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Fano resonances in low-energy electron transmission through crystalline films

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Abstract
It is shown that in crystalline films with a definite lattice symmetry there exist one-dimensional bands of bound electron states above the boundary of the continuous spectrum. The intensity of electron reflection near the state of complete transmission of low-energy electrons is found to have the form of a Fano resonance. We obtain the relationship between the Fano function parameters and physical characteristics of the system. The conditions for the electron transparency to arise near the bound state bands in the continuum are determined.

1. Introduction

Recently, considerable attention has been paid to physical situations in which bound electron states are embedded in a continuum [1]. Interference of these localized and propagating states results in the appearance of Fano resonances [2]. The Fano function gives the most general shape of the resonance line which involves the Breit–Wigner resonance [3] as a special case [1, 4].

Growing interest in Fano resonances in the physics of low-dimensional systems is due to the fact that they may provide important information on the system geometry and potential, and the effect of spatial confinement on the characteristics of excited states both below and above the vacuum level. Fano interference phenomena may potentially be used for the design of new types of quantum electronic devices such as Fano transistors [5] and Fano filters for polarized electrons [6]. There is an attractive idea to use Fano phenomena for lasing without inversion [7].

Present-day nanotechnologies make it possible to obtain various solid-state systems with the abovementioned properties (Aharonov–Bohm rings, two-dimensional electronic waveguides, nanotubes etc). Generation of such systems is often rather difficult. On the other hand, it is not rare for the bound electron states to arise above the vacuum level. They occur in many planar bounded crystals with a definite lattice symmetry [8]. Exposure to factors lowering the system symmetry (deformations, external fields etc) leads to transformation of these bands of localized states into resonances, and hence to changes in electron scattering.

In the present paper we analyze the role of the energy bands of bound states above the vacuum level in the transmission of low-energy electrons through a crystalline film.

In section 2, within the multiscattering approach, we show that near the energy of the complete electron transmission the reflection coefficient at the crystalline film is described by a Fano function. In section 3 we find the conditions for electron transparency, and we also derive the dependence of the energy of complete electron transmission on the parameters of energy bands of bound states and resonances. Section 4 contains the concluding remarks.

2. Fano resonances in films of symmetric crystals

Energy bands of bound electron states may exist in films with a definite lattice symmetry above the boundary of the continuous spectrum $E = \mathbf{k}^2$, where E is the energy and $\mathbf{k}$ is a reduced two-dimensional quasi-momentum (atomic units with energy in Ry are used).

The electron bound states and resonances of the film satisfy the homogeneous Lippmann–Schwinger equation:

$$\Psi_{\mathbf{k}}(\mathbf{r}, E) = -\int_{\Omega} G_{\mathbf{k}}^{(0)}(\mathbf{r}, \mathbf{r}'; E) V(\mathbf{r}') \Psi_{\mathbf{k}}(\mathbf{r}', E)\, \mathrm{d}\mathbf{r}', \qquad (1)$$

where Ω is the film unit cell infinite in z, and $V(\mathbf{r})$ is an effective single-particle potential which is assumed to be zero far away from the film surface when $|z| > z_0$ [9]. The potential $V(\mathbf{r})$ is invariant under transformations of the film symmetry group.

The Green function of free electrons of the crystalline film has the form:

$$G_{\mathbf{k}}^{(0)}(\mathbf{r},\mathbf{r}';E)=\frac{1}{2\pi S}\sum_{\mu}\int_{-\infty}^{+\infty}\frac{\exp[\mathrm{i}(\mathbf{k}+\mathbf{K}_\mu,\lambda)(\mathbf{r}-\mathbf{r}')]}{(\mathbf{k}+\mathbf{K}_\mu)^2+\lambda^2-E}\mathrm{d}\lambda$$
$$=\sum_{\mu}\frac{\exp[\mathrm{i}(\mathbf{k}+\mathbf{K}_\mu,\sqrt{E-(\mathbf{k}+\mathbf{K}_\mu)^2})(\mathbf{u}-\mathbf{u}',|z-z'|)]}{-2\mathrm{i}S\sqrt{E-(\mathbf{k}+\mathbf{K}_\mu)^2}}. \quad (2)$$

