TITLE: New Mathematical Tools for Quantum Technology
Abstract:
The principle of superposition is a key element for quantum technological phenomena connected with the generation and transfer of quantum information. In this contribution we work out the mathematical techniques for calculating i) the coherent generation of matter waves by radiation and, ii) the transfer and detection of information on an atomic scale. In this context, the use of single-particle Green functions in configuration space is shown to be a powerful tool for establishing a reliable and transparent description of experiments in Quantum Technology. As one of several examples we apply the method to the calculation of scanning tunneling images. Emphasis is put on a comparison with experiments.
The photoelectric effect in external fields

Christian Bracher\textsuperscript{a}, John B. Delos\textsuperscript{a}, Vassiliki Kanellopoulos\textsuperscript{b}, Manfred Kleber\textsuperscript{b,*}, Tobias Kramer\textsuperscript{b}

\textsuperscript{a} Physics Department, The College of William and Mary, Williamsburg, VA 23187-8795, USA
\textsuperscript{b} Physik Department T30, Technische Universität München, James-Franck-Str., 85747 Garching, Germany
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Abstract

Atoms and negative ions interacting with laser photons yield a coherent source of photoelectrons. Applying external fields to photoelectrons gives rise to interesting and valuable interference phenomena. We analyze the spatial distribution of the photocurrent using elementary quantum methods. The photoelectric effect is shown to be an interesting example for the use of coherent particle sources in quantum mechanics.

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1. Introduction

The wave–particle duality lies at the heart of quantum mechanics. Duality applies also to light whose nature had occupied the minds of scientists for centuries. Let us only mention the important milestones: in 1675 Isaac Newton had the idea that light was a stream of tiny particles \cite{1} whereas in 1678 his rival Christian Huygens suggested that light behaves like traveling waves. The matter should have been settled in favor of the wave hypothesis with Thomas Young’s seminal double-slit experiment (1801) \cite{2} (but it took another 30 years before British scientists would concede the point). However, in 1900 Max Planck found the famous radiation law \cite{3} that describes quantitatively the intensity of light emitted at different frequencies $\nu$ from a hot blackbody. To derive the spectral energy density Planck had to assume that the energy of light "is composed of a definite number of finite parts" (which Einstein later called energy quanta)

\begin{equation}
E_{\nu} = Nh\nu.
\end{equation}

\textsuperscript{*} Corresponding author.
E-mail address: manfred_kleber@ph.tum.de (M. Kleber).

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Planck was not sure about the meaning of this equation. He tended to believe that the division of radiation into small portions $h\nu$ was not a property of the radiation field itself but resulted from the interaction between light and matter in thermal equilibrium. He later said "I can characterize the whole procedure as an act of despair, since by nature I am peaceable, and opposed to doubtful adventures. However, I had already fought for six years... without arriving at any successful result. I was aware that this problem was of fundamental importance... hence a theoretical interpretation had to be found at any price, no matter how high it may be" [4].

At this point Albert Einstein took action. The title of his famous paper [5] reads "Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Geschichtspunkt." [Concerning an heuristic point of view toward the emission and transformation of light]. In his paper Einstein introduced independent energy quanta (the term photon was coined later) which characterize radiation and cannot be divided further. Einstein used a statistical-thermodynamic argument for the existence of such quanta: examining a formula he derived for the entropy of radiation, he found that high frequency (or low density) radiation "behaves, in a thermodynamic sense, as if it consists of mutually independent radiation quanta" of magnitude $h\nu$, and therefore "it is plausible to investigate whether the laws of the creation and transformation of light are so constituted as if light consisted of such quanta" [4,6].

In the last three sections of his 1905 paper [5] Einstein's applied the concept of independent energy quanta to explain Stokes' law of fluorescence (light emitted has a lower frequency than the light absorbed), the ionization of gases by ultraviolet light, and the photoelectric effect in solids. He predicted that the maximum kinetic energy of electrons released from the solid would be

$$K_{\text{max}} = h\nu - \phi,$$

where $\phi$ denotes the work function of the solid. At the time he was only able to state that this formula was "not in contradiction" with the available experiments.

