Physica E 59 (2014) 133–138

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Tunneling of Bloch electrons through a small-size contact

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HIGHLIGHTS

- A tunneling of Bloch waves through a contact of small diameter is studied.
- We use an inhomogeneous tunnel barrier of low transparency to describe the contact.
- The electron tunneling from the bulk-mode states into the surface states is studied.
- An asymptotically exact expression is derived for the conductance of the system.
- Prospects for the application of the results to the theory of STM are discussed.

ARTICLE INFO

Article history:
Received 16 September 2013
Received in revised form
19 December 2013
Accepted 7 January 2014
Available online 15 January 2014

Keywords:
STM
Bloch waves
Tunneling
Surface states
Local density of states
Conductance

ABSTRACT

For the first time the tunneling of Bloch waves through a contact of small diameter is studied in the framework of a model of an inhomogeneous tunnel δ-barrier of low transparency. The electron tunneling from bulk-mode states into the surface states localized near the contact interface is considered. An asymptotically exact expression (in the inverse height of the barrier) is derived for the conductance of the system. Prospects for the application of the obtained results to the theory of scanning tunneling microscopy are discussed.

1. Introduction

Currently the scanning tunneling microscope (STM) [1] is one of the most effective tools for characterization of conducting surfaces [2,3]. The theory of STM is addressed in a vast number of papers (for instance, see reviews [4,5]) that may be split into two groups: the works of the first group deal with the first principles calculations. They take into account the real crystal structure of the conductors and the particular shape of the STM-tip, ultimately providing the most detailed description of the experiment (see review [6] and cited literature). The main disadvantage of the above approach is the necessity of performing rather cumbersome numerical calculations for every given tip – sample pair.

The theories of the second group are based on somewhat simplified models of the tunnel barrier and on certain general assumptions about the electron wave functions. Like the theories of the first group they are frequently used for interpretation of the experimental results. In this case the standard tunnel effect theory approach yields the analytical representation for the current–voltage characteristics of the contact that provides their explicit functional dependences on physical parameters. The latter makes such an approach advantageous in terms of applicability to a wider range of problems.

One of the earliest and perhaps still the most popular theories of STM is the one by Tersoff and Hamann (TH) [7]. Their theoretical analysis of the tunnel current is based on Bardeen's approximation [8] where a tunneling matrix element is calculated using the wave functions within the barrier region for stand-alone individual electrodes. The authors [7] found that the STM conductance G is proportional to the electronic local density of states (LDOS) $\rho(\mathbf{r}, \varepsilon)$ at point $\mathbf{r}_0$ which represents the center of curvature of the contact (see. Fig. 1(a) following Bardeen's approximation [8] Chen had shown [9] that for more complex (non s-wave) symmetry of the wave function of the STM-tip the conductance G depends on derivatives of $\rho(\mathbf{r}, \varepsilon)$ with respect to the coordinates at the point $\mathbf{r}_0$.

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http://dx.doi.org/10.1016/j.physe.2014.01.008

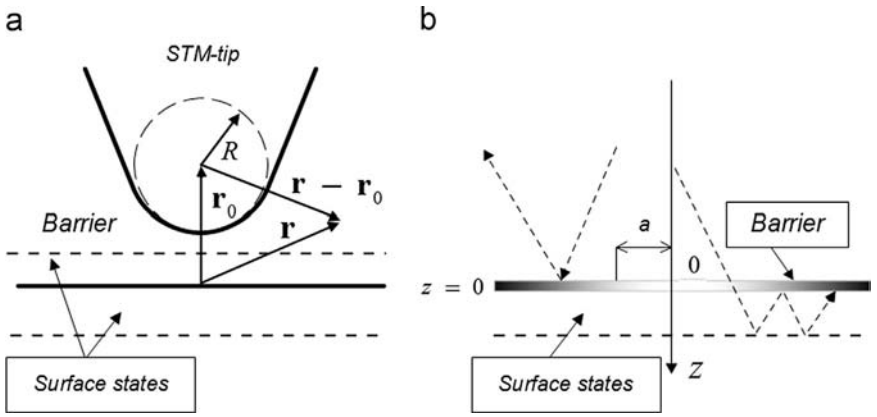

Fig. 1. (a) The model used by Tersoff and Hamman [7] to describe spatially inhomogeneous tunnel barrier in STM experiments. (b) Our model for the system containing an STM-tip and a sample, which exhibit Shockley-like surface states. The classical trajectories for transmitted and reflected electrons are shown by dashed arrows.

Experimental results demonstrate good qualitative agreement between the STM-images and the theoretical LDOS [7,9]. This provides an experimental justification for applying the formulas for the conductance G derived in the framework of the TH model and its modifications leaving existing discrepancies at the background. Nevertheless, this question cannot be neglected because in Bardeen's approximation [8] the wave function, which corresponds to tunneling from one electrode, does not satisfy the boundary conditions at the surface of the second conductor. As a result, the STM conductance becomes dependent on the LDOS, defined by the unperturbed wave function of the surface states at the point $\mathbf{r}_0$, which belongs to the STM-tip region (see Fig. 1a) where the solution of the Schrödinger equation which satisfies the boundary conditions at the tip – barrier region interface has a completely different form. The next question that arises in this context is about the dependence of the STM conductance on the contact size. It is obvious that at quite large radius R of the tip certain image "blurring" occurs (formally, in the limit of infinite contact radius, the conductance depends on the surface density of states averaged over the entire contact plane) which is absent in the TH theory [7]. Progress towards answering the above questions may result in alternative approaches to the problem.