Here S is the cross-section of the unit cell Ω by the crystal surface and $\mathbf{u}(\mathbf{u}')$ is the surface-parallel component of the vector $\mathbf{r}(\mathbf{r}')$. The summation is taken over the vectors of the reciprocal lattice of the film. Separating out the term with $\mathbf{K}_\mu = 0$ in equation (2), we can rewrite equation (1) for $z < -z_0$ in the form:

$$\Psi_{\mathbf{k}}(\mathbf{r},E)=\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{u}}\frac{\exp[-\sqrt{k^2-E}\,z]}{2\mathrm{i}S\sqrt{k^2-E}}$$
$$\times\int_{\Omega}\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{u}'}\exp[\sqrt{k^2-E}\,z']\,V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}',E)\mathrm{d}\mathbf{r}'$$
$$+\sum_{\mu}\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{K}_\mu)\mathbf{u}}\frac{\exp[-\sqrt{(\mathbf{k}+\mathbf{K}_\mu)^2-E}\,z]}{2\mathrm{i}S\sqrt{(\mathbf{k}+\mathbf{K}_\mu)^2-E}}$$
$$\times\int_{\Omega}\mathrm{e}^{-\mathrm{i}(\mathbf{k}+\mathbf{K}_\mu)\mathbf{u}'}\exp\left[\sqrt{(\mathbf{k}+\mathbf{K}_\mu)^2-E}z'\right]$$
$$\times V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}',E)\,\mathrm{d}\mathbf{r}'. \quad (3)$$

It is seen from equation (3) that, in the general case, at $E > k^2$ the first term is a nondecreasing function of z, and the state $\Psi_{\mathbf{k}}(\mathbf{r}, E)$ is no longer a discrete spectrum state bound in z. If, however,

$$\int_{\Omega}\mathrm{e}^{-\mathrm{i}\mathbf{k}\mathbf{u}'}\mathrm{e}^{\pm\sqrt{k^2-E}\,z'}\;V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}',E)\,\mathrm{d}\mathbf{r}'=0 \quad (4)$$

then $\Psi_{\mathbf{k}}(\mathbf{r}, E)$ remains a function quadratically integrable in Ω even above the boundary of the continuous spectrum. So, the states bound in z can exist above the continuous spectrum boundary $E = k^2$. Such a situation occurs in films of cubic crystals. Let us consider, for example, a (001) fcc film. In this case the Brillouin zone is a square of side $2\pi/A$, where A is the plane-lattice constant (figure 1).

Consider next a state with a wavevector $\mathbf{k}_{\bar{\Delta}}$ lying in the $\bar{\Delta}$ direction of the two-dimensional Brillouin zone ($\mathbf{k}_{\bar{\Delta}} = (k_{\bar{\Delta}}, 0, 0)$, $|k_{\bar{\Delta}}| < \pi/A$). According to the Wigner theorem [10], the eigenfunctions $\Psi_{\mathbf{k}}(\mathbf{r})$, being solutions of equation (1), must be transformed according to the irreducible representations of the group of wavevector $\mathbf{k}$. For the case under consideration the representations of this group, which is isomorphic to the group C_{2v} [11], are presented in table 1.

Consider the function $\Psi_{\mathbf{k}_{\bar{\Delta}}}^{\bar{\Delta}_3}(\mathbf{r})$ transforming in accordance with the representation $\bar{\Delta}_3$. The integral in equation (4) can be written for $E > \mathbf{k}_{\bar{\Delta}}^2$ as:

$$\int_{\Omega}\mathrm{e}^{-\mathrm{i}k_{\bar{\Delta}}\mathbf{u}}\left[\cos\left(\sqrt{E-k_{\bar{\Delta}}^2}\,z\right)\right.$$
$$\left.\pm\,\mathrm{i}\sin\left(\sqrt{E-k_{\bar{\Delta}}^2}\,z\right)\right]V(\mathbf{r})\Psi_{\mathbf{k}_{\bar{\Delta}}}^{\bar{\Delta}_3}(\mathbf{r})\,\mathrm{d}\mathbf{r}. \quad (5)$$