Einstein himself said that his theory was "very revolutionary", and indeed it was too much even for his admirers. Later, when Planck nominated him to the Prussian Academy of Sciences, he felt he had to apologize: "There is hardly one among the great problems... to which Einstein has not made an important contribution. That he may sometimes have missed the target in his speculations, as, for example, in his hypothesis of light quanta, cannot really be held too much against him, for it is not possible to introduce fundamentally new ideas, even in the most exact sciences, without occasionally taking a risk".

The photoelectric theory was finally put to the test a decade later by Robert Millikan, who showed that the formula was accurate to about 0.5%. Still, the hypothesis of light quanta was so incredible to him that he said: "Despite the apparently complete success of the Einstein equation, the physical theory of which it is designed to be the symbolic expression is found so untenable that Einstein himself, I believe, no longer holds it" [7].

Today the quantum theory of radiation is well established. However, we now know that the photoelectric effect is actually not a compelling argument for the existence of photons, because the Einstein relation can be derived from the Schrödinger equation using time-dependent perturbation theory [8], assuming a non-quantized, classical electromagnetic wave of frequency $\nu$. Phenomena that truly cannot be explained in terms of classical, non-quantized radiation fields include squeezing via non-linear optical processes, or the generation of non-classical light [9]. Recent beam-splitter experiments with single photons [10,11] exemplify Einstein's idea of the existence of indivisible photons.

2. Photoelectric effect as a two-step process

New knowledge is presently being gained by examining the photoelectric effect in applied static electric or magnetic fields. We may speak about this as a two-step process (Fig. 1). In the first step, the incoming photon transfers its energy to the bound electron and a photoelectron is created with an energy $E$ given by Eq. (2). In the second step it leaves the atom and propagates in the applied fields. The dynamics of the emitted electron is governed by the rules of quantum mechanics. In the following we consider a dilute gas of independent atoms where the interaction of the photoelectron with neighboring atoms can be neglected. Then, under steady-state conditions with many atoms
and monochromatic light we can calculate the photocurrent from Fermi's Golden Rule [12,13]:

\[ J(E) \propto \text{Im}(\langle \tilde{D}\psi | \tilde{G}(E) | \tilde{D}\psi \rangle), \]  

with the proportionality factor suppressed. Here \( \tilde{D}|\psi \rangle \) describes the action of the dipole operator \( \tilde{D} = \mathbf{e} \cdot \mathbf{r} \) on the initially bound state \( |\psi \rangle \) of the photoelectron under consideration. \( \tilde{G} \) is the quantum propagator (or single particle Green function) at fixed energy \( E = h\nu - E_0 \) for atoms. The work function must be replaced by the positive binding energy \( E_0 \) of the photoelectron. This formula says that the moving photoelectron has to be propagated with the Hamiltonian in the applied fields, and then matched with itself again [14].

\[
\langle \tilde{D}\psi | \tilde{G}(E) | \tilde{D}\psi \rangle
= \int d\mathbf{r} d\mathbf{r}' \langle \tilde{D}\psi | \mathbf{r} \rangle \langle \mathbf{r} | \tilde{G}(E) | \mathbf{r}' \rangle \langle \mathbf{r}' | \tilde{D}\psi \rangle. \]

The energy-dependent Green function

\[ G(\mathbf{r}, \mathbf{r}'; E) = \langle \mathbf{r} | \tilde{G}(E) | \mathbf{r}' \rangle \]

is the relative probability amplitude for an electron to travel from \( \mathbf{r} \) to \( \mathbf{r}' \). This formulation emphasizes the dynamical aspects of the propagation and opens the possibility of a semiclassical calculation of photocurrents with closed-orbit theories [15,16]. In general there are several classical orbits that link the points \( \mathbf{r} \) and \( \mathbf{r}' \). In quantum mechanics, these paths have to be weighted with complex amplitudes and coherently summed up [17].