In order to describe the STM experiments the model of an inhomogeneous infinitely thin tunnel barrier (Fig. 1b) was proposed [10], that later was considered in several theoretical papers [11–13]. A significant simplification of this model, as compared with the TH model, is in replacement of the three-dimensional inhomogeneous tunnel barrier by a two-dimensional one. Accordingly, in the two-dimensional model of the barrier there are no parameters characterizing the contact's shape that is mostly unknown. The obvious advantage of this model is in possibility of getting a consistent solution of the problem and finding the asymptotically exact wave function for transmitted electrons, which satisfies all the necessary boundary conditions.

In several papers (see a review [14]) the model of an inhomogeneous δ-barrier was used to describe the effect of single subsurface defect on the conductance measured by STM.

The conductance of the contact was analyzed theoretically [15] within the approximation of free electrons with quadratic anisotropic dispersion law.

In the present paper we consider for the first time the problem of a Bloch electron tunneling through an inhomogeneous δ-barrier from bulk-like states, which do not decay with distance from a boundary, into surface Shockley-like states [16]. An asymptotically exact (in the inverse amplitude of the barrier) formula for the conductance of the system is derived. Prospects for the application of the obtained results to the theory of scanning tunneling microscopy are discussed. It is found that the reason of the STM-image blurring is not only in the finite size of the tunneling area, but also in the diffraction of the electron waves in the contact area. The conditions under which the local density of states may be directly found from the STM conductance are formulated. It is shown that if the tunneling occurs into/from the bulk-like states, the proportionality of the conductance to the LDOS does not hold.

2. Model and the problem formulation

The model used for the solution of the problem is presented in Fig. 1b. We describe the inhomogeneous infinitely thin tunnel barrier by the potential [11]:

$$U(\mathbf{r}) = U_0 f(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\delta(z), \tag{2.1}$$

where $f(\boldsymbol{\rho})$ is an arbitrary function of two-dimensional vector $\boldsymbol{\rho}=(x,y)$, and it satisfies the following condition [11]:

$$f(\boldsymbol{\rho}) = \begin{cases} \sim 1, & \rho \lesssim a; \\ \to\infty, & \rho \gg a. \end{cases} \tag{2.2}$$

The parameter a plays the role of an effective contact radius in the plane $z=0$ with the center at the point $\boldsymbol{\rho}=\boldsymbol{\rho}_0$. We will assume further that this value is less than the electron Fermi wavelength $\lambda_F (a \le \lambda_F)$, and is much less than the length of localization of surface states.

The Schrödinger equation for the "surface states" is written in the following form [17]:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + W^{(\pm)}(\boldsymbol{\rho},z) + V_s(z)\Theta(z)\right)\psi^{(\pm)}(\mathbf{r}) = \varepsilon\psi^{(\pm)}(\mathbf{r}), \tag{2.3}$$

where ε and m are the electron mass and the energy respectively, $W^{(\pm)}(\boldsymbol{\rho},z)$ is a periodic function in $\boldsymbol{\rho}$ with the period of the two-dimensional "surface" lattice in the half-spaces $z>0$ and $z<0$, $V_s(z)$ is the potential that defines the appearance of bound (surface) state at $z>0$ near the interface. Here and below the upper index $(\pm)$ signifies that an appropriate function belongs to half-space $z \gtrless 0$ or $z \lessgtr 0$. The wave function $\psi^{(\pm)}(\mathbf{r})$ satisfies the boundary conditions

$$\psi^{(+)}(\boldsymbol{\rho},+0) = \psi^{(-)}(\boldsymbol{\rho},-0); \tag{2.4}$$

$$\psi_z^{(+)\prime}(\boldsymbol{\rho},+0) - \psi_z^{(-)\prime}(\boldsymbol{\rho},-0) = \frac{2m}{\hbar^2}U_0 f(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\psi^{(\pm)}(\boldsymbol{\rho},0). \tag{2.5}$$

The particular form of the boundary conditions at $\pm\infty$ depends on the formulation of the problem of electron tunneling.

