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# SEMICLASSICAL ASYMPTOTIC APPROXIMATIONS AND THE DENSITY OF STATES FOR THE TWO-DIMENSIONAL RADIALLY SYMMETRIC SCHRÖDINGER AND DIRAC EQUATIONS IN TUNNEL MICROSCOPY PROBLEMS

**J. Brüning,* S. Yu. Dobrokhotov,† M. I. Katsnelson,‡ and D. S. Minenkov†**

*We consider the two-dimensional stationary Schrödinger and Dirac equations in the case of radial symmetry. A radially symmetric potential simulates the tip of a scanning tunneling microscope. We construct semiclassical asymptotic forms for generalized eigenfunctions and study the local density of states that corresponds to the microscope measurements. We show that in the case of the Dirac equation, the tip distorts the measured density of states for all energies.*

**Keywords:** axially symmetric two-dimensional Schrödinger operator, axially symmetric two-dimensional Dirac operator, generalized eigenfunction, semiclassical approximation, density of states, tunnel microscopy

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## 1. Introduction

Our study is related to the question of how much the tip of a scanning tunneling microscope (STM) [1] affects the measured values. We study the influence of the potential induced by the microscope tip on the electronic states in a crystal. We consider the situation where the electron microscope tip is brought toward a two-dimensional crystal placed on the substrate. A potential difference $U_0$ is produced between the tip and the substrate, as a result of which a tunnel current arises between the tip and the crystal surface. This current is measured by the microscope and is proportional to the local density of states (LDOS)—and also to the electron density—at the point of the crystal under the tip (see [2], [3] and the references therein). At the same time, a potential $U(r)$ arises in the crystal, induced by the tip and distorting the measured LDOS. The mathematical setup of the problem is: it is required to construct semiclassical asymptotic forms for the generalized eigenfunctions of the stationary Schrödinger and Dirac equations on a plane with a radially symmetric potential $U(r)$ and to determine the LDOS at the point of maximum potential (i.e., under the tip).

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*Humboldt University, Berlin, Germany, e-mail: bruening@mathematik.hu-berlin.de.

†Institute for Problems in Mechanics, RAS, Moscow, Russia; Moscow Institute of Physics and Technology, Moscow, Russia, e-mail: dobr@ipmnet.ru, minenkov.ds@gmail.com.

‡Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands; Ural Federal University, Ekaterinburg, Russia, e-mail: M.Katsnelson@science.ru.nl.

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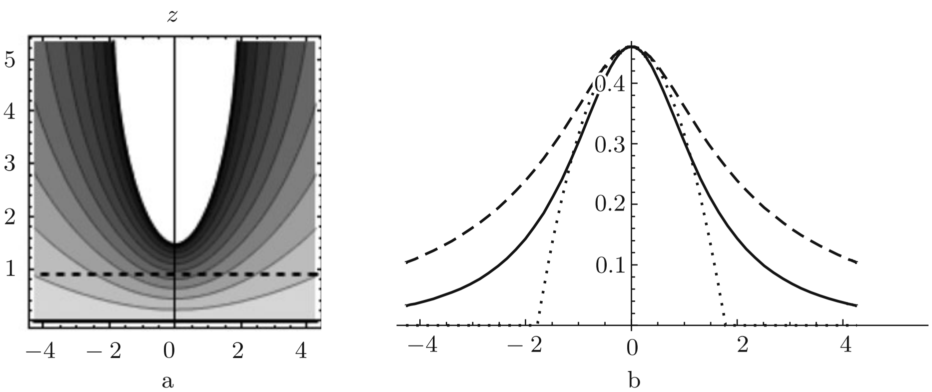


**Fig. 1**. (a) Equipotential lines of the electric field near the STM tip: the white region denotes the tip surface, the solid line $z = 0$ denotes the substrate, and the dashed line denotes the crystal surface. (b) Comparison of the potentials in the crystal induced by the tip (solid line), by a point charge (dashed line), and by a model parabolic potential (dotted line).

We consider a planar substrate and assume that the two-dimensional crystal is transparent for the field. Using the model in [4] for the electrostatic field of a tip next to a flat screen, we simulate the electric potential between the tip and the substrate, including the electrostatic potential $u(x, y, z)|_{z=z_{\mathrm{cryst}}}$ induced by the tip in the crystal (see Fig. 1). We then consider the two-dimensional Schrödinger equation in the case with a square crystal lattice or the two-dimensional Dirac equation for a crystal with a hexagonal lattice. In these equations, a radially symmetric potential $U(x, y) = q_e u(x, y, z)|_{z=z_{\mathrm{cryst}}}$ appears, induced by the microscope tip (here $q_e$ is the electron charge). We assume that the potential $U(r)$ decreases monotonically and vanishes at infinity. We assume that the mass $m(r)$ in the Dirac equation is radially symmetric and has a finite limit at infinity (not necessarily zero); for example, we can consider a constant mass.

After introducing characteristic energy and length scales $E_0$ and $L_0$, we obtain the dimensionless equations with a small (semiclassical) parameter before the derivatives. We consider the stationary Schrödinger equation

$$- h^2\Delta\psi - \big(E - U(r)\big)\psi = 0 \tag{1.1}$$

and the Dirac equation

$$\begin{pmatrix} m(r) & -ihe^{-i\varphi}\Big(\dfrac{\partial}{\partial r} - \dfrac{i}{r}\dfrac{\partial}{\partial\varphi}\Big) \\ -ihe^{i\varphi}\Big(\dfrac{\partial}{\partial r} + \dfrac{i}{r}\dfrac{\partial}{\partial\varphi}\Big) & -m(r) \end{pmatrix}\Psi - \big(E - U(r)\big)\Psi = 0, \tag{1.2}$$

where the coordinates are $x \in \mathbb{R}^2$, $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$,

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}$$

is the Laplace operator, $U(r) = U(|x|)$ is the potential, $m(r)$ is the mass, $h \ll 1$ is the semiclassical parameter arising as a result of passing to dimensionless variables: $h^2 \equiv \hbar^2/(2m_eE_0L_0^2)$ for the Schrödinger equation and $h \equiv \hbar v_{\mathrm{F}}/(E_0L_0)$ for the Dirac equation, where $\hbar$ is the Planck constant, $m_e$ is the electron mass, and $v_{\mathrm{F}}$ is the Fermi velocity. In the calculations, we use the STM tip parameters in [5], and the induced potential is depicted in Fig. 1.

