THE POSSIBILITY OF RESONANCE TRANSMISSION OF ELECTRONS IN CRYSTALS THROUGH A SYSTEM OF BARRIERS

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The transmission coefficient of a one-dimensional quantum-mechanical system consisting of two potential barriers is considered (see Fig. 1). When the energy of the incident particles coincides with that of a quasi-level in the well between the barriers, resonance occurs. The resonance transmission coefficient is unity when the barriers are equal, and decreases exponentially as the equality of the barriers is destroyed; this allows the transmission coefficient to be controlled by a small deformation of the barriers. It is shown that there exists in principle the possibility of resonant tunnelling of electrons in a semiconductor through the two closely situated thin dielectric layers, 2 and 4 in Fig. 2, which act as potential barriers of different height. An external electric field can make the barriers equal and control the resonance current. The conditions necessary for the realization of this effect in experiment are discussed. The magnitude of the resonance current depends on the shape of the Fermi surface of the main crystal. The character of the reflection and transmission of electrons through the dielectric barriers should be specular, and all mean free paths should be large compared with the thickness of the system.

1. It is well known that the quantum-mechanical one-dimensional system of two equal potential barriers, shown in Fig. 1b, has a property of resonance transmission. A detailed explanation of the physics of the phenomena and a calculation for the quasi-classical case can be found in Bohm's book.[1] The resonance transmission, or Ramsauer effect, occurs when the energy of the particle incident from region 1 on to the barrier 2 is the same as the energy of a quasi-level in the well 3 between the barriers. In the one-dimensional case such quasi-levels always exist. Resonance is accompanied by the establishment of an intense standing wave inside the resonant well. In the stationary state the incident wave from region 1 proceeds through the barrier 2 into the well 3, while simultaneously a wave of equal intensity flows out from the well on the other side through the barrier 4. When the energy of the incident particle is altered from the resonance value, the transmission coefficient falls exponentially. Because the system is symmetrical in the sense of the equality of the individual transmission coefficients of each barrier, nothing is changed if we take the waves to be incident not from region 1 but from region 5. The resonance transmission coefficient is a consequence of this symmetry.

It is well known that if a single potential barrier is situated in front of an impenetrable wall,

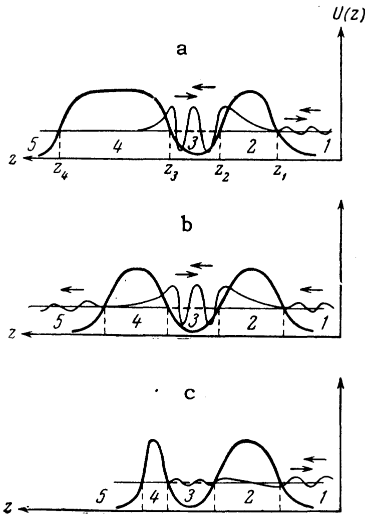

FIG. 1. Change in character of resonant penetration of waves in the well 3 with decreasing barrier 4.

then resonance in the quasi-levels is possible also. In Fig. 1a such a barrier 2 in front of a wall 4 is of finite thickness. The transmission coefficient of a barrier decreases exponentially as the width or height of the barrier is increased; therefore, the finite barrier 4, large compared with the smaller barrier 2, can act as a practically impenetrable wall. At resonance an intense standing wave is also set up in the well 3 in front of the wall. In the steady state resonance condition the wave incident from region 1 completely penetrates through the barrier 2 into the well 3, but a wave of exactly the same intensity flows out backwards from the well 3 to meet the incident wave. The steady state process of resonance reflection is energetically equivalent to a simple non-resonant reflection of the wave from barrier 2, but physically the two phenomena are greatly different, since, for non-resonance reflection, waves do not substantially penetrate into region 3 behind the barrier. In particular, therefore, the build-up process is completely different.