For clarity let us consider an electron wave ψ_{inc} which is incident on the tunnel barrier (2.1) from the region $z<0$. This wave ψ_{inc} is almost entirely reflected by the interface $z=0$ except a

small region of radius a near the point $\mathbf{r}=0$. The tunneling through this region causes the existence of a transmitted wave ψ_{tr} in the potential well at $z>0$. In this case at large distances from the contact $|\mathbf{r}|\gg a$, $z<0$ the wave function ψ_{inc} has to be a Bloch wave for half- space $\psi_0^{(-)}(\boldsymbol{\rho},z)$ [18,19].

$$\psi^{(-)}(\boldsymbol{\rho},z)\to\psi_0^{(-)}(\boldsymbol{\rho},z),\quad \mathbf{r}\to-\infty; \tag{2.6}$$

where

$$\psi_0^{(-)}(\boldsymbol{\rho},z)=\sqrt{\frac{1}{\Omega}}\sum_{\mathbf{G}}F_{\mathbf{G}}(\boldsymbol{\kappa},k_z;z)\exp[i(\boldsymbol{\kappa}+\mathbf{G})\boldsymbol{\rho}],\quad z\le 0, \tag{2.7}$$

$\boldsymbol{\kappa}$ and k_z are tangential and perpendicular to the boundary components of the electron wave vector [17], $\mathbf{k}$, $\mathbf{G}$ are two-dimensional reciprocal lattice vectors lying in the planes parallel to the contact plane; n represents band index, $\Omega=L_xL_y(L_z/2)$ is the volume of the region $z<0$ of our system, linear sizes of which $L_{x,y,z}\to\infty$ we assume to be much larger than any length parameter of the problem. We will use the extended zone scheme. For simplification of formulas we do not write the spin indexes. The function (2.7) is a standing Bloch wave and it satisfies the zero boundary condition at $z=0$,

$$\psi_0^{(-)}(\boldsymbol{\rho},z=0)=0, \tag{2.8}$$

and the normalization condition

$$\int_{\Omega}d\mathbf{r}\Theta(-z)|\psi_0^{(-)}(\mathbf{r})|^2=1 \tag{2.9}$$

The dependence on z coordinate of the coefficients $F_{\mathbf{G}}(\boldsymbol{\kappa},k_z;z)$ in the expansion (2.6) reflects the existence of the periodic lattice potential in z-direction in the half-space $z<0$. The equation for functions $F_{\mathbf{G}}(\boldsymbol{\kappa},k_z;z)$ can be obtained easily by substitution of the expression (2.6) for the wave function in the primary Schrödinger equation [18]

$$-\frac{\hbar^2}{2m}\frac{\partial^2F_{\mathbf{G}}}{\partial z^2}+\frac{\hbar^2}{2m}(\boldsymbol{\kappa}+\mathbf{G})^2F_{\mathbf{G}}+\sum_{\mathbf{g}}w(\mathbf{G}-\mathbf{g},z)F_g=\varepsilon^{(-)}F_{\mathbf{G}}; \tag{2.10}$$

where $w(\mathbf{g},z)$ is the Fourier transform of the function $W(\boldsymbol{\rho},z)$. The function $F_{\mathbf{G}}(\boldsymbol{\kappa},k_z;z)$ satisfies the boundary condition

$$F_{\mathbf{G}}(\boldsymbol{\kappa},k_z;0)=0, \tag{2.11}$$

and it corresponds to the zero total charge flow through any plane $z=const$ parallel to the interface

$$\begin{aligned}J&=\frac{|e|\hbar}{m}\int_S d\boldsymbol{\rho}\mathrm{Im}(\psi_0^{(-)*}(\boldsymbol{\rho},z)\psi_{0z}^{(-)\prime}(\boldsymbol{\rho},z))\\&=\frac{|e|\hbar}{m}\mathrm{Im}\sum_{\mathbf{G}}F_{\mathbf{G}}^*(\boldsymbol{\kappa},k_z;z)F_{\mathbf{G}z}'(\boldsymbol{\kappa},k_z;z)=0.\end{aligned} \tag{2.12}$$

where $S=L_xL_y$, and $L_{x,y}\to\infty$.

The amplitude of the transmitted wave ψ_{tr} vanishes far from the contact as a result of the effect of flow spreading at $\boldsymbol{\rho}\to\infty$ and the exponential damping of the wave function at classically inaccessible region at $z\to\infty$

$$\psi_{tr}^{(+)}(\rho,z)\to 0,\quad \mathbf{r}\to\infty. \tag{2.13}$$

Knowing the wave functions of transmitted electrons, one can calculate the charge current flow through the interface $z=0$ parallel to the z axis

$$J_z(\mathbf{k})=\frac{|e|\hbar}{mU_0^2}\mathrm{Im}(\psi_1^{(+)*}(\boldsymbol{\rho},0)\psi_{1z}^{(+)\prime}(\boldsymbol{\rho},+0)). \tag{2.14}$$

At zero temperature for the calculation of the total tunnel current it is enough to know the density of charge flow in one direction only. The sign of the applied voltage V corresponds to the possibility of electron tunneling from occupied states of the half-space $z\le 0$ into free states in the half-space $z\ge 0$ (Fig. 2).

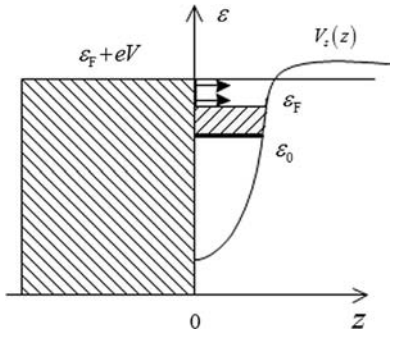

Fig. 2. Illustration of the tunneling process. The bias eV, applied to the tip, makes possible the electron transport from the bulk-type states to the surface Shockley-type ones.

