Study of resonant electron tunneling with a scanning tunneling microscope

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A resonant transparency has been found in a three-dimensional asymmetric potential barrier, serving as a model of a (microscopic proturberance)-vacuum-(defect in insulating film) structure. As the microscopic proturberance moves in a direction parallel to the surface of the film, the transparency above the defect may have not only a maximum but also a local minimum. The path traced out by the sharp point of a scanning tunneling microscope in a small neighborhood above the defect has been determined.

The resonant tunneling of electrons through a small set of point defects in an insulating film was studied in Ref. 1. It was shown in Ref. 2 that a scanning tunneling microscope[3] (recently constructed in the USSR[4]) is capable of observing single defects and thereby visualizing the internal structure of thin films. It appears that an experiment similar to that in Ref. 2, but in which there was the flexibility of varying not only the applied voltage and the temperature (as in Ref. 1) but also the distance from the sharp point to the defect, would make it possible to look at the process of resonant tunneling in an unaveraged "pure" form. A comparison of such an experiment with the theory would make it possible to study both the time-varying effects accompanying resonant tunneling and the resonant-tunneling dynamics proper—topics which have recently been the subject of some discussion.[5-7] In the present letter we derive a theory for the resonant tunneling of electrons from the sharp point of a scanning tunneling microscope through an unfilled level of a defect in the film of an insulator.

We write the Hamiltonian describing the motion of the electrons in the form $H = -\nabla^2/2 + V(\mathbf{r}) + \hat{u}(|\mathbf{r} - \mathbf{r}_0|)$. Here $V(\mathbf{r}) = V(z,\rho)$ is an axisymmetric potential, assumed to be semiclassical outside the film and outside the sharp point, while $\hat{u}$ is a well of zero radius, which serves as model of a defect. We assume that the film is wide enough that the nonresonant transparency is exponentially small. The resonant current will then be concentrated in a narrow tube containing the defect, and it will fall off quite rapidly as the microscopic protuberance is moved away from the point (x_0, y_0, z_3) (Fig. 1). In this tube, the electrons move along paths $\rho(z)$ which deviate only slightly from the z axis. In a first approximation in ρ, these paths satisfy the equation

$$\rho_{zz} + \frac{p_z}{p}\rho_z + \frac{V^0_{\rho\rho}}{p^2}\rho = 0, \quad p(z) = \sqrt{2(E - V(z,0))}, \quad V^0_{\rho\rho}(z) = \left.\frac{d^2V}{d\rho^2}\right|_{\rho=0} \qquad (1)$$

To calculate the transparency of the barrier $D(E)$, we assume that the displacement of the microscopic protuberance in the (x,y) plane, i.e., $s = \sqrt{x_0^2 + y_0^2}$, is much smaller than the scale length of the problem along the z axis.

In a small neighborhood of the defect, in which $V(z,\rho)$ can be assumed to remain constant, the wave function can be written[8]

$$\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \frac{\Psi_0(\mathbf{r}_0)\exp(-p_0|\mathbf{r} - \mathbf{r}_0|)}{(p_0 - \sqrt{2|E_0 - V(\mathbf{r}_0)|})|\mathbf{r} - \mathbf{r}_0|}, \quad p_0 = |p(0)|, \quad \mathbf{r}_0 = (x_0, y_0, 0), \qquad (2)$$

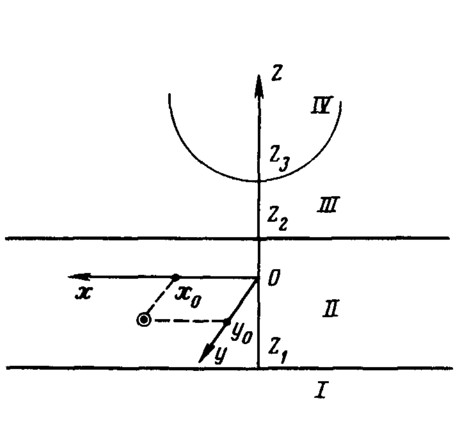

FIG. 1. I—Substrate; II—insulating film; III—vacuum; IV—sharp point of the scanning tunneling microscope.

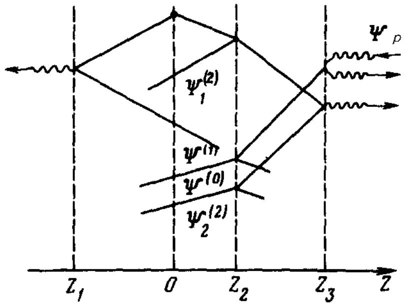

FIG. 2. Schematic diagram of the wave function of the problem.

where Ψ_0 is the wave function corresponding to the Hamiltonian $H - \hat{u}$, and E_0 is the energy of a bound state in the well. The solution Ψ_0 is found by the method illustrated in Fig. 2. In the film, the potential V is assumed to depend on only z, so that the Schrödinger equation allows separation of variables here. Continuing the standing spherical wave in (2) to the left, and requiring, after the joining at the boundary z_1, that there be only an outgoing wave to the left of z_1, we find the wave function $\Psi^{(1)}$. A continuation of the spherical wave to the right is carried out by making use of the asymptotic solution of the Schrödinger equation near the z axis, given in Ref. 9, and also by assuming that in a small neighborhood of the tip of the microscopic protuberance the boundary has the shape of a paraboloid of revolution, $z - z_3 = \rho^2/2R$. The functions $\Psi_1^{(2)}$ and $\Psi_2^{(2)}$ are found by requiring that after a systematic joining of the spherical wave at the film boundary z_2 and at the boundary of the microscopic protuberance the solution to the right of z_3 has the form of an outgoing wave. Furthermore, we continue the plane wave $\Psi_p = (2E)^{-1/4} \exp\{ip_x x + ip_y y - i[\sqrt{2E} - (p_x^2 + p_y^2)/\sqrt{2E}]z\}$, where[1] $p_{x,y} \ll \sqrt{2E}$ which is incident at a small angle, along with the corresponding outgoing wave across the boundary of the microscopic protuberance, having found a solution $\Psi^{(0)}$ which falls off exponentially inside the barrier. The wave function found in this manner, shown schematically in Fig. 2, satifies the boundary conditions of our problem within exponentially small terms. From the equation $\Psi^{(0)}(\mathbf{r}_0) + \Psi^{(1)}(\mathbf{r}_0) + \Psi_1{}^{(2)}(\mathbf{r}_0) + \Psi_2{}^{(2)}(\mathbf{r}_0) = \Psi_0(\mathbf{r}_0)$ which follows from (2), we can determine $\Psi_0(\mathbf{r}_0)$. We can then find the transparency $D(E)$ by calculating the flux of the wave function to the left of z_1 and averaging it over p_x and p_y.