If it is considered that the barrier 4 is not an absolutely impenetrable wall, but possesses some extremely small transmission coefficient, then a small flux of particles also proceeds from well 3 into region 5 through the barrier 4. Because the system of barriers is asymmetrical, when the wave is incident from the opposite side from region 5, the resonance process will be greatly different from that considered above. Despite resonance, there will be in practice simple reflection of the waves from the barrier 4, since the wave cannot sense small barriers separated from it by a high barrier. An increase of intensity of the standing wave in the well 3 between the barriers that is large compared with the incident wave cannot occur in this case, since the wave escapes more easily out of the well through the smaller barrier than it penetrates into it through the larger barrier.

The basic idea of the present work is as follows: if we start to deform potential barriers without destroying resonance, a continuous transition can exist from one of the resonance effects discussed above to the other. Thus, if we gradually start to diminish the width (or height) of the large barrier 4 in Fig. 1a, then, when the individual transmission coefficients of the barriers 2 and 4 become equal, the original resonance reflection is changed into resonance transmission, to which corresponds Fig. 1b. Further, when barrier 4 becomes smaller than barrier 2, as shown in Fig. 1c, the resonance transmission becomes a simple reflection from barrier 2. The general principles quoted above can be readily verified in a concrete calculation if the barriers are taken to have a simple shape allowing an exact solution; however, the formulae are cumbersome, and their behavior is difficult to follow. A very clear expression for the transmission coefficients of an arbitrary system of two barriers, which illustrates what has been said, above can be obtained[1)] in the quasi-classical approximation, by exactly the same method as in [1]:

$$T = 1 / \{\sin^2 J_3 \,\mathrm{ch}^2 (J_2 - J_4) + \cos^2 J_3 \,\mathrm{ch}^2 (J_2 + J_4 + \ln 4)\},$$
$$\hbar J_i = \int_{z_{i-1}}^{z_i} p_i \, dz, \qquad p = |\sqrt{2m[U(z) - E]}|. \quad (1)^*$$

Here J_i is the action integral taken in the i-th region between neighboring turning points; p is the classical momentum of the particle.

Resonance occurs under the usual quasi-classical condition

$$2\hbar J_3 = \oint p_3 \, dz = 2\pi\hbar (n + 1/2) \quad (n = 0, 1, 2, \ldots), \quad (2)$$

which determines the quasi-level in the well 3. Here $\cos J_3 = 0$, and the resonance transmission coefficient is simply equal to

$$T_{\mathrm{res}} = \mathrm{ch}^{-2} (J_2 - J_4), \quad (3)$$

i.e., depends on the ratio of the barriers, and tends to unity when $J_2 = J_4$. Owing to the exponential variation, the resonance transmission coefficient (3) is very sensitive to change of form of the barriers. Thus, there exists in principle the possibility of shutting off or turning on the resonance transmission at will by means of a small deformation of the barriers.

It is well known that the resonance effects considered are not specifically quantum-mechanical, but can occur for waves of any nature, including electromagnetic, acoustic, etc. For electromagnetic waves, resonant systems of one-dimensional barriers can be easily formed with dielectric layers at total internal reflection. For elastic waves in liquids, totally reflecting solid layers can serve as barriers. All the resonance effects mentioned above then occur, and an additional resonance diffraction effect associated with waves at inclined incidence.[2] The width of the potential barriers is here determined by the thickness of the totally reflecting layers, and the height by the material constants of the medium: the dielectric permittivity and magnetic permeability for electromagnetic waves in dielectrics, and the elastic moduli for elastic waves. If these constants are changed by any external factors, it is possible to control the resonance transparency.

2. There also exists in principle the possibility of the effect considered above occurring for electrons in crystals, and we discuss this further. It is well known that, in a number of semiconducting crystals and in certain metals, the conduction electrons possess an effective mass m* many times smaller than the mass of a free electron

[1)]I am grateful to M. Ya. Azbel', who, when acquainted with the original version of the article, obtained this formula and kindly suggested its use.