In the case of low transparency of the barrier, the latter causes the main drop of the electrical potential $V(\boldsymbol{\rho},z)$ [14]. We assume that $V(\boldsymbol{\rho},z<0)=V=const$, and $V(\boldsymbol{\rho},z>0)=0$. The conductance will be calculated in the linear in V approximation (Ohm's law approximation). It is true if $|eV|\ll\varepsilon_F$ (the Fermi energy is the same in both half-spaces). Accordingly it is enough to know the wave function at $V=0$.

We also neglect possible scattering processes in the region of electrical current spreading (the size of this region is of the order of the contact radius a) and presume an infinite electron mean free path. Under these assumptions, the formula for the tunnel current can be derived by integration of the flux (2.14) with respect to the incident momentum direction for the electrons with the Fermi energy, and by integration over $\boldsymbol{\rho}$ in the plane $z=0$[10]:

$$I=2eV\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\int_S d\boldsymbol{\rho}\Theta(v_z)J_z(\mathbf{k})\delta(\varepsilon_F-\varepsilon^{(-)}(\mathbf{k})), \tag{2.15}$$

where $\varepsilon=\varepsilon^{(-)}(\boldsymbol{\kappa},k_z)$ is the energy eigenvalue corresponding to the solution (2.7) of the Eq. (2.3), $v_z=\partial\varepsilon^{(-)}/\hbar\partial k_z$ is the electron velocity in the direction that is perpendicular to the interface The wave vector $\mathbf{k}$ belongs to the electron in the half-space $z<0$.

3. Asymptotic solution of Schrödinger equation for low transparency of tunnel barrier

Let us examine the solution of Eq. (2.3) by expanding in the small-parameter $1/U_0$ and taking into account only the lowest order corrections, which are proportional to $1/U_0$. The wave function ψ_{tr} of electrons transmitted through the barrier from the half-space $z<0$ into the half-space $z>0$ can be written in the form

$$\psi_{tr}^{(+)}(\rho,z)=\frac{1}{U_0}\psi_1^{(+)}(\rho,z),\quad z\ge 0, \tag{3.1}$$

which is non-zero only in the first approximation in $1/U_0$. The trial wave function $\psi^{(-)}(\boldsymbol{\rho},z)$ in the half-space $z<0$ we use is [15]:

$$\psi^{(-)}(\rho,z)=\psi_0^{(-)}(\rho,z)+\frac{1}{U_0}\psi_1^{(-)}(\rho,z), \tag{3.2}$$

where the second summand describes the perturbation of the standing wave (2.7) caused by the finite probability of tunneling through the contact. As a result of the boundary condition (2.6) the second summand in Eq. (3.2) vanishes at $\mathbf{r}\to-\infty$.

Substituting the expansions (3.1) and (3.2) in boundary conditions (2.4) and (2.5) and equating the terms of the same order in $1/U_0$ we get

$$\psi_1^{(-)}(\boldsymbol{\rho},-0)=\psi_1^{(+)}(\boldsymbol{\rho},+0) \tag{3.3}$$

$$-\psi_{0z}^{(-)\prime}(\boldsymbol{\rho},-0)=\frac{2m}{\hbar^2}f(\boldsymbol{\rho}-\boldsymbol{\rho}_0)\psi_1^{(\pm)}(\boldsymbol{\rho},0). \tag{3.4}$$

In the simplified boundary condition (3.4), which is obtained in zero approximation in $1/U_0$ the derivative of the wave function transmitted into the region $z>0$ $\psi_{tr}^{(+)}(\boldsymbol{\rho},z)=\frac{1}{U_0}\psi_1^{(+)}(\boldsymbol{\rho},z)$ is omitted, being negligible in comparison with the remaining terms. The derivative $\psi_{0z}^{(-)\prime}(\boldsymbol{\rho},-0)$ can be easily found from Eq. (2.6). The formula for the wave function of transmitted electron takes the form

$$\psi_1^{(+)}(\boldsymbol{\rho},0)=-\frac{\hbar^2}{2mf(\boldsymbol{\rho}-\boldsymbol{\rho}_0)}\psi_{0z}^{(-)\prime}(\boldsymbol{\rho},0), \tag{3.5}$$

where

$$\psi_{0z}^{(-)\prime}(\boldsymbol{\rho},0)=\sqrt{\frac{1}{\Omega}}\sum_{\mathbf{G}}F'_{\mathbf{G}z}(\boldsymbol{\kappa},k_z;0)\exp[i(\boldsymbol{\kappa}+\mathbf{G})\boldsymbol{\rho}],\quad k_z>0. \tag{3.6}$$

In order to find the wave function of the electrons that are transmitted into surface states we make the following additional assumption. We neglect any changes in the lattice potential in the direction normal to the interface at the characteristic length λ_s of the surface state damping and approximately take $W^{(+)}(\boldsymbol{\rho},z)\approx W^{(+)}(\boldsymbol{\rho},0)$.