3. Near-threshold effects

Applying this photoelectric formula to negative ions in an applied electric field gives a new way to measure the kinetic energy of the detached electron, and therefore the binding energy of the negative ion, with unprecedented precision. (Even today it is difficult to calculate ab initio the binding energy of the excess electron \( E_0 \) attached to a negative ion [21].)

The propagation of photoelectrons in a homogeneous external electric field has been experimentally studied by Blondel et al. [18–20]. The left-hand side in Fig. 2 illustrates the motion of a photoelectron subject to the electric force. The relevant Green function is that of a particle falling freely in a constant field [14,23,24]. Two classical trajectories lead from the source (the negative ion) to any point on the detector. As in Young's double-slit experiment, an interference pattern is produced by the electron waves that travel along these two paths. From the interference pattern

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**Fig. 1.** Two steps to create a photoelectron: (left panel) the photon transfers its energy \( h\nu \) to the initially bound electron, (right panel) the photoelectron escapes from the absorption region and propagates in the applied fields.

**Fig. 2.** Near-threshold detachment of oxygen ions: \( \text{O}^- \rightarrow \text{O} + e^- \) in the presence of a homogeneous electric force field \( \mathbf{F} \). The two possible classical trajectories for a photoelectron leading from the source \( \odot \) to any destination will give rise to interference on a distant detector screen. The fringe pattern in the current distribution depends sensitively on the energy. By counting the number of fringes the binding energy \( E_0 \) of the outer electron can be determined from Einstein's law [14,19–20].
one can determine the kinetic energy of the electrons and plot it against the photon energy to check Einstein’s law (2) (right panel of Fig. 2), and to determine the binding energy $E_0$ of the electron. Experimental results are reported in Ref. [19], Fig. 6. The recorded circular intensity fringes compare very well with the theoretical prediction [22]. They show a highly accurate verification of Einstein’s law which can be used to obtain the binding energy of $\text{O}^-$ with unprecedented accuracy [19,20].

Other new phenomena also appear in these experiments. For example, a static electric field opens up a sub-threshold ($E < 0$) tunneling regime which also has been confirmed by experiment [25]. An external magnetic field in combination with a crossed electric field can force the electron to stay in its initial bound state due to the lack of available final states [26,27]. Experimentally, a suppression of the photocurrent has been observed [28].

The photoelectric effect in neutral atoms subject to external fields reveals similarly intriguing interference phenomena [29,30]. Their interpretation has led to a new understanding of classical periodic orbits, and their bifurcation and proliferation as order changes to chaos [31–36]. Finally, we mention a recent prediction for photoionization of a neutral atom in parallel electric and magnetic fields: if the laser pulse is short, the released electrons will arrive at a detector in a chaotic pulse train [37].

4. Conclusions

Einstein’s theory of the photoelectric effect opened a door leading to the quantum theory of matter and radiation. A century later, the photoelectric effect still provides new insights into the wave–particle duality, and it provides new ways to measure the structure and spectra of atoms and ions.

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References

A simple method for simulating scanning tunneling images

B. Donner and M. Kleber
Physik-Department T30, Technische Universität München, James-Franck-Strasse, 85747 Garching, Germany

C. Bracher
Physics Department, The College of William and Mary, Williamsburg, Virginia 23187-8795

H. J. Kreuzer
Department of Physics and Atmospheric Science, Dalhousie University, Halifax, N.S. B3H 3J5, Canada

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Real-space observation of single atoms and electron surface states lies at the heart of scanning tunneling microscopy. The resolution of atomic structures depends on quantum mechanical features such as three-dimensional tunneling, the Pauli principle, the possibility of electron resonances, and the importance of multiple scattering events, which allow the current carrying electrons to detect single atoms and explore electronic properties of surfaces. We present a simple calculation that leads directly to experimentally observable quantities. The starting point of the calculation is the treatment of the scanning tunneling microscope (STM) as an open quantum system, with the tip being a point-like source (or sink) of electrons. Our STM image simulations of corral-like adsorbate structures bear strong resemblance to the experimental results by Crommie et al. [Science 262, 218–220 (1993); Physica D 83, 98–108 (1995)]. © 2005 American Association of Physics Teachers.