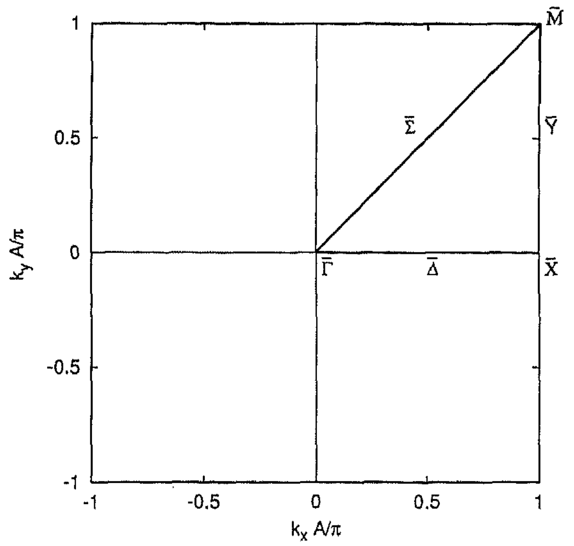

Figure 1. The two-dimensional Brillouin zone for fcc (001) crystal film.

Table 1. Irreducible representations of the group of vector $\mathbf{k}_{\bar{\Delta}}$. $\hat{E}$ is the identical transformation, $\hat{C}_2$ is the rotation through the angle π about the [100] axis and $\hat{\sigma}$ is the reflection in the plane $z = 0$.

$\bar{\Delta}$ (C_{2v})	$\hat{E}$	$\hat{C}_2$	$\hat{\sigma}$	$\hat{\sigma}\hat{C}_2$
$\bar{\Delta}_1$	1	1	1	1
$\bar{\Delta}_2$	1	−1	−1	1
$\bar{\Delta}_3$	1	1	−1	−1
$\bar{\Delta}_4$	1	−1	1	−1

It is easily seen that the functions

$$\exp(-\mathrm{i}\mathbf{k}_{\bar{\Delta}}\mathbf{u})\cos\left(\sqrt{E-k_{\bar{\Delta}}^2}z\right)$$

and

$$\exp(-\mathrm{i}\mathbf{k}_{\bar{\Delta}}\mathbf{u})\sin\left(\sqrt{E-k_{\bar{\Delta}}^2}z\right)$$

transform according to the representations $\bar{\Delta}_1$, and $\bar{\Delta}_2$, respectively. The above integral is equal to zero as a consequence of the well-known selection rule for matrix elements of the operators of scalar quantities. This suggests that the states of said symmetry may exist in the continuous spectrum. The same is true for the states transforming according to the representation $\bar{\Delta}_4$. Similarly, one can demonstrate that for $E > \mathbf{k}^2$ bands of bound states may exist along the $\bar{\Sigma}$ direction ($\mathbf{k}_{\bar{\Sigma}} = (k_{\bar{\Sigma}}, k_{\bar{\Sigma}}, 0)$, $|k_{\bar{\Sigma}}| < \pi/A$) of the Brillouin zone of the (001) fcc film.

The wavefunction of a scattered electron satisfies the equation:

$$\Psi_{\mathbf{k}}(\mathbf{r},E)=\exp[\mathrm{i}(\mathbf{k},k_z)\mathbf{r}]-\int_{\Omega}G_{\mathbf{k}}^{(0)}(\mathbf{r},\mathbf{r}';E)$$
$$\times V(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}',E)\,\mathrm{d}\mathbf{r}' \quad (6)$$

where $k_z = +\sqrt{E-k^2}$. In the case of scattered electrons of low energies lying below the threshold of appearance of a nonspecular beam, in the asymptotic region $z \to -\infty$