Eq. (3.5) reduces the problem of finding the wave function $\psi_1^{(+)}(\boldsymbol{\rho},z)$ of the transmitted electrons to a solution of the simplified Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2+W^{(+)}(\boldsymbol{\rho},0)+V_s(z)\right)\psi_1^{(+)}(\boldsymbol{\rho},z)=\varepsilon\psi_1^{(+)}(\boldsymbol{\rho},z),\quad z\geq 0, \tag{3.7}$$

with the given value $\psi_1^{(+)}(\boldsymbol{\rho},0)$ at the interface $z=0$ (3.5). Note that in spite of the substantial simplification made the variables in Eq. (3.7) cannot be separated because of the dependence of the wave function values on coordinate $\boldsymbol{\rho}$ at the interface $z=0$. We expand the function $\psi_1^{(+)}(\boldsymbol{\rho},z)$ as an integral

$$\psi_1^{(+)}(\boldsymbol{\rho},z;\boldsymbol{\kappa},k_z)=\frac{S}{(2\pi)^2}\int d\boldsymbol{\kappa}'\Psi_1(\boldsymbol{\kappa}',z;\boldsymbol{\kappa},k_z)\psi_s^{(+)}(\boldsymbol{\rho};\boldsymbol{\kappa}'). \tag{3.8}$$

In (3.8) the two-dimensional Bloch wave functions are used as a basis. Vector $\boldsymbol{\kappa}'$ runs through all vectors in 2D first Brillouin zone

$$\psi_s^{(+)}(\boldsymbol{\rho};\boldsymbol{\kappa})=\frac{1}{\sqrt{S}}\sum_{\mathbf{G}}f_{\mathbf{G}}(\boldsymbol{\kappa})\exp[i(\boldsymbol{\kappa}+\mathbf{G})\boldsymbol{\rho}]. \tag{3.9}$$

The functions (3.9) are orthonormal. Coefficients $f_{\mathbf{G}}(\boldsymbol{\kappa})$ of the expansion satisfy the equation

$$\frac{\hbar^2}{2m}(\boldsymbol{\kappa}+\mathbf{G})^2f_{\mathbf{G}}(\boldsymbol{\kappa})+\sum_{\mathbf{g}}\tilde{w}(\mathbf{G}-\mathbf{g})f_{\mathbf{g}}(\boldsymbol{\kappa})=\varepsilon_{\parallel}^{(+)}f_{\mathbf{G}}(\boldsymbol{\kappa}); \tag{3.10}$$

where $\tilde{w}(\mathbf{g})$ is the Fourier transform of the function $W(\boldsymbol{\rho},0)$, and $\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa})$ is the energy of motion in the plane parallel to the interface.

Substituting the expansion (3.8) to the Schrödinger Eq. (3.7), we find the equation for the coefficients $\Psi_1(\boldsymbol{\kappa}',z;\boldsymbol{\kappa},k_z)$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1}{\partial z^2}+V_s(z)\Psi_1=\varepsilon_{\perp}\Psi_1, \tag{3.11}$$

where $\varepsilon_{\perp}=\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')$. The inverse transform of Eq. (3.8) and the boundary condition (3.5) at $z=0$ give a "boundary condition" for the function $\Psi_1(\boldsymbol{\kappa}',z;\boldsymbol{\kappa},k_z)$,

$$\Psi_1(\boldsymbol{\kappa}',0;\boldsymbol{\kappa},k_z)=-\frac{\hbar^2}{2m}\int_S\frac{d\boldsymbol{\rho}'}{f(\boldsymbol{\rho}'-\boldsymbol{\rho}_0)}\psi_{0z}^{(-)\prime}(\boldsymbol{\rho}',0;\boldsymbol{\kappa},k_z)\psi_s^{(+)*}(\boldsymbol{\rho}';\boldsymbol{\kappa}'). \tag{3.12}$$

In accordance with the boundary condition (2.13) at $z\to\infty$ the function $\Psi_1(\boldsymbol{\kappa}',z;\boldsymbol{\kappa},k_z)$ must satisfy the following condition

$$\Psi_1(\boldsymbol{\kappa}',z\to\infty;\boldsymbol{\kappa},k_z)\to 0. \tag{3.13}$$

The particular form of a solution of the Eq. (3.11), which satisfies the boundary conditions (3.12) and (3.13) depends on the potential $V_s(z)$, which for realistic models has a complex form (see, for example, [20]). In what follows we are not going to define in detail the functional form of $V_s(z)$ in Eq. (3.11). We limit ourselves to a more general assumption such that there is only one discrete energy level $\varepsilon_{\perp}=\varepsilon_0$ in the potential well at $U_0\to\infty$ in the energy range of interest, $\varepsilon\leq\varepsilon_F$, where ε_F is the Fermi energy (Fig. 2).

