first $k_0 - \mathcal{N}$ layers, the effective boundary condition can be written in the form

$$D_{k_0-\mathcal{N}+k} = \sum_{l=0}^{\mathcal{N}-1} T_{kl}^{(k_0)} D_{k_0+l}, \qquad k=0,1,\ldots,\mathcal{N}-1. \tag{13}$$

The matrix $\hat{T}$ is expressed in terms of the constants of the Hamiltonian in the obvious way, with the help of the first k_0 lattice equations. It is an analytic function of **q** and ε. Substituting (7) into (13), we find the expression

$$S_{ik} = -\left(\frac{x_k^+}{x_i^-}\right)^{k_0} \frac{\det \hat{B}_{ik}}{\det \hat{B}}, \tag{14}$$

where

$$B_{mj} = (x_j^-)^{-m} - \sum_{l=0}^{\mathcal{N}-1} T_{\mathcal{N}-m,l}\,(x_j^-)^l, \qquad m,j=1,2,\ldots,\mathcal{N}, \tag{15}$$

and the matrix B_{ik} is found from B in (15) by replacing x_i^- by x_k^+ in column i. Certain analytic properties of S_{ik} in (14) can be seen for an arbitrary matrix $\hat{T}$. The determinants in (14) vanish whenever two roots of the dispersion relation coalesce, since the two corresponding columns are identical in such a case. We thus have

$$S_{ik} = S_{ik}^{(0)}\,(x_k^+/x_i^-)^{k_0} f_{ik}(q,\varepsilon), \tag{16}$$

where $S_{ik}^{(0)}$ is given by (10), and f_{ik} is the ratio of two polynomials of degree $\mathcal{N}$ in x_j^-, which are symmetric with respect to all x_j^-. The numerator differs from the denominator only in that x_i^- is replaced by x_k^+. Correspondingly, we have

$$P_{ik} = P_{ik}^{(0)}\,|f_{ik}|^2, \tag{17}$$

where $P_{ik}^{(0)}$ is given by (12).

Expressions (16) and (17) can be used to follow the threshold and resonant features of multichannel scattering. At fixed values of the energy ε and quasimomentum **q** of a quasiparticle, the dispersion relation (6) has $2\mathcal{N}$ solutions, of which $2L$, $L \leqslant \mathcal{N}$, are real and correspond to waves propagating in the interior of the crystal. As **q** or ε changes, the number L changes and can take on all values from 0 to $\mathcal{N}$. In terms of quantum scattering theory,[14] complex p_j correspond to virtual levels, and a unit change in L corresponds to the appearance or disappearance of one more reaction channel. The number of real roots is determined by the number of crossings of a constant-energy surface $\varepsilon(p_1,p_2,p_3) = \varepsilon$ by lines $p_2 = q_2 + N_2 p_1$, $p_3 = q_3 + N_3 p_1$ (when jumps in **q** in the first zone are taken into account, these equations determine not one line but an entire family of parallel straight lines). The number of real roots, L, may change either without a change in the topology of the constant-energy surface or as a result of a topological transition. In the former case, the secant is nearly tangent to the constant-energy surface, and a slight change can eliminate two crossing points. Near a topological transition,[15] on the other hand, slight changes in ε result in the appearance or disappearance of isolated regions of the constant-energy surface, with the result that the number of real p_j may also change. In such cases, the scattering matrix has some specific anomalies near the threshold. Let us assume that $\varepsilon = \varepsilon_\alpha$ corresponds to a threshold $x_\alpha^+ = x_\alpha^-$, i.e., $v_\alpha = 0$. Near the threshold we have $\varepsilon - \varepsilon_\alpha = (p - p_\alpha)^2/2m_\alpha$, and S_{ik} and P_{ik} are expanded in powers of $p - p_\alpha = [2m_\alpha(\varepsilon - \varepsilon_\alpha)]^{1/2}$. Far from the threshold, they are expanded in powers of ε (Ref. 12). Furthermore, at the threshold the ratio $P_{ik}^{(0)}$ given by (12) has a discontinuity in its derivative with respect to $(\varepsilon - \varepsilon_\alpha)^{1/2}$ (below the threshold, $P_{ik}^{(0)}$ is completely independent of complex P_l). This discontinuity must persist in P_{ik} in (17), since there is no basis for its cancellation by virtue of f_{ik} for any matrix $\hat{T}$.