To calculate the LDOS, we can use two approaches. One of them is to consider the problem in a bounded region $r = \sqrt{x^2 + y^2} \le R$ with boundary conditions at $r = R$ (e.g., with the Dirichlet conditions

$\psi|_{r=R} = 0$ for the Schrödinger equation) and calculate the density of states for a discrete spectrum $E_k$ by the formula [6]

$$\mathrm{LDOS}(E_k)|_{r=0} = |\psi_k(0)|^2 D(E_k) = \frac{|\psi_k(0)|^2}{\Delta E_k}, \qquad \Delta E_k \equiv E_{k+1} - E_k. \tag{1.3}$$

Another variant is to consider the problem in an unbounded region $(x, y) \in \mathbb{R}^2$ with conditions normalizing the eigenfunctions of the continuous spectrum to the delta function, $\iint_{\mathbb{R}^2} \psi_k \psi_{k_1}^* \, dx = \delta(k - k_1)$, and determine the LDOS for the continuous spectrum as (see, e.g., [7])

$$\mathrm{LDOS}(E)|_{r=0} \equiv \int |\psi(0, E(k))|^2 \delta(E(k) - E)\, dk = |\psi(0, E)|^2 \left(\frac{dE(k)}{dk}\right)^{-1}\Bigg|_{E(k)=E}. \tag{1.4}$$

The dependence of the energy $E(k)$ on the radial wave number $k$ has the form $E(k) = h^2k^2$, $dE(k)/dk = 2h^2k = 2h\sqrt{E(k)}$, for the Schrödinger equation and $E(k) = hk$, $dE(k)/dk = h$, for the Dirac equation.

As shown in [6], these two approaches are equivalent for exact eigenfunctions. In the limit $R \to \infty$, the LDOS of the discrete spectrum passes into the LDOS of the continuous spectrum. In the case of a finite region, we can formulate an exact mathematical result for the asymptotic approximation of the wave functions: because the problem is radially symmetric and hence effectively one-dimensional, the asymptotic approximations are the asymptotic wave functions, i.e., approximate the exact solutions. The asymptotic approximations have the form of Bessel functions [8]. The final formulas depend on the size $R$ of the area and are quite cumbersome. In the case of an infinite region, the asymptotic formulas have a simple, clear form, but a theorem that the presented formulas are asymptotic to the solutions does not exist, so far as we know. Nevertheless, if we formally use the obtained asymptotic formulas for the problem with an unbounded region, normalize them to the delta function, and calculate the LDOS for them, then the answer for the LDOS coincides with the limit of the asymptotic LDOS for a bounded region with $h = \mathrm{const} > 0$ as $R \to \infty$.

The answer for the LDOS calculated in the case of an infinite region for the "asymptotic wave function" has a simple, clear form and is physically reasonable.

The paper is structured as follows. In Sec. 2, we separate the variables for the radially symmetric potential and mass. In this case, the Dirac system is reducible to two equations of the type of a perturbed Schrödinger equation with an effective potential depending on the initial potential, the energy level, and the mass (see [9]). In Sec. 3, we present formulas for the leading term of the asymptotic approximation in the case of an infinite region and the LDOS for these asymptotic approximations. The results are presented in Fig. 2. In Appendix A, we present semiclassical asymptotic approximations of the solution (see Fig. 3) and the procedure for normalizing them to the delta function. In Appendix B, we write exact solutions of the Schrödinger equation in the case of a parabolic potential (see Fig. 4). For the Dirac equation, we write an exact solution only for the energy level $E = U(0)$ and zero mass (see Fig. 5).

## 2. Separation of variables and reduction of the Dirac equation to scalar equations

Because of the symmetry, the variables in Eqs. (1.1) and (1.2) can be separated, after which the problem becomes effectively one-dimensional. With the substitution $\psi(x) = e^{il\varphi}\psi(r)$, $l \in \mathbb{Z}_+$, Schrödinger equation (1.1) passes into

$$-h^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{l^2}{r^2}\right)\psi - \big(E - U(r)\big)\psi = 0.$$

In the vicinity of $r=0$, the solutions have the form $\psi = cJ_l\bigl(\frac{r}{h}\sqrt{E-U_0}\bigr)$, and hence $\psi(0)=0$ if $l\neq 0$. Only solutions with zero angular momentum contribute to the LDOS at $r=0$, and it suffices to consider the one-dimensional equation

$$-h^2\biggl(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\biggr)\psi - n^2(r)\psi = 0, \qquad n^2(r) = E-U(r). \tag{2.1}$$

Similarly, substituting $\Psi(x) = \bigl(e^{il\varphi}\psi_1(r),\ e^{i(l+1)\varphi}\psi_2(r)\bigr)^{\mathrm{T}}$, where the superscript T denotes conjugation, in the Dirac equation yields (see, e.g., [9])

$$\begin{gathered}\psi_2 = -ih\frac{1}{v_+}\biggl(\frac{\partial}{\partial r}-\frac{1}{r}\biggr)\psi_1, \qquad v_+(r) = E-U(r)+m(r),\\ -h^2\biggl(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{l^2}{r^2}\biggr)\psi_1 + h^2\frac{v_+'}{v_+}\biggl(\frac{\partial}{\partial r}-\frac{l}{r}\biggr)\psi_1 - \bigl((E-U)^2-m^2\bigr)\psi_1 = 0\end{gathered}$$

or, equivalently,

$$\begin{gathered}\psi_1 = -ih\frac{1}{v_-}\biggl(\frac{\partial}{\partial r}+\frac{l+1}{r}\biggr)\psi_2, \qquad v_-(r) = E-U(r)-m(r),\\ -h^2\biggl(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{(l+1)^2}{r^2}\biggr)\psi_1 + h^2\frac{v_-'}{v_-}\biggl(\frac{\partial}{\partial r}+\frac{l+1}{r}\biggr)\psi_2 - \bigl((E-U)^2-m^2\bigr)\psi_2 = 0.\end{gathered}$$