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I. INTRODUCTION

During the last two decades developments in technology and research have greatly advanced our understanding of nature at the atomic level. A particularly spectacular tool is the scanning tunneling microscope (STM), which records the spatial variations of the tunneling current in the junction between a sharp metallic tip and a conducting probe surface. With such a device it is possible to resolve individual atoms. Tersoff and Hamann related the STM image to the electronic states of the probe surface. This relation was illustrated spectacularly by Crommie et al., whose images of standing electron waves within a “quantum corral” ring of iron atoms placed on a copper surface harboring a two-dimensional electron gas have become a staple of textbooks.

When Feynman gave his famous lectures, the controlled emission of single electrons and the manipulation of single quantum particles was still a dream. Feynman introduced the visionary idea that an electron gun consisting of a tungsten wire that emits electrons could be used for a double-slit interference experiment. But he remarked that “you should not try to set up this experiment” because the “trouble is that the apparatus would have to be made on an impossibly small scale” to show the quantum interference effects in which he was interested. Little could he anticipate the advent of nanotechnology.

The tip of the STM and the probe surface provide an open quantum system where electrons are free to enter and leave. The usual textbook description of scattering invokes the limit of infinitely distant particle sources and detectors, which is appropriate in particle physics. However, quantum scattering is not limited to asymptotic problems where particles are generated (and observed) far from the scattering region. In the STM an electric current flows through a macroscopic wire that ends in a sharp tip. Its apex can be viewed as a source (or sink) of electrons that leave (enter) the tip by tunneling through the surface potential barrier between tip and sample surface. The apex of a good tip is ultrasharp, consisting of a single atom, and can be modeled very accurately as a point-like entity. The emission of particles from point-like sources was considered long before the advent of mesoscopic physics. Schwinger introduced sources as a means of describing quantum dynamics. Furthermore, the wave functions generated by point-like structures are most naturally interpreted in terms of the trajectories of classical physics. In particular, the current variations recorded in the STM image are directly linked to the backscattering amplitude.

We present a tutorial approach for understanding the subtle and fascinating quantum mechanical principles that rule the dynamics of a scanning tunneling microscope and small scale quantum electrical transport. Our method incorporates the important physical features of three-dimensional quantum motion in external fields, but it is not intended to replace high accuracy ab initio calculations that rely on purely numerical methods. To be specific, we consider a conducting sample surface that harbors a two-dimensional noninteracting electron gas in the presence of adatoms. For slow electrons, s-wave scattering prevails, which is appropriately described by a zero-range potential interaction. In this case, we obtain an analytic solution for the scattering problem which forms the basis for the calculation of the observed surface roughness or corrugation. We will show that scattering resonances play an essential role for resolving atoms and detecting electron surface states. Simulated STM images of several corral-like adsorbate structures serve as examples that illustrate the method.

In the following, some basic analytic results will serve as input for a straightforward calculation of real STM images of quantum corrals. In particular, we show how to model the apex of a STM as a source (or sink) of electrons, calculate three-dimensional tunneling across a vacuum barrier and determine the tunneling current, construct the $T$ matrix for multiple scattering between the tip, adatoms, and a surface, and...
understand why surface states and surface electron waves are imaged even though the tunneling current flows in the direction orthogonal to the surface.

II. THE SOURCE MODEL OF STM

The principal idea behind our description of a scanning tunneling image is that the open tip–surface system (see Fig. 1) supports stationary tunneling wave functions with nonvanishing current density \( j(r) \). (We use the independent electron approximation and thus neglect many-body effects.) If the electrons flow from the tip to the surface, the corresponding tunneling process starts at the apex of the tip. For a very large separation between tip and surface, the tunneling current drops to zero, with the apex states becoming the eigenstates \( \psi_{\text{spec}}(r; \varepsilon) \) of the unperturbed tip. The eigenstates satisfy the stationary Schrödinger equation:

\[
    [E - H_\varepsilon] \psi_{\text{spec}}(r; \varepsilon) = 0,
\]

with \( H_\varepsilon \) the tip Hamiltonian; \( E \) is one of the eigenvalues in the continuous spectrum of the apex states of the tip wire system. For finite separations and in the presence of an electric field between the tip and the surface, Eq. (1) is changed to

\[
    (E - H_\varepsilon - W(r)) \psi_{\text{spec}}(r; \varepsilon) + \psi_{\text{spec}}(r; \varepsilon) = 0,
\]

where the scattering contribution \( \psi_{\text{spec}}(r; \varepsilon) \) represents the small part of the apex wave function due to the coupling \( W(r) \) between the two electrodes in the presence of the external voltage and the elastic scattering potential of the adsorbed atoms and the substrate. We use Eq. (1) to rewrite Eq. (2) as

\[
    (E - H_\varepsilon - W(r)) \psi_{\text{spec}}(r; \varepsilon) = W(r) \psi_{\text{spec}}(r; \varepsilon),
\]

The right-hand side of Eq. (3) can be viewed as a source term for the tunneling wave function \( \psi_{\text{spec}}(r; \varepsilon) \) because the leads of the STM feed the apex of the tip with electrons, which replace those that traverse the potential barrier between the tip and the surface. We define the source function

\[
    S(r; \varepsilon) = W(r) \psi_{\text{spec}}(r; \varepsilon),
\]

and recast Eq. (3) in the form

\[
    (E - H_\varepsilon - W(r)) \psi_{\text{spec}}(r; \varepsilon) = S(r; \varepsilon),
\]

which is an inhomogeneous stationary Schrödinger equation with a source term centered about the apex of the tip. The idea of treating scattering out of a particle source is not new. However, the STM analogy allows us to apply the idea to experiments like those of Refs. 4 and 5.

We now turn to the mathematical aspects of Eq. (5). The solution to this inhomogeneous equation is formally given in terms of the convolution integral

\[
    \psi_{\text{spec}}(r; \varepsilon) = \int d^3r' G(r, r'; \varepsilon) S(r'; \varepsilon),
\]

which involves the (one-particle) energy Green function \( G(r, r'; \varepsilon) \) of the unperturbed wave function \( \psi_{\text{spec}}(r; \varepsilon) \). Because this polarization is small, the source function \( S(r; \varepsilon) \) is roughly proportional to \( \psi_{\text{spec}}(r; \varepsilon) \), a feature that occurs in other problems such as photodissociation.

In the presence of a strongly localized isotropic electron source, with the point-like apex of the tip located at \( r' \), we have approximately

\[
    S(r; \varepsilon) = S_0(\varepsilon) \delta(r - r'),
\]

and the desired solution to Eq. (6) is given by

\[
    \psi_{\text{spec}}(r; \varepsilon) = S_0(\varepsilon) G_{\text{ret}}(r, r'; \varepsilon),
\]

where the source strength \( S_0(\varepsilon) \) is specified in Appendix A. (Point-like sources of more complicated orbital character, such as p- and d-wave tips, have been invoked to explain the atomic resolving power of the STM.\textsuperscript{22,23} Although easily accommodated within the point source formalism,\textsuperscript{24} we will restrict ourselves to simple s-wave emission for the sake of clarity. As shown in Appendix B, the choice of a simple point-like source is an excellent approximation for an atomically sharp tip.)

Equation (7) does not specify a unique solution for the Green function, because an eigenfunction of the full Hamiltonian \( H_\varepsilon + W(r) \) can always be added to \( G(r, r'; \varepsilon) \). This freedom lets us incorporate boundary conditions into the theory. For electrons that leave the tip we have to use the retarded Green function \( G_{\text{ret}}(r, r'; \varepsilon) \) (outgoing-wave boundary condition). If the tip acts as a sink, we would employ its time-reversed counterpart, the advanced Green function \( G_{\text{adv}}(r, r'; \varepsilon) \) (incoming-wave boundary condition). The retarded Green function is best visualized as the relative probability amplitude that a particle arrives at point \( r \) if it has been created at point \( r' \).