Thus let us write the solution of Eq. (3.11) as

$$\Psi_1(\boldsymbol{\kappa}',z;\boldsymbol{\kappa},k_z)=C(\boldsymbol{\kappa}';\boldsymbol{\kappa},k_z)\chi(z;\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')), \tag{3.14}$$

where the function $\chi(z;\varepsilon_{\perp})$ vanishes at $z\to\infty$. The wave function of the bounded (surface) state in the one-dimensional potential well formed by the potential $V_s(z)$ and the infinite wall at $z\leq 0$ satisfy the boundary condition

$$\chi(0,\varepsilon_0)=0,\quad \chi(z\to\infty,\varepsilon_0)\to 0, \tag{3.15}$$

and also the normalization condition

$$\int_0^{\infty}dz\chi^2(z,\varepsilon_0)=1. \tag{3.16}$$

Substituting the Eq. (3.14) in the boundary condition (3.12), we obtain the equation for the coefficient $C(\boldsymbol{\kappa}';\boldsymbol{\kappa},k_z)$

$$C(\boldsymbol{\kappa}';\boldsymbol{\kappa},k_z)\chi(0;\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}'))=-\frac{\hbar^2}{2m}\int_S\frac{d\boldsymbol{\rho}'}{f(\boldsymbol{\rho}'-\boldsymbol{\rho}_0)}\psi_{0z}^{(-)\prime}(\boldsymbol{\rho}',0;\boldsymbol{\kappa},k_z)\psi_s^{(+)*}(\boldsymbol{\rho}';\boldsymbol{\kappa}'). \tag{3.17}$$

This equation is valid for all $\boldsymbol{\kappa}'$ with the exception of a single point, at which $\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')=\varepsilon_0$, and the solution $\chi(z,\varepsilon_0)=0$ in accordance with the condition (3.15). In order to avoid the divergence that appears as a result of division by $\chi(0;\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}'))$ which in fact has no physical meaning we employ a standard approach of the mathematical physics (see for example [21]). We introduce an infinitesimal damping of energy levels by means of substitution $\varepsilon\to\varepsilon-i\gamma$. Then the wave function which is the inverse transform (3.8) of the solution Ψ_1 (3.14) can be presented as the limit

$$\psi_1^{(+)}(\boldsymbol{\rho},z;\boldsymbol{\kappa},k_z)=-\tfrac{\hbar^2}{2m}\lim_{\gamma\to 0}\int_S\tfrac{d\boldsymbol{\rho}'}{f(\boldsymbol{\rho}'-\boldsymbol{\rho}_0)}\psi_{0z}^{(-)\prime}(\boldsymbol{\rho}',0;\boldsymbol{\kappa},k_z)\times$$

$$\int d\boldsymbol{\kappa}'\psi_s^{(+)*}(\boldsymbol{\rho}';\boldsymbol{\kappa}')\psi_s^{(+)}(\boldsymbol{\rho};\boldsymbol{\kappa}')\frac{\chi(z,\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')-i\gamma)}{\chi(0,\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')-i\gamma)}, \tag{3.18}$$

It is easily to note that as the result of orthogonality of the functions $\psi_s^{(+)}(\boldsymbol{\rho};\boldsymbol{\kappa}')$ at $z=0$ formula (3.18) transforms itself into (3.5).

4. Conductance of the system

Substituting the function $\psi_1(\boldsymbol{\rho},z)$ (3.18) and its derivative at $z=+0$ in (2.15), one obtains the following formula for the conductance of the system $G=I/V$

$$G(\boldsymbol{\rho}_0)=\frac{e^2\hbar^5}{2m^3U_0^2}\mathrm{Im}\int_S\frac{d\boldsymbol{\rho}}{f(\boldsymbol{\rho}-\boldsymbol{\rho}_0)}\int_S\frac{d\boldsymbol{\rho}'}{f(\boldsymbol{\rho}'-\boldsymbol{\rho}_0)}D^{(-)}(\varepsilon_F;\boldsymbol{\rho},\boldsymbol{\rho}')D^{(+)}(\varepsilon_F;\boldsymbol{\rho},\boldsymbol{\rho}'), \tag{4.1}$$

where

$$D^{(-)}(\varepsilon_F;\boldsymbol{\rho},\boldsymbol{\rho}')=\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\Theta(v_z)\psi_{0z}^{(-)\prime *}(\boldsymbol{\rho},0;\mathbf{k})\psi_{0z}^{(-)\prime}(\boldsymbol{\rho}',0;\mathbf{k})\delta(\varepsilon^{(-)}(\mathbf{k})-\varepsilon_F), \tag{4.2}$$

$$D^{(+)}(\varepsilon_F;\boldsymbol{\rho},\boldsymbol{\rho}')=\lim_{\gamma\to 0}\frac{S}{(2\pi)^2}\int d\boldsymbol{\kappa}'\psi_s^{(+)*}(\boldsymbol{\rho}';\boldsymbol{\kappa}')\psi_s^{(+)}(\boldsymbol{\rho};\boldsymbol{\kappa}')\frac{\chi(z,\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')-i\gamma)}{\chi(0,\varepsilon-\varepsilon_{\parallel}^{(+)}(\boldsymbol{\kappa}')-i\gamma)}. \tag{4.3}$$

Note, that interchanging the integration variables $\boldsymbol{\rho}\rightleftarrows\boldsymbol{\rho}'$ formally corresponds to the complex conjugation of functions $\psi_s^{(+)}$ and $\psi_{0z}^{(-)\prime}$ in the Eqs. (4.2) and (4.3). Therefore the imaginary part

of the integrand in Eq. (4.3) is defined by the existence of a pole $\varepsilon_{\parallel} = \varepsilon_F - \varepsilon_0 + i\gamma$ of the integrand at $\chi(0,\varepsilon_0) = 0$ which matches the discrete energy level $\varepsilon_{\perp} = \varepsilon_0$ in the potential well $V_s(z)$ with an infinite potential wall at $z = 0$.