$$\Psi_{\mathbf{k}}(\mathbf{r}, E) = \exp(\mathrm{i}\mathbf{ku})\left[\exp(\mathrm{i}k_z z) + a_-(\mathbf{k}, E)\exp(-\mathrm{i}k_z z)\right] \tag{7}$$

where $a_-(\mathbf{k}, E)$ is the amplitude of mirror reflection. In view of (6) and (2) we get:

$$a_-(\mathbf{k}, E) = \frac{1}{2\mathrm{i}Sk_z}\int_\Omega \mathrm{e}^{-\mathrm{i}(\mathbf{k},-k_z)\mathbf{r}}\, V(\mathbf{r})\,\Psi_{\mathbf{k}}(\mathbf{r}, E)\,\mathrm{d}\mathbf{r}. \tag{8}$$

On the other hand,

$$\Psi_{\mathbf{k}}(\mathbf{r}, E) = \mathrm{e}^{\mathrm{i}(\mathbf{k},k_z)\mathbf{r}} - \int_\Omega G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E)\, V(\mathbf{r}')\,\mathrm{e}^{\mathrm{i}(\mathbf{k},k_z),\mathbf{r}'}\,\mathrm{d}\mathbf{r}' \tag{9}$$

where $G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E)$ is the one-electron Green function corresponding to the Hamiltonian $\hat{H} = -\Delta + V(\mathbf{r})$ of the film.

The bands of bound electron states $E_n(\mathbf{k})$ situated above the continuous spectrum boundary form no surfaces in $\mathbf{k}$ space. When the vector $\mathbf{k}$ deviates from the direction along which is realized a state with wavefunction exponentially decreasing for $|z| \to \infty$, this state transforms to a quasi-stationary state with a finite lifetime. Thus, if along particular directions of the two-dimensional Brillouin zone there exist bands of bound states $E_n(\mathbf{k})$, lying above the continuous spectrum boundary, there exists a surface of resonances $E_n^{(R)}(\mathbf{k})$ 'stretched' over these bands:

$$E_n^{(R)}(\mathbf{k}) = \mathcal{E}_n^{(R)}(\mathbf{k}) - \mathrm{i}\Gamma_n(\mathbf{k}), \qquad (\Gamma(\mathbf{k}) > 0). \tag{10}$$

$$E_n^{(R)}(\mathbf{k}_{\bar{\Delta}}) = \mathcal{E}_n^{(R)}(\mathbf{k}_{\bar{\Delta}}) = E_n(\mathbf{k}_{\bar{\Delta}}), \qquad (\Gamma(\mathbf{k}_{\bar{\Delta}}) = 0). \tag{11}$$

In the neighborhood of a resonance

$$G_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E) = \frac{\Psi_{n\mathbf{k}}^{(R)}(\mathbf{r})\Psi_{n\mathbf{k}}^{(R)*}(\mathbf{r}')}{E_n^{(R)}(\mathbf{k}) - E} + \tilde{G}_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E) \tag{12}$$

where $\Psi_{n\mathbf{k}}^{(R)}(\mathbf{r})$ is the wavefunction of a resonance state of 'energy' $E_n^{(R)}(\mathbf{k})$. The function $\tilde{G}_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E)$ analytically depends on $\mathbf{k}$ and E. In what follows we omit the subscript n.

Since the film considered is symmetric with respect to the reflection in the plane $z = 0$, the wavefunctions of resonance and stationary states, being solutions of the homogeneous Lippmann–Schwinger equation, will be either even or odd with respect to z for any $\mathbf{k}$:

$$\Psi_{\mathbf{k}}^{(R),j}(\mathbf{r}) = (-1)^j\,\Psi_{\mathbf{k}}^{(R),j}(\hat{\sigma}\mathbf{r}), \tag{13}$$

where $j = 1$ for states of the odd type and $j = 2$ for those of the even type. In view of equations (8), (9) and (12), we get

$$a_-(\mathbf{k}, E) = a_-^{(0)}(\mathbf{k}, E) - \frac{(-1)^j}{2\mathrm{i}Sk_z}\frac{|W^{(j)}(\mathbf{k}, E)|^2}{E^{(R)}(\mathbf{k}) - E}, \tag{14}$$