The resonant properties of S_{ik} and P_{ik} become obvious if we rewrite the factors in (10) in the form

$$\frac{1 - x_j^-/x_k^+}{1 - x_j^-/x_i^-} = \frac{x_i^-}{x_k^+}\left(1 - \frac{x_i^- - x_k^+}{x_i^- - x_j^-}\right). \tag{18}$$

Since the partial amplitudes f_{ik} are continuous at the points $x_i^- = x_j^-$ and $x_i = x_k^+$, S_{ik} has some structural features near these points which are described by (18). In the specular channel, we have $f_{ik} \to 1$ as $x_i^- \to x_k^+$, since we have $\hat{B}_{ik} \to \hat{B}$ in (14) in this case. The corresponding expressions for S_{ik} and P_{ik} are analogs of the Breit-Wigner formulas for multichannel scattering by a coherent surface.

The lattice model discussed above contains the basic properties of multichannel surface scattering, but it does not fully incorporate the specific features of the particular quasiparticles. We now discuss the range of applicability of (10) and (12) without the factors f_{ik} in (16) for the various quasiparticles.

For electrons in metals, distortions of the spectra near the surface can be ignored if the characteristic value of the pseudopotential V is small in comparison with the Fermi energy ε_F (Ref. 16). The boundary condition $D_k = 0$ can be used outside the crystal if the work function satisfies $U \gg \varepsilon_F$. If the various bands are far apart, interband transitions are of minor importance. For narrow-band electrons, the surface distortions turn out not to be small in comparison with the width of the band, and a quasiparticle may reflect in layers far from the surface. For metals, f_{ik} in (16) differs from unity by quantities of order $\varepsilon_F / U \ll 1$ and $V/\varepsilon_F \ll 1$. Incorporating the complex roots with large imaginary parts $|\operatorname{Im} p_j| \gtrsim U/\varepsilon_F, \varepsilon_F/V$ in products (10) and (12) is thus attempting to go beyond the accuracy of the treatment.

For phonons, there are two circumstances to be taken into consideration. First, the lattice Hamiltonian of phonons is written not for the scalar quantity $c_{\mathbf{n}}$ in (1) but for the displacement vector $\mathbf{u}_{\mathbf{n}}$. In general, therefore, we would be dealing with a three-band situation, and surface scattering would be accompanied by interband transitions. Purely single-band transitions refer to the case in which the polarization vector is parallel to the surface and perpendicualr to $\mathbf{q}$.

Second, for a free crystal the uniform shift of the crystal as a whole, $\mathbf{u}_{\mathbf{n}} \to \mathbf{u}_{\mathbf{n}} + \delta\mathbf{u}$, does not alter the state of the phonon system. In Eqs. (4′) we accordingly have

$$\varepsilon = -\omega^2 + \sum_{l=-\mathscr{N}}^{\mathscr{N}} t_l(0). \tag{19}$$

The boundary condition which we have used, $D_k = 0$ at $k < 0$, corresponds to a reflection of phonons from a crystal boundary which is rigidly fixed. The absence of distortions of the strength constants in the surface layer with a fixed crystal boundary is equivalent in practice to the nearest-neighbor approximation. Interband transitions are also inconsequential.

