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# Tunneling of Bloch electrons through a small-size contact

N.V. Khotkevych-Sanina *, Yu. A. Kolesnichenko

*B.I. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Lenin Ave, Kharkov 61103, Ukraine*

## 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.

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## 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 $\delta$-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 $\mathbf{r}_0$.

* Corresponding author. Tel. +380 573410868.
*E-mail addresses:* khotkevych@ilt.kharkov.ua, nkhotkevych@yahoo.com (N.V. Khotkevych-Sanina).

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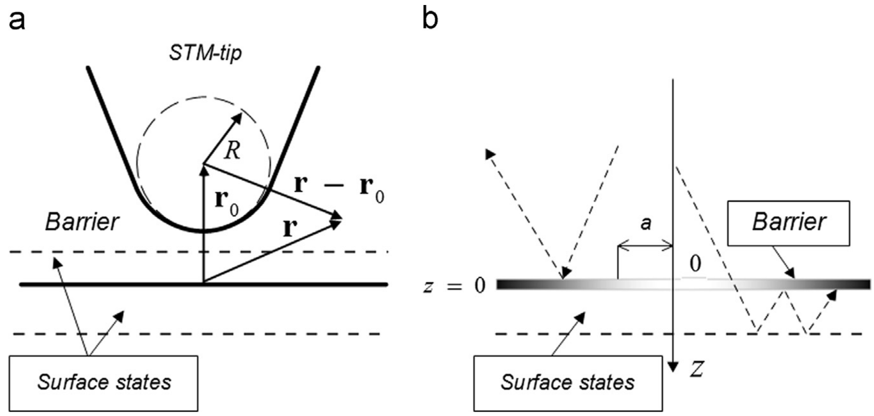


**Fig. 1.** (a) The model used by Tersoff and Hamman [7] to describe spatially inhomogeneous tunnel barrier in STM experiments. (b) Our model for the system containing an STM-tip and a sample, which exhibit Shockley-like surface states. The classical trajectories for transmitted and reflected electrons 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 $\delta$-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 $\delta$-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 $\varepsilon$ 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 $z \ge 0$ or $z \le 0$. 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 $\psi_{inc}$ which is incident on the tunnel barrier (2.1) from the region $z<0$. This wave $\psi_{inc}$ is almost entirely reflected by the interface $z=0$ except a