Before we write the result, let us determine the solutions $\rho_j^{1,2}$ of Eq. (1) by means of the initial conditions $\rho_j^1(z_j) = \rho_{jz}^2(z_j) = 0$ and $\rho_{jz}^1(z_j) = \rho_j^2(z_j) = 1$. We also introduce the matrix $T = \|t_{ij}\|$ through the relation $\rho_3^k(z) = t_{1k}\rho_2^1(z) + t_{2k}\rho_2^2(z)$. We introduce the notation

$$S_j = \int_0^{z_j} |p|\,dz, \quad \tau_j = \int_0^{z_j} \frac{dz}{|p|}, \quad p_j^{\pm} = \lim_{z \to z_j \pm 0} |p(z)|,$$

$$t_{0j} = R^{-1} t_{1j} + t_{2j}, \quad q_j = t_{j2} + \tau_2 p_2^{+} t_{j1}.$$

Our final expression for $D(E)$ is then

$$D(E) = \frac{2\pi^2 \Gamma_+ \Gamma_-}{(E - \widetilde{E}_0)^2 + {}^1/_4(\Gamma_+ + \Gamma_-)^2}, \tag{3}$$

where the decay widths Γ_+ and Γ_- are given by

$$\Gamma_+ = \frac{8p_2^+ p_2^- p_3^+ (p_3^-)^2 \, e^{-2S_3 - as^2}}{(p_2^+ + p_2^-)^2 \, [(p_3^+)^2 + (p_3^-)^2] q_0 q_1}, \quad \Gamma_- = \frac{2p_1^+ p_1^- \, e^{-2S_1}}{[(p_1^+)^2 + (p_1^-)^2]\tau_1}, \quad a = \frac{p_2^+ t_{01}}{q_0}. \tag{4}$$

To save space, we will not write out the expresion for $\widetilde{E}_0$. An analytic expression for T can be found easily in the case in which equation of motion (1) can be integrated in quadrature in the vacuum, e.g., in the case in which the potential V is spherically symmetric and independent of ρ. In the simple model of a uniform barrier, with $p_0 = p_1^+ = p_2^+ = p_2^- = p_3^-$, we have $q_0 = R^{-1} z_3 + 1$, $q_1 = z_3$, $a = p_0 (R + z_3)^{-1}$. In this case, the result in (3), (4) in the limit $R = \infty$ follows from the theory of Ref. 10. It can be shown directly that the transparency in (3) does not depend on the direction which we select for the incident wave. This conclusion is also demonstrated by the symmetry of expression (3).

If we have $\Gamma_+ < \Gamma_-$ at $s = 0$, the penetrability of the barrier as a function of the horizontal coordinates of the microscopic protuberance has a maximum above the defect, at the point $s = 0$. In the opposite case, $\Gamma_+ > \Gamma_-$, in which the microscopic protuberance and the defect lie close to the film surface, the point $s = 0$ corresponds to a local minimum of the penetrability (the maximum transparency now on the circle $s =$ const, defined by the equality $\Gamma_+ = \Gamma$).

In a scanning tunneling microscope with the feedback which is ordinarily used, which tracks a level of constant current $j = \int F(E) D(E) dE$ [$F(E)$ as expressed in terms of the electron state density and a Fermi distribution function[11]], as the sharp point moves in from a region far from the defect it passes over the defect into the region with $\Gamma_+ < \Gamma_-$. Part of the region $\Gamma_+ > \Gamma_-$ may be unstable. At sufficiently small values of Γ_+, Γ_-, and the shift of the level $\widetilde{E}_0$, the function $F(E)$ can be taken through the integral sign, and we find $j = \pi F(\widetilde{E}_0) \Gamma_+ \Gamma_- (\Gamma_+ + \Gamma)^{-1}$. In this case, the condition for a constant current takes the form $\Gamma_+ =$ const. Also using (4), we find an expression which determines the path, $z_3(s)$, traced out by the tip of the sharp point of the scanning tunneling microscope in a small region above the defect—an expression which is independent of the temperature and the state density of the electrons—where in S_3 it is necessary to allow for the z_3 dependence of V, which keeps the applied voltage constant. For the model of a uniform barrier, the radius of curvature of path (5) at the tip is $d = R + z_3$. The expressions derived here could easily be corrected to allow for the differences in the effective masses in the different regions.

The method of detecting the jumps of electrons which are filling and leaving a defect (as the temperature is lowered, these jumps become significantly less frequent[12]) and also the method of inelastic tunneling spectroscopy for scanning tunneling microscopy[13] would in principle make it possible to observe this effect and to study it to some extent. A study of resonant tunneling would supplement these methods and would make it possible to obtain new information about a defect.

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[1)]At $z>z_3$ we assume $V(z,\rho)=0$.

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