Solutions with $l=0$ when $\psi_1(0)\neq 0$ and with $l=-1$ when $\psi_2(0)\neq 0$ contribute to the LDOS at $r=0$. We have

$$-h^2\biggl(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\biggr)\psi_1 - n_1^2\psi_1 + h^2\frac{v_+'}{v_+}\frac{\partial}{\partial r}\psi_1 = 0, \qquad \psi_2 = -ih\frac{1}{v_+}\psi_1', \tag{2.2}$$

for $l=0$ and

$$-h^2\biggl(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\biggr)\psi_2 - n_1^2\psi_2 + h^2\frac{v_-'}{v_-}\frac{\partial}{\partial r}\psi_1 = 0, \qquad \psi_1 = -ih\frac{1}{v_-}\psi_2', \tag{2.3}$$

for $l=-1$, where

$$n_1 = \sqrt{(E-U)^2-m^2}, \qquad v_\pm(r) = E-U(r)\pm m(r).$$

At zero mass, the case $l=-1$ is symmetric to the case $l=0$ under interchanging $\psi_1$ and $\psi_2$.

We consider Eqs. (2.1) and (2.2) in the domain $r\in\mathbb{R}_+$ and supplement them with the smoothness condition at $x=0$ and the condition of normalization to the delta function:

$$\begin{aligned}&\psi'(0)=0, \qquad &&\iint_{\mathbb{R}^2}\psi_k\psi_{k_1}^*\,dx = \delta(k-k_1),\\ &\psi_1'(0)=0, \qquad &&\iint_{\mathbb{R}^2}\Psi_k\Psi_{k_1}^*\,dx = \iint_{\mathbb{R}^2}\bigl(\psi_{1,k}\psi_{1,k_1}^*+\psi_{2,k}\psi_{2,k_1}^*\bigr)\,dx = \delta(k-k_1),\end{aligned} \tag{2.4}$$

where $k$ is the wave vector modulus and $\psi_k = \psi(x;E(k))$. For Eq. (2.3), the smoothness condition is $\psi_2'(0)=0$.

As a rule, it is impossible to separate variables in the case of a nonsymmetric potential, and the adiabatic method must be used [10], [11].

## 3. The leading asymptotic terms and their LDOS

For Eqs. (2.1)–(2.3), the asymptotic solutions are given by the Maslov canonical operator [12], for which it is convenient to use the representation recently obtained in [13]:

$$\psi(x) = \oint \varphi(x,\theta,h)e^{(i/h)\Phi(x,\theta)}\,d\theta, \qquad \Phi(x,\theta) = T(x\mathbf{n}(\theta)), \qquad \mathbf{n}(\theta) = (\cos\theta, \sin\theta),$$

where the eikonal $T(r) = \int_0^r n(r)\,dr$ is equal to $T(r) = \int_0^r \sqrt{E-U}\,dr$ for Schrödinger equation (2.1) and to $T(r) = \int_0^r \sqrt{(E-U)^2 - m^2}\,dr$ for effective equations (2.2) and (2.3) to which the Dirac equation is reduced. This representation can also be used in the case where the potential $U(x)$ has no symmetries. In such a representation, we can quite simply determine corrections to the leading asymptotic term. With the symmetry taken into account, it becomes the Bessel integral [8]:

$$\begin{aligned} \psi(r,h) &= \int e^{(i/h)T(r,h)\cos\eta}\,\varphi(r,h)\,d\eta = 2\pi\varphi(r,h)\,J_0\biggl(\frac{1}{h}T(r,h)\biggr), \\ T(r,h) &= T(r) + hT_1(r) + \dots, \qquad \varphi(r,h) = \varphi_0(r) + h\varphi_1(r) + \dots, \end{aligned} \tag{3.1}$$

where $T_k(r), \varphi_k(r) \in C^\infty(\mathbb{R}_+)$.

For the Schrödinger equation, the leading asymptotic term for over-barrier states $E > U(0)$ becomes

$$\psi(r) = \frac{\sqrt[4]{E}}{\sqrt{2\pi h}} \frac{\sqrt{T(r)}}{\sqrt{r}\,\sqrt[4]{E-U(r)}}\,J_0\biggl(\frac{1}{h}T(r)\biggr)(1+O(h)). \tag{3.2}$$

For $E < U(0)$ in the classically forbidden region (for $r < r_0(E)$, where $r_0(E)$ is the turning point, $U(r_0(E)) = E$), the leading asymptotic term has the form

$$\psi(x) = \frac{\sqrt[4]{E}}{\sqrt{2\pi h}} \exp\biggl\{-\frac{1}{h}\int_0^{r_0(E)} \sqrt{U(r)-E}\,dr\biggr\} \frac{\sqrt{T_{\mathrm{tun}}(r)}}{\sqrt{r}\,\sqrt[4]{U(r)-E}}\,J_0\biggl(\frac{1}{h}T_{\mathrm{tun}}(r)\biggr)(1+O(h)), \tag{3.3}$$

where

$$T_{\mathrm{tun}}(r) = \int_0^r |n(r)|\,dr = \int_0^r \sqrt{U(r)-E}\,dr.$$

The LDOS at zero for over-barrier energies and for classically forbidden states is respectively equal to

$$\begin{aligned} \mathrm{LDOS}_{\mathrm{Sch}}(E) &= \frac{1}{4\pi h^2}(1+O(h)), && E > U(0), \\ \mathrm{LDOS}_{\mathrm{Sch}}(E) &= \frac{1}{4\pi h^2}\exp\biggl\{-\frac{2}{h}\int_0^{a(E)} \sqrt{U(r_1)-E}\,dr_1\biggr\}(1+O(h)), && E < U(0). \end{aligned} \tag{3.4}$$

The LDOS for above-barrier states (the first equation in (3.4)) coincides with the LDOS with a zero potential. The LDOS for under-barrier energies is exponentially small. Plots of the LDOS are presented in Fig. 2.