To perform the integration in Eq. (4.3) it is necessary to know the explicit form of the wave functions. However in order to determine its imaginary part it is possible to exploit more general considerations. If an analytical function $\chi(\varepsilon)$ has a simple zero $\varepsilon = \varepsilon_0$ only, it can always be presented in the form $\chi(\varepsilon) = (\varepsilon - \varepsilon_0)X(\varepsilon)$ and $X(\varepsilon) \neq 0$, were $X(\varepsilon_0) = \chi'_{\varepsilon}(\varepsilon_0)$ [22]. Applying the well-known symbolic relation [23]

$$\lim_{\gamma \to 0} \frac{1}{\varepsilon - i\gamma} = V.p.\frac{1}{\varepsilon} + i\pi\delta(\varepsilon) \tag{4.4}$$

we obtain

$$\begin{aligned} &\mathrm{Im}\, D^{(+)}(\varepsilon_F; \boldsymbol{\rho}, \boldsymbol{\rho}') = \tfrac{\pi S}{(2\pi)^2} \tfrac{\chi'_z(0,\varepsilon_0)}{\chi'_{\varepsilon}(0,\varepsilon_0)} \int d\boldsymbol{\kappa}' \times \\ &\psi_s^{(+)*}(\boldsymbol{\rho}'; \boldsymbol{\kappa}') \psi_s^{(+)}(\boldsymbol{\rho}; \boldsymbol{\kappa}') \delta(\varepsilon^{(+)}(\boldsymbol{\kappa}') + \varepsilon_0 - \varepsilon_F). \end{aligned} \tag{4.5}$$

By using the properties of the Wronskian of one-dimensional Schrödinger equation (see, for example, [24]), the boundary and normalization conditions (3.15) and (3.16), one can find the relation

$$\chi'_z(0,\varepsilon_0)\chi'_{\varepsilon}(0,\varepsilon_0) = \frac{2m}{\hbar^2}, \tag{4.6}$$

connecting the derivatives in energy and in coordinate at the interface. Substituting Eqs. (4.5) and (4.6) in the Eq. (4.1) we finally get

$$\begin{aligned} &G(\boldsymbol{\rho}_0) = \tfrac{\pi e^2 \hbar^5}{m^2 U_0^2} (\chi'_z(0,\varepsilon_0))^2 \int_S \tfrac{d\boldsymbol{\rho}}{f(\boldsymbol{\rho} - \boldsymbol{\rho}_0)} \int_S \tfrac{d\boldsymbol{\rho}'}{f(\boldsymbol{\rho}' - \boldsymbol{\rho}_0)} \\ &\rho_s^{(+)}(\varepsilon_F - \varepsilon_0; \boldsymbol{\rho}, \boldsymbol{\rho}') \tilde{\rho}_v^{(-)}(\varepsilon_F; \boldsymbol{\rho}, \boldsymbol{\rho}'), \end{aligned} \tag{4.7}$$

where

$$\begin{aligned} &\tilde{\rho}_v^{(-)}(\varepsilon_F; \boldsymbol{\rho}, \boldsymbol{\rho}') = \tfrac{\Omega}{(2\pi)^3} \tfrac{\hbar^2}{m^2} \int d\mathbf{k} \Theta(v_z) \times \\ &\psi_{0z}^{(-)*}(\boldsymbol{\rho}, 0; \mathbf{k}) \psi_{0z}^{(-)\prime}(\boldsymbol{\rho}', 0; \mathbf{k}) \delta(\varepsilon^{(-)}(\mathbf{k}) - \varepsilon_F), \end{aligned} \tag{4.8}$$

$$\begin{aligned} &\rho_s^{(+)}(\varepsilon_F - \varepsilon_0; \boldsymbol{\rho}, \boldsymbol{\rho}') = \tfrac{S}{(2\pi)^2} \int d\boldsymbol{\kappa}' \times \\ &\psi_s^{(+)*}(\boldsymbol{\rho}'; \boldsymbol{\kappa}') \psi_s^{(+)}(\boldsymbol{\rho}; \boldsymbol{\kappa}') \delta(\varepsilon^{(+)}(\boldsymbol{\kappa}') + \varepsilon_0 - \varepsilon_F). \end{aligned} \tag{4.9}$$