\[
    W(r) = -F_z + \alpha \delta(z - z_0) + \sum_{j=1}^{N} W_{ad}(r, r_j).
\]

The first term on the right-hand side of Eq. (10) accounts for the bulk-vacuum transition potential of the surface and the applied external voltage. It is shown in Appendix B why even a uniform force field will lead to realistic STM images. The second term in Eq. (10) represents a strongly reflecting...
surface at \( z = z_w \). The reason for introducing such a term is that we wish to consider a situation where the transmitted electrons have an energy in the band gap of the bulk of the conducting sample surface.\(^{25}\) In this case the surface reflects strongly and behaves like a flat table (with its composing atoms being treated here as a continuum). To be specific, we assume that the sample surface contains a two-dimensional electron gas whose unoccupied states allow the tunneling (transmitted) electrons to spread on the surface. A nonzero external electric field may lead to a very small transmission, but the majority of the tunneling electrons will still flow along the surface before eventually being released into the bulk. Simulating such a situation means that \( \alpha \) is finite but large, which gives rise to strong reflection when the electrons arrive at the surface. The \( N \) adsorbed atoms at \( r = r_j \) are considered individually (see Fig. 1) and scatter electrons elastically.

In Appendix A we will show that independent of the specific form for \( W(r) \), an intrinsic particle current (the number of electrons per second and per energy) always is associated with the inhomogeneous Schrödinger equation (9):

\[
\frac{dN(r', E)}{dE} = \frac{4}{\hbar^2} |S_0|^2 \text{Im}[G(r', r'; E)] = \frac{\sigma_0(r'; E)}{e^2},
\]

where \( \sigma_0 \) is the tunneling conductivity between the tip and the sample surface (atoms included), and spin degeneracy already is included. [For simplicity, \( G(r, r'; E) \) in the following will denote the retarded energy Green function \( G_{rt} \) given by Eq. (7).] As shown in Appendix A, a three-dimensional \( s \)-like orbital tip state as represented by the source term (8) is approximately given by

\[
|S_0|^2 = \frac{\hbar^2}{mk_f},
\]

where \( \hbar k_f \) denotes the Fermi momentum of the tip metal, and \( m \) the electron mass. Equation (12) is valid for small voltages and low temperatures. By utilizing the identity\(^{26,26}\)

\[
\text{Im}[G(r, r'; E)] = -m \text{Im}[G(r, r'; E)],
\]

we can express the conductivity \( \sigma_0(r'; E) \) in terms of the local density of states \( n(r'; E) \) of the probe surface in the presence of the STM tip at the apex position \( r' \). (Alternatively, the variations in the local density of states can be linked to the closed classical orbits that begin and end at the point source.\(^{15–17}\))

In thermal equilibrium, both the tip and the surface show an occupation density \( f(E) = [1 + \exp((E - E_f)/kT)]^{-1} \), where the respective Fermi energies are shifted by the bias. In the source-sink model, Eq. (13) for the average differential particle number current can be cast in the form

\[
\frac{dN(r', E)}{dE} = \frac{4 \pi \hbar}{mk_f} [f(E) - f(E + eV)] n(r'; E),
\]

with \( V \) the applied bias voltage and \( E = E_f \). Equation (14) results from Eqs. (11)–(13), with the expression inside the square brackets a consequence of the Pauli principle, which allows transport from occupied to empty levels only. For low temperatures and in the vicinity of the Fermi level, the square brackets can be replaced by \( \pm 1 \), depending on whether the electrons flow from tip to probe or vice versa.

We note that Eq. (14) agrees with the \( s \)-wave tip model of Refs. 2 and 3, according to which the tunneling current is proportional to the Fermi-level local density of states \( n(r'; E) \) of the probe at the apex of the tip. In the more general treatment presented here, \( n(r'; E) \) is the local density of states of the probe in the presence of the tip and the applied electric field. Indeed, the source formalism is not based on perturbation theory, but instead is an extension of the approach of Refs. 2 and 3. Therefore, it also can be applied in principle to small separations between tip and probe where one expects a non-negligible coupling between the two electrodes.