In the case of the Dirac equation with zero mass, the effective potential has the form $n_1^2(r) = |E-U(r)|$, and the classically forbidden region is absent. The leading asymptotic term is written as

$$\psi_1(r) = \frac{1}{\sqrt{2}\sqrt{2\pi h}} \frac{\sqrt{T(r)}}{\sqrt{r}}\,J_0\biggl(\frac{1}{h}T(r)\biggr)(1+O(h)), \tag{3.5}$$

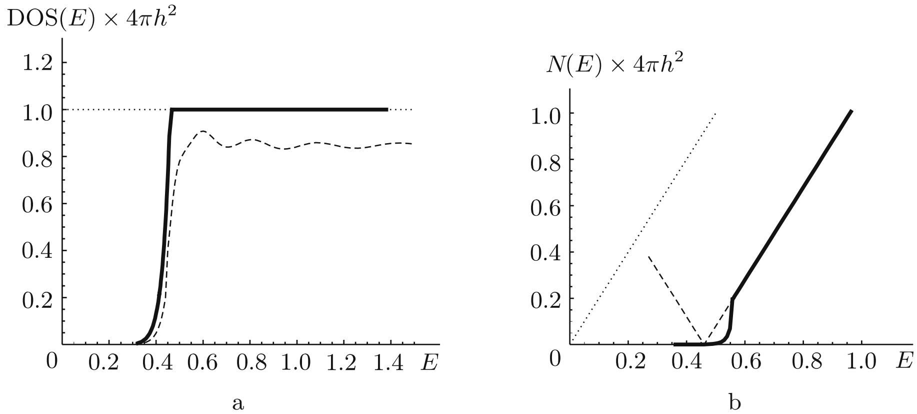


**Fig. 2**. (a) The LDOS for the Schrödinger equation corresponding to the leading asymptotic term for the tip potential (solid line), for the exact solution for a parabolic potential (dashed line), and for the exact solution without a potential (dotted line). (b) The LDOS for the Dirac equation corresponding to the leading asymptotic term for the potential in the case of a nonzero mass (solid), for the potential in the case of a zero mass (dashed line), and for the potential with no mass and no potential (dotted line). The maximum induced potential is equal to $U(0) = 0.46$, the mass is chosen as $m = 0.1$ in the Dirac equation, and the semiclassical parameter is $h = 0.1$ in both cases.

and the LDOS (with the symmetry with respect to the pseudospin components $\psi_1$ and $\psi_2$ taken into account) is equal to

$$\mathrm{LDOS}_{\mathrm{Dir}}(E) = \frac{|E - U(0)|}{2\pi h^2}\,(1 + O(h)). \tag{3.6}$$

If $E < U(0)$ in this case, then we can speak of the density of "hole" states. The LDOS with a zero potential is equal to $E/2\pi h^2$. The presence of a potential leads to a "shift" of this dependence: the LDOS decreases by a constant value $U_0/2\pi h^2$ for all energies $E > U(0)$ above the barrier (see Fig. 2).

In the case of the Dirac equation with a nonzero mass, the effective potential in (2.2) and (2.3) is equal to $n_1^2(r) = (E - U(r))^2 - m(r)^2$ and can take negative values, i.e., a classically forbidden region appears. With a nonzero mass, the symmetry with respect to the pseudospin components is broken.

We consider several regimes:

**Regime 1:** $E > U(0) + m(0)$. In this case, for all $r \in \mathbb{R}_+$, the effective potential is positive, and the wave functions are oscillating.

**Regime 2:** $U(0) - m(0) < E < U(0) + m(0)$. In this case, there is one turning point $r_-$, for which $v_-(r_-) = E - U(r_-) - m(r_-) = 0$. For $r > r_-$, the effective potential is positive, and the wave functions are oscillating. In the classically forbidden region $r < r_-$, the effective potential is negative, and the wave functions decay exponentially.

**Regime 3:** $U(\infty) + m(\infty) < E < U(0) - m(0)$. In this case, there exist two turning points $r_+ < r_-$ such that $v_\pm(r_\pm) = E - U(r_\pm) \pm m(r_\pm) = 0$. The effective potential is positive for $r > r_-$ and for $r < r_+$. For $r_+ < r < r_-$, the effective potential is negative, and we have a tunneling wave function here. For $r < r_+$, stationary states have a discrete spectrum of the energies $E_j$: these are either quasistationary (Gamov) states, which go to infinity with time, or states that come from infinity with resonance (Klein) tunneling (analogous effects were described in [14]).

The leading term for the LDOS at zero in these three cases has the form (the semiclassical asymptotic approximations of the wave functions and the derivation of the normalization constants are presented in

Appendix A)

$$
\begin{aligned}
&\text{Regime 1:} \qquad \mathrm{LDOS}_{\mathrm{Dir}}(E) = \frac{v_+(0)+v_-(0)}{4\pi h^2} = \frac{E-U(0)}{2\pi h^2},\\
&\text{Regime 2:} \qquad \mathrm{LDOS}_{\mathrm{Dir}}(E) = \frac{m(0)}{2\pi h^2}\,\exp\biggl\{-\frac{2}{h}\int_0^{r_-(E)} |n_1|\,dr\biggr\},\\
&\text{Regime 3:} \qquad \mathrm{LDOS}_{\mathrm{Dir}}(E_j^\pm) = \frac{|v_\pm(0)|}{16\pi h\,\Delta E_j^\pm}\,\exp\biggl\{-\frac{2}{h}\int_{r_+(E_j^\pm)}^{r_-(E_j^\pm)} |n_1|\,dr\biggr\}.
\end{aligned}
\tag{3.7}
$$

In the last formula, $\Delta E_j^\pm \equiv E_{j+1}^\pm - E_j^\pm$ is the distance between the energy levels $E_j^\pm$. The energy $E_j^+$ corresponds to the angular momentum $l=0$, and $E_j^-$ corresponds to $l=-1$ (see Appendix A).