where

$$a_-^{(0)}(\mathbf{k}, E) = \frac{1}{2\mathrm{i}Sk_z}\left\{\int_\Omega \cos(2k_z z)V(\mathbf{r})\,\mathrm{d}\mathbf{r} - \int_\Omega\int_\Omega \mathrm{e}^{-\mathrm{i}(\mathbf{k},-k_z)\mathbf{r}}V(\mathbf{r})\tilde{G}_{\mathbf{k}}(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\mathrm{e}^{\mathrm{i}(\mathbf{k},k_z)\mathbf{r}'}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\right\} \tag{15}$$

is the background scattering amplitude analytical [4, 11] in $\mathbf{k}$ and E, and

$$W^{(j)}(\mathbf{k}, E) = \int_\Omega \mathrm{e}^{-\mathrm{i}(\mathbf{k},k_z)\mathbf{r}}V(\mathbf{r})\Psi_{\mathbf{k}}^{(R),j}(\mathbf{r})\,\mathrm{d}\mathbf{r}. \tag{16}$$

Complete transmission occurs for electrons of energy E_t such that $a_-(\mathbf{k}, E_t) = 0$, and hence defined by the simultaneous equations

$$\operatorname{Re} a_-^{(0)}(\mathbf{k}, E) = \frac{(-1)^j|W^{(j)}(\mathbf{k}, E)|^2}{2Sk_z\Gamma(\mathbf{k})}\frac{1}{\varepsilon^2(\mathbf{k}, E) + 1}, \tag{17}$$

$$\operatorname{Im} a_-^{(0)}(\mathbf{k}, E) = \frac{(-1)^j|W^{(j)}(\mathbf{k}, E)|^2}{2Sk_z\Gamma(\mathbf{k})}\frac{\varepsilon(\mathbf{k}, E)}{\varepsilon^2(\mathbf{k}, E) + 1} \tag{18}$$

where

$$\varepsilon(\mathbf{k}, E) = \frac{E - \mathcal{E}^{(R)}(\mathbf{k})}{\Gamma(\mathbf{k})} \tag{19}$$

is the dimensionless energy parameter used in the Fano resonance theory. If equations (17) and (18) are solvable simultaneously, then, under the assumption that the background scattering is constant over the width of the resonance [4], and hence for E close to E_t, we obtain

$$a_-(\mathbf{k}, E) = \frac{(-1)^{j+1}}{2Sk_z(E_t)}\frac{|W^{(j)}(\mathbf{k}, E_t)|^2}{\Gamma(\mathbf{k})}\cos(\delta(\mathbf{k}, E_t)) \times \mathrm{e}^{\mathrm{i}\delta(\mathbf{k},E_t)}\frac{\varepsilon(\mathbf{k}, E) - \tan\delta(\mathbf{k}, E_t)}{\varepsilon(\mathbf{k}, E) + \mathrm{i}}, \tag{20}$$

where, according to (17) and (18), the phase of the background scattering amplitude is

$$\tan\delta(\mathbf{k}, E_t) = \varepsilon(\mathbf{k}, E_t). \tag{21}$$

The reflection coefficient $R(\mathbf{k}, E) = |a_-(\mathbf{k}, E)|^2$ can be written as

$$R(\mathbf{k}, E) = R_0(\mathbf{k}, E_t)\frac{[\varepsilon(\mathbf{k}, E) + q]^2}{\varepsilon^2(\mathbf{k}, E) + 1}, \tag{22}$$

where

$$q = -\tan\delta(\mathbf{k}, E), \tag{23}$$

and

$$R_0(\mathbf{k}, E_t) = \frac{|W^{(j)}(\mathbf{k}, E_t)|^4}{4S^2\Gamma^2(\mathbf{k})(E_t - k^2)}\frac{1}{q^2(\mathbf{k}, E_t) + 1}. \tag{24}$$

Expression (22) coincides with the Fano function providing the most general description of the resonance line shape [4]. Figure 2 presents the dependence of the reflection coefficient on the energy position of the scattered electron with respect to the transparency energy, described by the dimensionless variable $\varepsilon_t = (E - E_t)/\Gamma$, and on the spacing between the energies of the complete electron transmission and the resonance, given by the parameter $\varepsilon(E_t) = (E_t - \mathcal{E}^{(R)})/\Gamma$. One can see rapid flattening of the reflection zero dip at Fano antiresonance as the distance of the resonance energy from the electron transparency energy increases. For small Γ this picture does not actually depend on the resonance width.