*ch = cosh.

m, a de Broglie wavelength of the order of tens of angstroms, and a large mean free path of order 10^4-10^6 Å. Such electrons can penetrate thin nonconducting layers of thickness $d \sim 100$ Å by the tunnel effect. These electrons sense the non-conducting layers macroscopically as one-dimensional potential barriers of a height $U \sim 1$ eV determined by the width of the forbidden gap. If two such barriers are situated sufficiently close to one another, the resonance effects considered above can occur in principle. In this case it is especially easy to control the resonance transparency, since a small change of the applied voltage is sufficient to deform the potential barriers.

We consider the plane layer system of a crystalline medium shown in Fig. 2a. The shaded media 1, 3, and 5, correspond to an electronic conductor, and the unshaded ones, 2 and 4, to a dielectric. We shall consider the electrons in the conductors as a free Fermi gas which might be degenerate or nondegenerate. In Fig. 2b the potential energy of electrons is shown under the simplifications taken. U_i is the bottom of the conduction band in the i-th region. It is assumed for simplicity that the barriers 2 and 4 have equal widths (this is not necessary in principle) and different heights, i.e., $d_2 = d_4$ and $U_4 > U_2$. The quasi-levels of electrons in the well 3 are shown by broken lines; the number of these levels depends on the width of the well and the height of the walls.

We switch on an identical electric field $\mathscr{E}$ in the direction 5 to 1 in both the dielectric layers. The potential energy of the electrons is thereby lowered by the amount $V = e\mathscr{E}d_2$ (e is the electronic charge) in the medium 3 and by 2V in the medium 5. As a result we obtain the potential energy shown in Fig. 2c. Because of the great steepness of the barriers it is impossible to use here the quasi-classical expressions (1)–(3); the problem, however, does permit an exact solution with the aid of Airy functions. We assume for simplicity that the effective

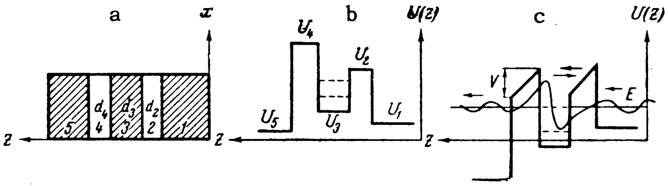

FIG. 2. System of crystalline conductors (a) separated by dielectric layers 2 and 4, and the potential energy of the electrons without the field (b) and after turning on the field (c).

height of each of the barriers is sufficiently large and that it is permissible to use the asymptotic representation for the Airy functions, [3] and we find that at resonance the transparency of the system is a maximum and is given as before by formula (3), where it is now necessary to put

$$J_2 = \frac{2}{3}\{|\xi_r|^{3/2} - |\xi_l|^{3/2}\} + \ln\left\{\frac{k_1}{k_3}\left[|\xi_r|^{-1/2} + \frac{\xi'^2}{k_1^2}|\xi_r|^{1/2}\right]\right.$$
$$\left.\times\left[|\xi_l|^{1/2} + \frac{k_3^2}{\xi'^2}|\xi_l|^{-1/2}\right]\right\},$$
$$J_4 = \frac{2}{3}\{|\xi_r+\delta|^{3/2} - |\xi_l+\delta|^{3/2}\}$$
$$+ \ln\left\{\frac{k_3}{k_5}\left[|\xi_r+\delta|^{-1/2} + \frac{\xi'^2}{k_3^2}|\xi_r+\delta|^{1/2}\right]\right.$$
$$\left.\times\left[|\xi_l+\delta|^{1/2} + \frac{k_5^2}{\xi'^2}|\xi_l+\delta|^{-1/2}\right]\right\};$$
$$k_i = p_i/\hbar, \qquad \xi_r = -(U_2 - E)\,d_2\xi'/V,$$
$$\xi_l = -[(U_2 - V) - E]\,d_2\xi'/V,$$
$$\delta = [V - (U_4 - U_2)]\,d_2\xi'/V, \qquad \xi' = [2mV/d_2\hbar^2]^{1/3}. \tag{4}$$

It is not difficult to show that the quasi-classical action integrals in (1) exactly coincide with the first terms in (4).