For large energies, the LDOS is the same as in the massless case and is equal to the LDOS without a tip minus the value $U(0)/2\pi h^2$, which is the same for all energies $E > U(0)+m(0)$. In the forbidden region $E < U(0)+m(0)$, just as in the case of the Schrödinger equation, the LDOS is exponentially small. Plots of the LDOS are presented in Fig. 2.

Therefore, in the case of the Schrödinger equation, the STM tip only distorts the LDOS for energies that are less than the induced potential (the LDOS becomes exponentially small), and the LDOS for large energies remains the same (in the leading term; see Fig. 2). In the case of the Dirac equation, the STM tip also distorts the states with large energies: the LDOS is decreased by the value $U(0)/2\pi h^2$ (i.e., the linear dependence of the LDOS on the energy is "shifted" in the abscissa by the value of the induced potential). In addition, in the presence of a mass $m$, the LDOS with energies less than $U(0)+m$ becomes exponentially small.

## 4. Summary

Using semiclassical asymptotic approximations for the generalized eigenfunctions of the two-dimensional radially symmetric Schrödinger and Dirac operators, we have studied the LDOS. This research allows estimating and comparing the effects of the influence of an STM tip on the measured results obtained by scanning.

## Appendix A: Semiclassical asymptotic approximations

**A.1. Normalization to the delta function.** We consider Schrödinger equation (2.1). In the over-barrier region, the asymptotic approximation is expressed in terms of the Bessel function and at large arguments has the form

$$
\begin{aligned}
\psi &= C_\infty(E)\frac{\sqrt{T(r)}}{\sqrt{r}\,\sqrt[4]{E-U(r)}}J_0\biggl(\frac{1}{h}T(r)\biggr)(1+O(h)) =\\
&= C_\infty(E)\frac{1}{\sqrt{r}}\sin\biggl(\frac{1}{h}\sqrt{E}\,r + O(1)\biggr)(1+O(h)), \quad r\to\infty.
\end{aligned}
$$

The constant $C_\infty(E)$ is determined from normalization condition (2.4). Following the procedure described in [7], we consider the equation for two close wave numbers $k$ and $k_1$ (where $E(k) = h^2k^2$) and apply complex conjugation, denoted by the asterisk, to the equation for $k_1$:

$$
\psi_k'' + \frac{1}{r}\psi_k' + \biggl(k^2 - \frac{U}{h^2}\biggr)\psi_k = 0, \qquad \psi_{k_1}^{*\prime\prime} + \frac{1}{r}\psi_{k_1}^{*\prime} + \biggl(k_1^2 - \frac{U}{h^2}\biggr)\psi_{k_1}^* = 0.
$$

Subtracting one equation from the other, we obtain

$$(k_1^2 - k^2) r \psi_k \psi_{k_1}^* = (r \psi_{k_1}^* \psi_k' - r \psi_k \psi_{k_1}^{*\prime})',$$

and hence

$$\iint_{\mathbb{R}^2_{xy}} \psi_k \psi_{k_1}^* \, dx \, dy = 2\pi \lim_{R\to\infty} \int_0^R \psi_k \psi_{k_1}^* r \, dr = \lim_{R\to\infty} \frac{2\pi R}{k_1^2 - k^2} (\psi_{k_1}^* \psi_k' - \psi_k \psi_{k_1}^{*\prime}) \big|_{r=R}.$$

Using the asymptotic representation at infinity and taking into account that $\psi_k'(0) = 0$, we obtain

$$\int_0^R \psi_k \psi_{k_1}^* r \, dr = \frac{|C_\infty|^2}{2(k_1^2 - k^2)} \big( (k - k_1) \sin((k_1 + k)R + O(1)) + (k + k_1) \sin((k_1 - k)R + O(1)) \big).$$

We consider the weak limit at $R \to \infty$,

$$\lim_{R\to\infty} \sin((k + k_1)R) = 0, \qquad \lim_{R\to\infty} \frac{\sin(R(k - k_1))}{k - k_1} = \pi \delta(k - k_1).$$

As a result, we finally have

$$\lim_{R\to\infty} 2\pi \int_0^R \psi_k \psi_{k_1}^* r \, dr = \lim_{R\to\infty} \frac{\pi |C_\infty|^2}{k_1 - k} \sin((k_1 - k)r + O(1)) = \pi^2 |C_\infty|^2 \delta(r),$$

whence we obtain the value of the normalization constant $C_\infty = 1/\pi$.

Analogous considerations hold for the Dirac equation. Let $u = \psi_1 \sqrt{r}$ and $w = \psi_2 \sqrt{r}$. We consider the system for the wave number $k$ and the conjugate system for the wave number $k_1$. We respectively multiply the first and second equations in the system for $k$ by $-u_{k_1}^*$ and $-w_{k_1}^*$ and the first and second equations for $k_1$ by $u_k$ and $w_k$. We then sum the four obtained equalities. As a result, we obtain

$$(u_k u_{k_1}^* + w_k w_{k_1}^*)(k_1 - k) = i \frac{\partial}{\partial r} (u_k w_{k_1}^* + u_{k_1}^* w_k).$$