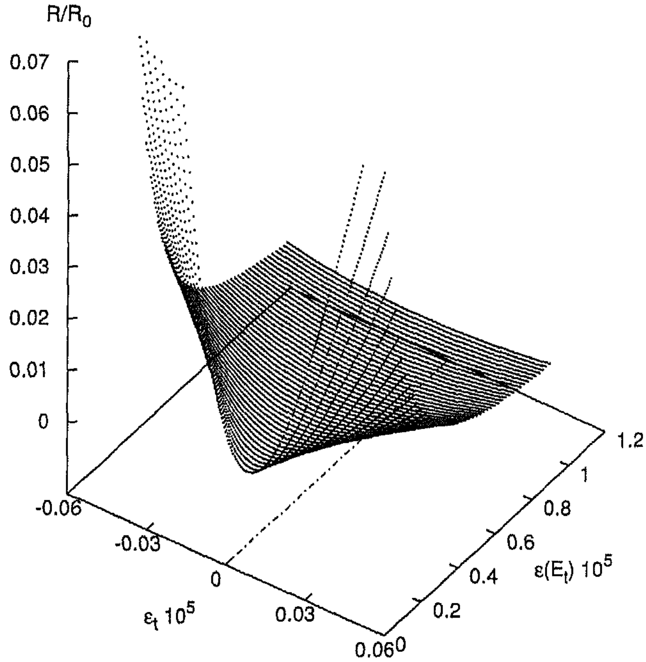

Figure 2. The reflection coefficient.

3. Electron transmission near the bound states in the continuous spectrum

3.1. The solvability condition for transparency equations

Let us separate out the real and imaginary parts in the second term on the right of equation (15):

$$a_0 + \mathrm{i}b_0 = \int_\Omega \int_\Omega \mathrm{e}^{-\mathrm{i}(\mathbf{k},-k_z)\mathbf{r}} V(\mathbf{r}) \times \tilde{G}_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) V(\mathbf{r}')\mathrm{e}^{-\mathrm{i}(\mathbf{k},k_z)\mathbf{r}'}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'. \tag{25}$$

The simultaneous system of (17) and (18), the solvability of which is the condition for the existence of electron transmission, can be written in the form:

$$a_0 + \mathrm{i}b_0 = \int_\Omega \cos(2k_z z) V(\mathbf{r})\,\mathrm{d}\mathbf{r} - \frac{(-1)^j |W^{(j)}(\mathbf{k},E)|^2}{(\mathcal{E}^{(R)}(\mathbf{k}) - E)^2 + \Gamma^2(\mathbf{k})}\left[\mathcal{E}^{(R)}(\mathbf{k}) - E + \mathrm{i}\Gamma(\mathbf{k})\right]. \tag{26}$$

Let us estimate the ratio a_0/b_0. Consider the resonance for $k_z d$ of the order of unity, where d is the half-thickness of the film. Away from the resonance, for small k_z ($k_z d \ll 1$) the singular term in expression (12) may be neglected. So

$$G_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) = \tilde{G}_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E). \tag{27}$$

On the other hand, for small k_z, according to (2),

$$G^{(0)}_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) \approx -\frac{1}{2\mathrm{i}Sk_z}\mathrm{e}^{\mathrm{i}k(\mathrm{u}-\mathrm{u}')}. \tag{28}$$