Resonance occurs when the energy E of the external electron coincides with a quasi-level of electronic energy in the well 3 and is given by the condition $k_3d_3 = (k_3d_3)_{res} + \epsilon_0$ where

$$\exp(ik_3d_3)_{res} = i\left[\frac{(|\xi_r+\delta|^{-1/4} - i\xi'k_3^{-1}|\xi_r+\delta|^{1/4})(|\xi_l|^{1/4} + ik_3(\xi')^{-1}|\xi_l|^{-1/4})}{(|\xi_r+\delta|^{-1/4} + i\xi'k_3^{-1}|\xi_r+\delta|^{1/4})(|\xi_l|^{1/4} - ik_3(\xi')^{-1}|\xi_l|^{-1/4})}\right]^{1/2}, \tag{5}$$

$$\varepsilon_0 = \frac{2k_3^{-1}\xi'(|\xi_l+\delta|^{1/2} - k_5^2(\xi')^{-2}|\xi_l+\delta|^{-1/2})\exp[-4/3(|\xi_r+\delta|^{3/2} - |\xi_l+\delta|^{3/2})]}{(|\xi_l+\delta|^{1/2} + k_5^2(\xi')^{-2}|\xi_l+\delta|^{-1/2})(|\xi_r+\delta|^{-1/2} + k_3^{-2}\xi'^2|\xi_r+\delta|^{1/2})}$$

$$-\frac{2k_3(\xi')^{-1}(|\xi_r|^{-1/2} - k_1^{-2}\xi'^2|\xi_r|^{1/2})\exp[-4/3(|\xi_r|^{3/2} - |\xi_l|^{3/2})]}{(|\xi_r|^{-1/2} + k_1^{-2}\xi'^2|\xi_r|^{1/2})(|\xi_l|^{1/2} + k_3^2(\xi')^2|\xi_l|^{-1/2})}. \tag{6}$$

The expression (6) is an exponentially small correction of the same order as the individual transparency of either of the barriers; therefore the resonance condition is determined with great accuracy by equation (5), which is consequently the approximate resonance condition and determines the position and number of the quasi-levels.

As the field is increased the difference in height of the barriers diminishes and, when $V \approx U_4 - U_2$, tends to zero. Then $J_2 = J_4$ and $T_{res} = 1$, i.e., the conditions for resonance tunnel penetration of electrons from medium 1 to medium 5 through the system of barriers occur. When the field is further increased the barrier 4 goes below barrier 2, the symmetry is destroyed, and the system loses its transparency. Consequently, the curve of resonance current with increasing V goes through a maximum and thereafter decreases. If unequal voltages are applied separately to layers 2 and 4, then, by displacing the potential of the layer 3 relative to the potentials of the media 1 and 5, we can destroy the symmetry of the barriers and thereby control the resonance current. If the field is applied in the opposite direction, then the original existing asymmetry of the barriers will be increased and the resonance transparency will not arise.

3. We now evaluate the requirements which must be satisfied in order that the effect considered can appear in real systems. Because the electrons fall on a system of barriers from the original crystal 1 in Fig. 2a, its properties are very important. The properties of the resonator layer 3 and the dielectric barriers 2 and 4, which together determine the sharpness of resonance, are also important. The purpose of the conductor 5 is to collect and lead away the electrons proceeding through the barrier; its properties should not, therefore, play a great part, and for this conductor a normal metallic coating can be used.

We have considered above one-dimensional motion along the z axis. Proceeding to the three-dimensional case, and assuming that the longitudinal component of the quasi-momentum p_x is preserved, we find that all the results obtained previously remain in force if we replace E by $E - p_x^2/2m^*$. This means that resonance is possible only for those conduction electrons in crystal 1 that lie close to the section of constant-energy surface by the plane $p_{1z} = p_{1z\,res}$. To calculate the total resonance current, therefore, it is necessary to know the shape of the constant-energy surface in crystal 1 and the density of states in the conduction band. It is also necessary to take into account that resonance penetration of electrons falling on the barrier at inclined incidence should be accompanied by the phenomenon of resonance diffraction.[2] However, such a calculation has been given by us previously. It is obvious physically that for a nonspherical shape of constant energy surface, which provides a great anisotropy of the electronic properties, a significant fraction of the conduction electrons in crystal 1 can participate in the resonance transmission. Therefore the effect considered should depend strongly on the shape of the Fermi surface in crystal 1.