At infinity, we have the asymptotic representations

$$\begin{aligned}
\frac{u(r)}{\sqrt{r}} = \psi_1 &= \frac{C}{\sqrt{2}\sqrt{2\pi h}} \frac{\sqrt{v_+ T}}{\sqrt{r n_1}} J_0\left(\frac{T}{h}\right)(1 + O(h)) = \\
&= \frac{C}{\pi\sqrt{2}} \frac{\sqrt{v_+}}{\sqrt{r n_1}} \cos\left(\frac{T}{h} - \frac{\pi}{4}\right)(1 + O(h)), \\
\frac{w(r)}{\sqrt{r}} = \psi_2 &= \frac{n_1}{v_+} \frac{iC}{\sqrt{2}\sqrt{2\pi h}} \frac{\sqrt{v_+ T}}{\sqrt{r n_1}} J_1\left(\frac{T}{h}\right)(1 + O(h)) = \\
&= \frac{iC}{\pi\sqrt{2}} \frac{\sqrt{n_1}}{\sqrt{r v_+}} \sin\left(\frac{T}{h} - \frac{\pi}{4}\right)(1 + O(h)).
\end{aligned}$$

Moreover, $T(r)/h = (r/h)\sqrt{E^2 - m(\infty)^2} + O(1)$. The normalization condition becomes

$$
\begin{aligned}
\delta(k - k_1) = & \iint_{\mathbb{R}^2_{xy}} \langle \Psi_k, \Psi^*_{k_1}\rangle dx\, dy = \iint_{\mathbb{R}^2_{xy}} (\psi_{1k}\psi^*_{1k_1} + \psi_{2k}\psi^*_{2k_1}) dx\, dy = \\
& = 2\pi \int_0^\infty (\psi_{1k}\psi^*_{1k_1} + \psi_{2k}\psi^*_{2k_1}) r\, dr = 2\pi i \lim_{r\to\infty} \frac{u_k w^*_{k_1} + u^*_{k_1} w_k}{k_1 - k} = \\
& = \lim_{r\to\infty} \frac{C^2}{\pi(k_1 - k)} \biggl\{ \sqrt[4]{\frac{E + m_\infty}{E - m_\infty} \frac{E_1 - m_\infty}{E_1 + m_\infty}} \times \\
& \quad \times \cos\biggl(\frac{r}{h}\sqrt{E^2 - m^2_\infty} + O(1)\biggr) \sin\biggl(\frac{r}{h}\sqrt{E_1^2 - m^2_\infty} + O(1)\biggr) - \\
& \quad - \sqrt[4]{\frac{E_1 + m_\infty}{E_1 - m_\infty} \frac{E - m_\infty}{E + m_\infty}} \times \\
& \quad \times \cos\biggl(\frac{r}{h}\sqrt{E_1^2 - m^2_\infty} + O(1)\biggr) \sin\biggl(\frac{r}{h}\sqrt{E^2 - m^2_\infty} + O(1)\biggr) \biggr\} = \\
& = \frac{2C^2}{2\pi} \pi \delta(k_1 - k)
\end{aligned}
$$

(here the limit is also understood in the sense of weak convergence). Hence, the normalization constant is $C = 1$.

**A.2. Asymptotic approximations near turning points and in the classically forbidden region.** For completeness of the exposition, we present the asymptotic formulas for the Dirac equation near the turning points and in the classically forbidden region $U(\infty) + m(\infty) < E < U(0) - m(0)$. The two turning points $r_+ < r_-$ are determined from the equation $v_\pm(r_\pm) = E - U(r_\pm) \pm m(r_\pm) = 0$. We set

$$
c_2 = \bigl(U'(r_+) - m'(r_+)\bigr)\bigl(E - U(r_+) - m(r_+)\bigr) > 0.
$$

Let $l = 0$. Then we have

$$
\psi_1 = \begin{cases}
\dfrac{1}{2\sqrt{\pi h}} \dfrac{\sqrt{v_+ T}}{\sqrt{n_1 r}} J_0\biggl(\dfrac{1}{h}\displaystyle\int_{r_-}^r n_1(r)\, dr\biggr), & r > r_-, \\
\dfrac{1}{\sqrt{2\pi}} \dfrac{\sqrt{v_+(r_-)}}{\sqrt[6]{h c_1}\sqrt{r_-}} \operatorname{Ai}\biggl((r_- - r)\dfrac{\sqrt[3]{c_1}}{h^{2/3}}\biggr), & r - r_- = O(h), \\
\dfrac{1}{2\sqrt{\pi h}} \dfrac{\sqrt{v_+ T}}{\sqrt{n_1 r}} \exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-} |n_1| dr\biggr\} J_0\biggl(i\dfrac{1}{h} T(r)\biggr), & r_+ < r < r_-, \\
\dfrac{1}{2\sqrt{2\pi}} \dfrac{\sqrt[6]{h}\sqrt{-U'(r_+) + m'(r_+)}}{\sqrt[3]{c_2}\sqrt{r_+}} \times & \\
\quad \times \exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-} |n_1| dr\biggr\} \operatorname{Bi}'\biggl((r - r_+)\dfrac{\sqrt[3]{c_2}}{h^{2/3}}\biggr), & r - r_+ = O(h), \\
\dfrac{1}{4\sqrt{\pi h}} \dfrac{\sqrt{|v_+(r)| T(r)}}{\sqrt{n_1(r)\, r}} \times & \\
\quad \times \exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-} |n_1| dr\biggr\} J_0\biggl(\dfrac{1}{h}\displaystyle\int_0^r n_1\, dr\biggr), & r < r_+.
\end{cases}
$$