For a crystal with a free surface, Eqs. (4′) with $0 \leqslant k < \mathscr{N}$ differ from the equations far from the surface, even if we ignore the distortions of the strength constants. The absence of jumps across the surface for phonons means that in the layer $0 \leqslant k < \mathscr{N}$ the value of ε in (4′) depends on k:

$$\varepsilon_k = -\omega^2 + \sum_{l=-k}^{\mathscr{N}} t_l(0).$$

The first $\mathscr{N}$ equations.

$$\varepsilon_k D_k = \sum_{l=-k}^{\mathscr{N}} t_l(\mathbf{q}) D_{k+l}, \qquad k = 0, 1, \ldots, \mathscr{N}-1, \tag{20}$$

determine the matrix $\hat{T}$ given by (13) when distortions of the strength constants are ignored. In the long-wave limit in this case, an antinode forms at the free end of the crystal, while a node forms at the pinned end.

For delocalized vacancies (vacancyons) in solid ^{4}He, Eqs. (10) and (12) are applicable because of the small value of the change in the density at the liquid-crystal interface (this small value means that the distortion of the characteristics of the spectrum of vacancyons near the surface is slight) and because inelastic processes are strongly suppressed at the boundary at low temperatures. At low temperatures, however, the wavelength of the vacancyons satisfies $\lambda \gg a$ (a is the distance between atoms), and we can expect significant effects of the multichannel nature of the situation at large values $N \sim \lambda a$.

The matrices $\hat{S}^{(0)}$ and $\hat{P}^{(0)}$ can also serve as a basis for constructing a perturbation theory[13] in the inhomogeneity of the surface.

3. QUANTIZATION OF THE SPECTRUM OF PLATES

We consider a crystal plate bounded by surfaces with indices $N = (1, N_2, N_3)$ and consisting of Z layers. We assume $Z/2 > k_0$ [used to generate the scattering matrix (14)]. In principle, the scattering matrices for the scattering at the different surfaces of the plate, $\hat{S}^{(1)}$ and $\hat{S}^{(2)}$, may be different. A wave which is incident with respect to the first surface is a reflected wave for the second. This matching condition, which determines the spectrum of eigenstates of quasiparticles in the plate, takes the form

$$\det\left[\delta_{jm} - \sum_{l=1}^{\mathscr{N}} \left(\frac{x_l^-}{x_j^+}\right)^Z S_{jl}^{(2)*} S_{lm}^{(1)}\right] = 0, \qquad j, m = 1, 2, \ldots, \mathscr{N}. \tag{21}$$

The dispersion relation (21) differs from the one ordinarily used[17] in that it incorporates not only real but also complex states p_j. Because of the factors $(x_l^-/x_j^+)^Z$, the order of the matrix (21) can be reduced significantly, since shallow surface levels make a real contribution. A semiclassical quantization[15] incorporates only adiabatic invariants corresponding to real p_j. Equation (21) also makes it possible to incorporate shallow surface states, by perturbation theory, for example.

The quantization condition[10] $E_n = \varepsilon(\mathbf{q}, p_z = \pi n/Z)$ which is frequently used, incorporates neither complex roots nor surface distortions of the crystal. If distortions near the surface are ignored, we should replace S in (21) by $\hat{S}^{(0)}$ from (10). In this case, (21) incorporates not only internal waves but also surface waves.

The determinant (21) vanishes at $x_i = x_j$. This result means that the energies ε corresponding to extrema of the function $\varepsilon(\mathbf{q}, p)$ are exact eigenvalues for the energy of the quasiparticles in the plate and bound the series. Minima of the spectrum can be identified with ground states for quasiparticles, and maxima with ground states for quasiholes.