Using the relation [9] between the Green functions $G_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E)$ and $G^{(0)}_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E)$

$$G_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) = G^{(0)}_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) - \int_\Omega G^{(0)}_{\mathbf{k}}(\mathbf{r},\mathbf{r}'';E) V(\mathbf{r}'') G_{\mathbf{k}}(\mathbf{r}'',\mathbf{r}';E)\,\mathrm{d}\mathbf{r}'' \tag{29}$$

according to (28) we get

$$G_{\mathbf{k}}(\mathbf{r},\mathbf{r}';E) \approx -\frac{\mathrm{e}^{\mathrm{i}k\mathrm{u}}}{2\mathrm{i}Sk_z}\left[\mathrm{e}^{-\mathrm{i}k\mathrm{u}'} - \frac{\langle V\rangle}{\langle V\rangle - \mathrm{i}k_z/d}\right], \tag{30}$$

where

$$\langle V\rangle = \frac{1}{2dS}\int_\Omega V(\mathbf{r})\,\mathrm{d}\mathbf{r} \tag{31}$$

is the mean inner potential of the film. In view of (27) the condition for the existence of electron transparency (26) can be written as

$$a_0 + \mathrm{i}b_0 = \frac{\langle V\rangle[\int_\Omega \cos(k_z z) V(\mathbf{r})\mathrm{d}\mathbf{r}]^2}{2dS\,[\langle V\rangle^2 + (k_z/d)^2]} \times \left(1 + \mathrm{i}\frac{k_z}{d\langle V\rangle}\right). \tag{32}$$

For small k_z

$$\left|\frac{b_0}{a_0}\right| = \left|\frac{k_z}{d\langle V\rangle}\right| \ll 1. \tag{33}$$

Then, using the assumption that the background scattering depends only weakly on energy, we obtain the transparency condition near the resonance:

$$\int_\Omega \cos(2k_z z) V(\mathbf{r})\mathrm{d}\mathbf{r} - a_0 \approx (-1)^j \left|W^{(j)}(\mathbf{k},E)\right|^2 \times \frac{(\mathcal{E}^{(R)}(\mathbf{k}) - E) + \mathrm{i}\Gamma(\mathbf{k})}{(\mathcal{E}^{(R)}(\mathbf{k}) - E)^2 + \Gamma^2(\mathbf{k})}. \tag{34}$$

This equation can be approximately solved with respect to E if

$$\Gamma(\mathbf{k}) \ll \left|\mathcal{E}^{(R)}(\mathbf{k}) - E\right|. \tag{35}$$

3.2. Transparency energy

According to (11) resonances with small $\Gamma(\mathbf{k})$ satisfying (35) arise when the surface-parallel component of the momentum of an incident electron lies near the direction along which a band of bound states is realized above the boundary of the continuous spectrum. By (34), in this case the energy of transmission is

$$E_t = \mathcal{E}^{(R)}(\mathbf{k}) - \frac{(-1)^j \left|W^{(j)}(\mathbf{k},E)\right|^2}{\int_\Omega \cos(2k_z z) V(\mathbf{r})\,\mathrm{d}\mathbf{r} - a_0(\mathbf{k},E)} \tag{36}$$

and condition (35) gives

$$\left|\int_\Omega \cos(2k_z z) V(\mathbf{r})\,\mathrm{d}\mathbf{r} - a_0(\mathbf{k},E)\right| \ll \frac{\left|W^{(j)}(\mathbf{k},E)\right|^2}{\Gamma(\mathbf{k})}. \tag{37}$$

In particular, near the direction $\bar{\Delta}$ of the 2D Brillouin zone of the film of cubic crystals, $\mathbf{k} = (k_{\bar{\Delta}}, k_y)$ where k_y is close to zero. Since the dispersion law of the resonance $E^{(R)}(\mathbf{k})$ is invariant under symmetry transformations of the film considered, in the $\bar{\Delta}$ direction $\partial\mathcal{E}^{(R)}(\mathbf{k}_{\bar{\Delta}})/\partial k_y = 0$ and $\partial\Gamma(\mathbf{k}_{\bar{\Delta}})/\partial k_y = 0$. By virtue of condition (4), the expansion of $|W^{(j)}(\mathbf{k},E_t)|^2$ in powers of k_y begins with the quadratic term