Let $l=-1$. Then we have

$$\psi_2=\begin{cases}\dfrac{1}{2\sqrt{\pi h}}\dfrac{\sqrt{v_-T}}{\sqrt{n_1 r}}J_0\biggl(\dfrac{1}{h}\displaystyle\int_{r_-}^{r}n_1(r)\,dr+\dfrac{\pi}{2}\biggr), & r>r_-,\\ -\dfrac{1}{\sqrt{2\pi}}\dfrac{\sqrt[6]{h}\sqrt{-U'(r_-)-m'(r_-)}}{\sqrt[3]{c_1}\sqrt{r_-}}\mathrm{Ai}'\biggl((r_--r)\dfrac{\sqrt[3]{c_1}}{h^{2/3}}\biggr), & r-r_-=O(h),\\ \dfrac{1}{2\sqrt{\pi h}}\dfrac{\sqrt{|v_-|T}}{\sqrt{n_1 r}}\exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-}|n_1|\,dr\biggr\}J_0\biggl(i\dfrac{1}{h}T(r)\biggr), & r_+<r<r_-,\\ \dfrac{1}{2\sqrt{2\pi}}\dfrac{\sqrt{|v_-(r_+)|}}{\sqrt[6]{hc_2}\sqrt{r_+}}\times & \\ \quad\times\exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-}|n_1|dr\biggr\}\mathrm{Bi}\biggl((r-r_+)\dfrac{\sqrt[3]{c_2}}{h^{2/3}}\biggr), & r-r_+=O(h),\\ \dfrac{1}{4\sqrt{\pi h}}\dfrac{\sqrt{|v_-(r)|T(r)}}{\sqrt{n_1(r)\,r}}\times & \\ \quad\times\exp\biggl\{-\dfrac{1}{h}\displaystyle\int_{r_+}^{r_-}|n_1|dr\biggr\}J_0\biggl(\dfrac{1}{h}\displaystyle\int_0^r n_1\,dr\biggr), & r<r_+.\end{cases}$$

The discrete spectrum $E_j^{\pm}$ corresponding to resonance tunneling is determined from

$$l=0:\quad \frac{1}{h}\int_0^{r_+(E_j^+)}\sqrt{(E_j^+-U(r))^2-m(r)^2}\,dr=2\pi\biggl(j+\frac{1}{4}\biggr),$$

$$l=-1:\quad \frac{1}{h}\int_0^{r_+(E_j^-)}\sqrt{(E_j^--U(r))^2-m(r)^2}\,dr=2\pi j$$

(here $j\in\mathbb{N}$). Plots of the asymptotic representations are shown in Fig. 3.

## Appendix B: Exact solutions for a parabolic potential

Asymptotic representations (3.2), (3.3), and (3.5) are applicable for energies $|E-U(r)|\ge\varepsilon>0$. To study the behavior of the LDOS for energies $E\sim U(0)$, we consider the problem with the potential

$$U(r)=\begin{cases}U_0-\omega^2r^2, & r\le r_0,\\ 0, & r\ge r_0,\end{cases}\qquad r_0=\frac{\sqrt{U_0}}{\omega}.$$

Equation (1.1) then becomes

$$h^2\frac{\partial^2\psi}{\partial r^2}+h^2\frac{1}{r}\frac{\partial\psi}{\partial r}+\bigl((E-U_0)+\omega^2r^2\bigr)\psi=0,$$

and its exact solution in terms of the Kummer confluent hypergeometric function[1] is known:

$$\psi(r)=\begin{cases}Ce^{(i\omega/2h)r^2}{}_1F_1\biggl(\dfrac{1}{2}-i\dfrac{E-U_0}{4h\omega};\,1;\,-i\dfrac{\omega}{h}r^2\biggr), & r\le r_0,\\ \dfrac{\sqrt[4]{E}}{\sqrt{2\pi h}}J_0\biggl(\dfrac{1}{h}\sqrt{E}\,r+\theta_0\biggr), & r\ge r_0,\end{cases}$$

[1] The Kummer confluent hypergeometric function is defined as the series

$$ {}_1F_1(a;b;z)=\sum_{k=0}^{\infty}\frac{a_k}{b_k}\frac{z^k}{k!},\qquad a_0=b_0=1,\quad a_k=a(a+1)\cdots(a+k-1).$$