If $\boldsymbol{\kappa}\boldsymbol{\rho} < k_F a \ll 1$ then we can neglect the coordinate dependence of the functions $\psi_s(\boldsymbol{\rho}, \boldsymbol{\kappa})$ by taking their values at the center of the contact $\boldsymbol{\rho} = \boldsymbol{\rho}' = \boldsymbol{\rho}_0$, and as a result the equation for the conductance takes the form:

$$G(\boldsymbol{\rho}_0) = \frac{\pi e^2 \hbar^5 S_{eff}^2}{2m^2 U_0^2} (\chi'_z(0,\varepsilon_0))^2 \rho_{2D}^{(+)}(\varepsilon_F - \varepsilon_0; \boldsymbol{\rho}_0) \tilde{\rho}_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0) \tag{4.10}$$

where

$$S_{eff} = \int_S \frac{d\boldsymbol{\rho}}{f(\boldsymbol{\rho})} \simeq \pi a^2, \tag{4.11}$$

is the effective cross sectional area of the contact, and

$$\rho_{2D}^{(+)}(\varepsilon, \boldsymbol{\rho}_0) = \rho_s^{(+)}(\varepsilon, \boldsymbol{\rho}_0, \boldsymbol{\rho}_0) = \frac{S}{(2\pi)^2} \int d\boldsymbol{\kappa}' \left|\psi_s^{(+)}(\boldsymbol{\rho}_0; \boldsymbol{\kappa}')\right|^2 \delta(\varepsilon^{(+)}(\boldsymbol{\kappa}') + \varepsilon_0 - \varepsilon_F) \tag{4.12}$$

is the local density of 2D surface states.

The function $\tilde{\rho}_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0)$ differs from the local density of 3D surface states by presence of the derivative of the $\psi_0^{(-)}(\boldsymbol{\rho}_0, z; \mathbf{k})$ function with respect to z

$$\begin{aligned} &\tilde{\rho}_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0) = \rho_s^{(+)}(\varepsilon_F - \varepsilon_0; \boldsymbol{\rho}_0, \boldsymbol{\rho}_0) \\ &= \frac{\Omega}{(2\pi)^3} \frac{\hbar^2}{m^2} \int d\mathbf{k} \Theta(v_z) |\psi_{0z}^{(-)\prime}(\boldsymbol{\rho}_0, 0; \mathbf{k})|^2 \delta(\varepsilon^{(-)}(\mathbf{k}) - \varepsilon_F). \end{aligned} \tag{4.13}$$

Note that a similar result had been obtained in paper [9] for the p_z surface state at the tip. By using the boundary condition (2.8) it is easy to derive that

$$\tilde{\rho}_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0) = \frac{\hbar^2}{m^2} \left[\frac{\partial^2}{\partial z^2} \rho_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0, z)\right]_{z=0}, \tag{4.14}$$

where

$$\rho_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0, z) = \frac{\Omega}{(2\pi)^3} \int d\mathbf{k} \Theta(v_z) \left|\psi_0^{(-)}(\boldsymbol{\rho}_0, z; \mathbf{k})\right|^2 \delta(\varepsilon^{(-)}(\mathbf{k}) - \varepsilon_F), \tag{4.15}$$

is the local density of 3D surface states. An order-of-magnitude estimate of the function $\tilde{\rho}_{3D}^{(-)}$ is $\tilde{\rho}_{3D}^{(-)}(\varepsilon_F; \boldsymbol{\rho}_0) \approx v_{zF}^2 \rho_{3D}(\varepsilon_F)$, where v_{zF} is the maximum value of the electron group velocity along the z axis on the Fermi surface, and $\rho_{3D}(\varepsilon_F)$ is the bulk density of states.

5. Conclusion

Thus, in the framework of the model of an inhomogeneous barrier of arbitrary shape and large amplitude U_0 we obtained an asymptotically exact solution at $1/U_0 \to 0$ for the tunnel conductance of the system. The result (4.10) does not depend on the direction of the current in the Ohm's law approximation. In the case of electron tunneling from the surface states into the states corresponding to waves propagating from the boundary into the sample, we, naturally, get the formula (4.10).

From our results several physical conclusions can be made, which may be used for the interpretation of STM images.

(i). The blurring of the STM-image (i.e. dependence of the STM conductance on the lateral coordinates) is defined not only by the finite size of the area S_{eff} (4.11), through which the tunneling occurs. It is also defined by electron wave diffraction on the inhomogeneous barrier. As a result of this the wave function of transmitted through the barrier electrons $\psi_1^{(+)}(\boldsymbol{\rho}, z)$ (3.18) and the density of charge flow (2.14) have a nonlocal relationship with the wave function in the half-space, from which the tunneling takes place.

(ii). A local relation between the STM conductance and LDOS exists only in the case when the characteristic radius a of the region S_{eff} is much less than the Fermi wave length of the electron $\lambda\!\!\!^{-}_F = 1/k_F$. Such limitation seems to be physical by nature, because $\lambda\!\!\!^{-}_F$ is a scale of changing of the amplitude of the electron wave function.

(iii). In the case of tunneling from/into bulk states the STM conductance is **not** proportional to the density of states of the investigated sample. This result is rather obvious, and it is similar to the one obtained for a planar tunnel junction [25]. This result is a consequence of the fact that the electrical current depends on the electron velocity in the direction perpendicular to the sample surface, which is not included in the density of states. Certainly, the function (4.2) reflects the main features of the electron density of states. However, in the case of strongly anisotropic dispersion law its difference from LDOS can be quite substantial.

The above conclusions are not just formal consequences of the proposed model but reflect really existing physical factors that influence the conductivity of small-size tunnel junctions.

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