The exact (not semiclassical) quantization procedure proposed here is important for experiments with thin films, which exhibit oscillatory effects associated with the discrete nature of the energy spectrum.[18]

4. INTERACTION OF QUASIPARTICLES WITH A TWINNING PLANE

Let us examine the transmission of quasiparticles through a twinning plane with indices (110). The motion along the a_3 axis separates out, and we are not interested in it. For the wave function D_k in (3), we assume that the $k = 0$ plane is a twinning plane. We restrict the analysis to the nearest-neighbor approximation. Above and below the $k = 0$ plane, the spectrum is $\varepsilon_{1,2}(q,p) = 2t_{1,2}\cos p + 2t_{2,1}\cos(q - p)$. The presence of a twinning plane in the crystal gives rise to slight distortions of the parameters of the Hamiltonian near the boundary. We assume that distortions occur only in the first layer. Above the twinning plane, there are one incident wave and one reflected wave, while below the twinning plane there is only a single transmitted wave. These waves are related by the equations

$$(\varepsilon-t_0)D_0=(t_4+t_3e^{iq})D_1+(t_3+t_4e^{-iq})D_{-1},$$

$$\varepsilon D_{\pm 1}=e^{\pm iq/2}(t_1e^{\mp iq/2}+t_2e^{\pm iq/2})D_{\pm 2}$$

$$+e^{\mp iq/2}(t_4e^{\pm iq/2}+t_3e^{\mp iq/2})D_0,$$

where t_0, t_3, and t_4 characterize surface distortions. When a wave of unit amplitude is incident on the boundary, the amplitude of the transmitted wave is

$$T=\left\{1-i\left[\varepsilon\left(1-\frac{A^2}{B^2}\right)+t_0\frac{A^2}{B^2}\right](4A^2-\varepsilon^2)^{-1/2}\right\}^{-1}, \qquad (22)$$

and that of the reflected wave is $R = T - 1$. Here $A^2 = t_1^2 + t_2^2 + 2t_1t_2\cos q$, and $B^2 = t_3^2 + t_4^2 + 2t_3t_4 \cos q$. The transmission coefficient $\mathscr{D} = |T|^2$ is given by

$$\mathscr{D}=\left\{1+\left[\varepsilon\left(1-\frac{A^2}{B^2}\right)+t_0\frac{A^2}{B^2}\right]^2(4A^2-\varepsilon^2)^{-1}\right\}^{-1}, \qquad (23)$$

and the reflection coefficient is $\mathscr{R}\equiv|1-T|^2=1-\mathscr{D}$.

If deformations of the crystal near the twinning boundary are ignored ($t_0 = 0$, $t_1 = t_4$, $t_3 = t_2$, the reflection coefficient vanishes, and the transmission coefficient is unity. In this case, the reflection of quasiparticles from the twinning plane is caused exclusively by distortions of the crystal lattice. Furthermore, we have $\mathscr{R} = 0$ for those values of q for which we have $B^2/A^2 = 1 - t_0/\varepsilon$. In the long-wave limit, $\varepsilon^2 \to 4A^2$, the electron transmission coefficient vanishes, while the reflection coefficient becomes unity, even if the surface distortions are very weak. The existence of a mirror symmetry for a twin leads to a situation[19] which is quite different from the general case of bicrystals.[20–22].

If we do not use the nearest-neighbor approximation, we would always need to introduce some additional tunneling constants in the Hamiltonian in order to incorporate the tunneling of quasiparticles across the twinning boundary. The reason is that for lattice sites near the boundary all the coordination spheres other than the first are quite different from those for sites in the interior of the crystal.

A local level for electrons, determined by the vanishing of the denominator in (23), is $\varepsilon_0 = 4A^2 + t_2{}^0$ in the simplest case, $A^2 = B^2$. A level of this type may be manifested in anomalies of superconductivity in crystals with twins.[23]

For phonons, the applicability of (22) and (23), with (19), reduces to $t_0 = 0$, $t_1 + t_2 = t_3 + t_4$, $\varepsilon = -\omega^2 + 2(t_1 + t_2)$. In the long-wave limit, expression (22) becomes

$$T\approx 1+iq\frac{(t_1t_2-t_3t_4)}{(t_1+t_2)[\omega^2(t_1+t_2)/q^2-t_1t_2]^{1/2}}$$

which is analogous to the result of Ref. 24 and makes it possible to relate the distortions of the constants of the Hamiltonian to the surface tension in the twinning plane.

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