The resonance discussed by us occurs due to the presence of discrete energy levels in the thin conducting layer 3. It is well known that in an infinite conductor the energy levels form a continuous band, but in the case of a thin film, instead of the continuous band a series of discrete levels occurs; this is associated with the formation of standing waves. The energy levels of particles in a one-dimensional rectangular well with infinite walls can be written as follows:

$$E_n = \frac{\pi^2\hbar^2}{2m^* d_3^2} n^2 = (0.0038\,\text{eV}) \left(\frac{m}{m^*}\right) \left(\frac{100\,\text{Å}}{d_3}\right)^2 n^2 \quad (n = 1, 2, \ldots). \tag{7}$$

Substituting $m^* = 0.1\,m$, $d_3 = 200\,\text{Å}$, we obtain, for example, with $E_n \approx 2$ eV, which corresponds to $n = 15$, a value of $E_{n+1} - E_n \approx 0.28$ eV. Thus, for energies of the order of the Fermi energy the distance between neighboring levels is sufficiently large.

For smaller effective masses and larger film thicknesses the distance between the levels is still greater. However, in the real case of conducting films, the discrete levels occur only when reflection of the electrons from both surfaces of the film is of a specular character. In the opposite case of diffuse reflection, the levels are greatly smeared out. Whether reflection is diffuse or specular depends on the relation between the de Broglie wavelength of the electron and the inhomogeneities of the film surface, which in the best case amount to several interatomic distances. One might think that, in semiconductor films where the effective mass of the electrons is sufficiently small and the de Broglie wavelength is particularly large, the conditions for specular reflection ought to be satisfied; however this question is still, apparently, inadequately investigated.

In metallic films the reflection of electrons is usually of a diffuse character. Nevertheless, discrete levels exist and determine a number of effects. It is, however, very curious[2)] that for bismuth, which is a semi-metal, reflection of conduction electrons from the surface of a crystal is specular.[4] In all cases when the surface of thin crystals was specular for visible light, the reflection of conduction electrons had a strictly specular character. The authors explain this by the very

[2)]I am grateful to L. V. Keldysh, who drew my attention to this fact.

large de Broglie wavelength of conduction electrons in bismuth, associated with the small Fermi energy and the small effective mass. The mean free path in the experiments amounted to millimeters, i.e., the conditions necessary for the existence of the effect we have considered were realized with ease. It is true that the plates of bismuth used in [4] were too thick for the energy levels to be discrete.

The insulating layers 2 and 4 must be very thin in order to possess adequate transparency, since for large film thicknesses, because of the exponential dependence, resonance becomes possible only for excessively large increases in the amplitude of the standing wave inside the resonator 3; this is unrealistic because of the finite density of states in the film 3 and the presence of scattering. Because the transmission coefficient of a single dielectric film is determined simultaneously by the thickness of the film, the width of the forbidden gap, and the effective mass of the carriers, a wide choice of possibilities exists here. In order to equalize the barriers it is necessary to apply to the film a constant voltage of the order of fractions of the forbidden gap. Because this voltage is smaller than the ionization potential of the dielectric, the only requirements which the films must satisfy is to possess finite transparency and minimum scattering.

The calculation made did not take into account scattering of electrons, which plays an important part, because the resonance considered is a coherent effect. Scattering in crystal 1 means that instead of plane monochromatic waves, wave packets occur comparable with the mean free path. Scattering inside the layers 2 and 4 leads to additional broadening of the quasi-levels. The process is therefore equivalent to the transmission of wave packets of finite extent through a resonant layer system possessing absorption. The greater the mean free path of the electrons in crystal 1 compared with the thickness of the system, and the smaller the scattering inside the layers, the sharper will be the resonance curves that can be obtained by increasing the thickness of the barriers. Scattering imposes a limit on the attainable resonance parameters according to the same laws as applied for light waves in the presence of two totally reflecting barriers.[5]

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