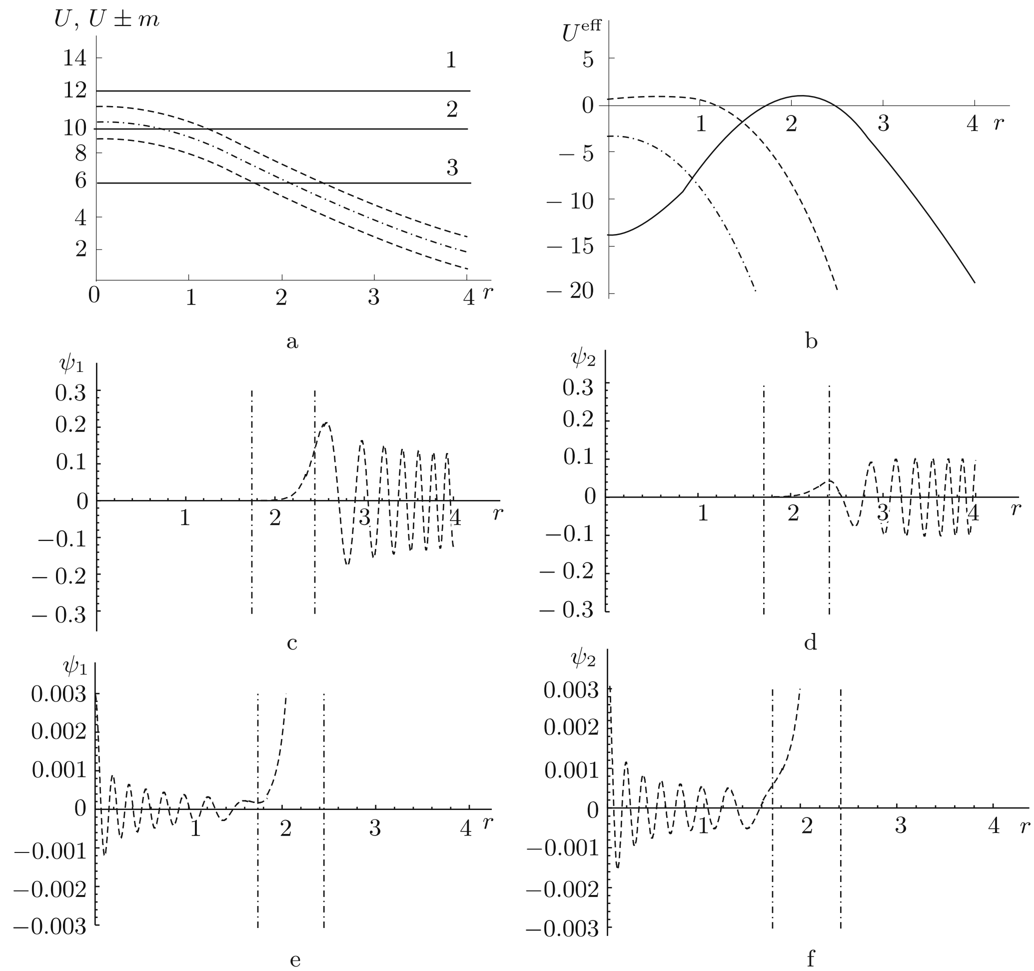


**Fig. 3**. (a) The potential $U(r)$ (dot-dashed line) and functions $U(r) \pm m$ (dashed line). (b) The effective potentials in the cases $E > U(0) + m(0)$ (dot-dashed line), $U(0) - m(0) < E < U(0) + m(0)$ (dashed line), and $E < U(0) - m(0)$ (solid line). Asymptotic representations in different scales (c,e) for $\psi_1(r)$ and (d,f) for $\psi_2(r)$ in case 3. Vertical lines in the plots mark the two turning points $r_\pm$ where $E - U(r_\pm) \pm m(r_\pm) = 0$.

where the constant $C$ and the phase shift $\theta_0$ are determined from the condition for the continuity of the solution and its logarithmic derivative at $r_0$:

$$\frac{\psi'}{\psi}\bigg|_{r=r_0-0} = \frac{\psi'}{\psi}\bigg|_{r=r_0+0}, \qquad C = \frac{\psi(r_0+0)}{\psi(r_0-0)}.$$

Solutions for $U_0 = u_{\text{tip}}(0)$ and $\omega^2 = u''_{\text{tip}}(0)/2$ are presented in Fig. 4, the LDOS for such a potential in comparison with the asymptotic LDOS is shown in Fig. 2. The discrepancy between the values of the exact and asymptotic solutions at $r = 0$ is within $O(h)$. This discrepancy cannot be decreased by calculating corrections to the leading term, because the potential chosen for the exact solution is not smooth.

For the Dirac equation (for effective Schrödinger equations (1.2)), we present an exact solution in the case of a zero mass and a parabolic potential with $E = U_0$, where $v(r) = \omega^2 r^2$ for $r < r_0$ and $v(r) = E$ for $r \geq r_0$. In this case, the equation becomes

$$h^2 \frac{\partial^2}{\partial r^2}\psi_1 - h^2 \frac{1}{r}\frac{\partial}{\partial r}\psi_1 + \omega^4 r^4 \psi_1 = 0, \quad r \leq r_0.$$

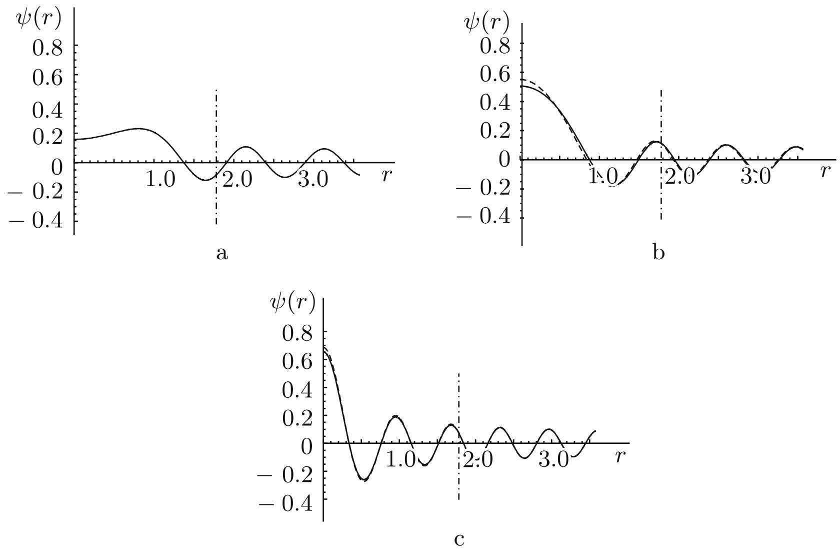


**Fig. 4**. Exact solutions of the Schrödinger equation with a parabolic potential (solid line) and the asymptotic values with the tip potential (dashed line) for $E - U(0) = -0.05$, 0.05, and 0.5 (respectively in (a), (b), and (c)).

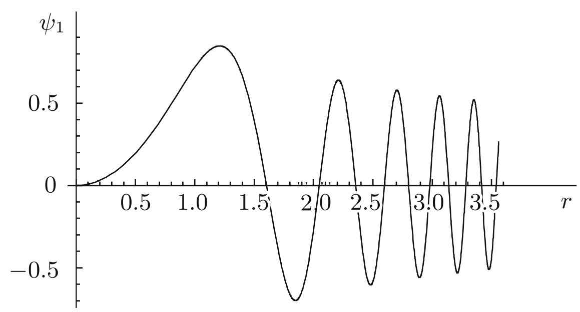


**Fig. 5.** An exact solution for the Dirac equation with $E = U(0)$ and $m \equiv 0$.

The solution with a parabolic potential is expressed in terms of the Bessel function:

$$\psi_1(r) = \begin{cases} Cr\, J_{1/3}\left(\dfrac{\omega^2}{3h} r^3\right), & r \le r_0, \\ \dfrac{1}{\sqrt{2}\sqrt{2\pi h}} J_0\left(\dfrac{1}{h} Er + \theta_0\right), & r \ge r_0. \end{cases}$$

The constant $C$ and the phase shift $\theta_0$ are determined as before from the continuity condition for the solution and its logarithmic derivative at $r_0$. Because the function $rJ_{1/3}(r)$ vanishes at $r = 0$, the STM LDOS is also zero for $E = U(0)$. The solution is depicted in Fig. 5.

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