$$\left|W^{(j)}(\mathbf{k},E)\right|^2 = \left|\tilde{W}^{(j)}(\mathbf{k}_{\bar{\Delta}},E)\right|^2 k_y^2 + o(k_y^2), \tag{38}$$

where

$$\tilde{W}^{(j)}(\mathbf{k}_{\bar{\Delta}}, E) = \int_{\Omega} \mathrm{e}^{-\mathrm{i}\sqrt{E-k_{\bar{\Delta}}^2}z} V(\mathbf{r}) U_{\mathbf{k}_{\bar{\Delta}}}^{(R),j}(\mathbf{r})\,\mathrm{d}\mathbf{r} \qquad (39)$$

and $U_{\mathbf{k}_{\bar{\Delta}}}^{(R),j}(\mathbf{r}) = \exp(-\mathrm{i}\mathbf{k}_{\bar{\Delta}}\mathbf{u})\Psi_{\mathbf{k}_{\bar{\Delta}}}^{(R),j}(\mathbf{r})$ is the periodic part of the Bloch function of a bound state with energy $E(\mathbf{k}_{\bar{\Delta}})$. Therefore the ratio $|W^{(j)}(\mathbf{k}, E_{\mathrm{t}})|^2/\Gamma(\mathbf{k})$ appearing in condition (37) remains finite at any k_y as small as desired. In the approximation quadratic in k_y the transmission energy is

$$E_{\mathrm{t}} = E(\mathbf{k}_{\bar{\Delta}}) + \left[\frac{1}{2}\frac{\partial^2 \mathcal{E}^{(R)}(\mathbf{k}_{\bar{\Delta}})}{\partial k_y^2} + \frac{(-1)^{j+1}|\tilde{W}^{(j)}(\mathbf{k}_{\bar{\Delta}}, E)|^2}{\int_{\Omega}\cos\left(2\sqrt{E-\mathbf{k}_{\bar{\Delta}}^2}\,z\right)V(\mathbf{r})\mathrm{d}\mathbf{r} - a_0(\mathbf{k}_{\bar{\Delta}}, E)} \right] k_y^2. \qquad (40)$$

In the case of smallness of the expression in square brackets the electron transparency is attained at a scattered electron energy close to the energy of a bound state with quasi-momentum corresponding to the surface-parallel component of the scattered electron momentum.

4. Conclusion

We have shown that for crystalline films the line shape of electron reflection near the electron transparency point has the form of a Fano resonance. This result is in agreement with the conclusion drawn by some authors that the Fano function gives the most general description of the resonance line shape, provided that the background scattering is constant over the width of the resonance [1, 4]. The analysis performed in this work allowed us to relate the parameters of this function to physical quantities that characterize both the scattered electron $(E, \mathbf{k})$ and the film material entering, through the scattering potential, in the matrix element $W^{(j)}(\mathbf{k}, E)$. We have found the conditions for electron transparency. It is shown that they can be fulfilled for electron scattering with a surface-parallel component of the momentum, close to the 2D Brillouin zone direction along which electron confinement is realized above the vacuum level. An expression for the energy of complete electron transmission is obtained by means of the fact that the dispersion law of resonances generated by these bound states is invariant under symmetry transformations of the film considered. In the case of electron scattering with tangential momentum $\mathbf{k}$, corresponding to the quasi-momentum of an embedded bound state, this energy is close to the bound state energy $E(\mathbf{k})$. The results obtained may be applied to ultrathin quantum-dimensional films required for the modern nano and picotechnology. As the film thickness increases, provided that the band of bound energy states is not a surface-state band, the size-quantized bands approach each other, forming in the limit projected energy bands of the bulk crystal. In this case the results obtained in this paper describe the known effect of a drastic change in electron transmission at the bulk band boundary [12, 13]. At present, this is successfully used in experimentally determining the band structure of photoemission final states [14].

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