The advantage of the present approach is that we do not need to calculate the density of states directly, which would require a rather involved numerical calculation. We can circumvent this difficulty by calculating the Green function with the correct boundary conditions directly from the model potential (10).

III. DETERMINATION OF THE GREEN FUNCTION

For surface potentials \( W(r) \) of the general form (10), a convenient route that leads to the Green function \( G(r, r'; E) \) consists of the following three steps.

A. One-dimensional problem

For the moment, we omit the terms \( W_{d0}(r, r_j) \) which correspond to the adsorbate atoms in the model potential \( W(r) \) given by Eq. (10). The remaining potential is

\[
\tilde{W}(z) = -Fz + \alpha \delta(z - z_w),
\]

which is translationally invariant along the surface and therefore no longer depends on the coordinates \( x \) and \( y \), which we formally drop. Standard techniques\(^{27–29}\) let us calculate the corresponding one-dimensional Green function \( G_{1D}(z, z'; E) \). The result is

\[
G_{1D}^0(z, z'; E) = \frac{G_{1D}^0(z, z'; E) - G_{1D}^0(z, z'; E)}{G_{1D}^0(z, z'; E) - \alpha^{-1}}.
\]

Here \( G_{1D}^0(z, z'; E) \) denotes the one-dimensional Green function for the linear potential problem \( \tilde{W}(z) \) of Eq. (15) with \( \alpha = 0 \). In other words, \( G_{1D}^0(z, z'; E) \) is the Green function for a uniformly accelerated particle.\(^{30,31}\) Its explicit form, a product of Airy functions, is given in Appendix B. [The method works as well with more sophisticated choices for \( \tilde{W}(z) \).] Knowledge of \( G_{1D}^0(z, z'; E) \) allows one to proceed to the next step in the calculation.

B. The background Green function

Because the STM is a three-dimensional device, we must calculate the Green function in physical space. As before, we neglect the atomic contributions \( W_{d0}(r, r_j) \) in Eq. (10), and obtain the three-dimensional background Green function \( G_{1D}^0(r, r'; E) \) for a particle in the bulk-surface transition potential \( \tilde{W}(r) = \tilde{W}(z) \) from its one-dimensional counterpart \( G_{1D}^0(z, z'; E) \). We do so by integrating over all momentum components \( \hbar k_z \) parallel to the surface (see Appendix C),
\[ G_{3D}^{a}(r,r';E) = G_{3D}^{a}(z,z';\Delta \rho;E) \]
\[ = \frac{1}{2\pi} \int_{0}^{\infty} dk_{x}k_{y}J_{0}(k_{z}\Delta \rho)G_{1D}^{a}(z,z';E-E_{x}), \]

(17)

where \( J_{0}(k_{z}\Delta \rho) \) is the usual cylindrical Bessel function of order zero, and \( E_{x} = \hbar^{2}k_{z}^{2}/2m \) is the kinetic energy of motion in the lateral motion. The lateral distance between \( r \) and \( r' \) is \( \Delta \rho = [(x-x')^{2} + (y-y')]^{1/2} \).

For the numerical evaluation of Eq. (17) it is advisable to use a high-accuracy fast Hankel transform. \cite{32} For \( \alpha = 0 \), the Green function \( G_{2D}^{a}(r,r';E) \) is known in closed form. \cite{31,34}

Also see Appendix B. We assume that the electron moves in the barrier potential with its full mass \( m \); trivial modifications in Eq. (17) will accommodate an effective mass tensor \( m^{*} \).

By construction, \( G_{3D}^{a}(r',r';E) \) is independent of the lateral position \((x',y')\) of the tip and thus cannot give rise to corrugation. Hence, for \( z' = \) constant, \( G_{3D}^{a}(r',r';E) \) is linked to a constant background current.

C. Dyson equation for \( G(r,r';E) \)

The full solution of the model problem defined by Eqs. (9) and (10), \( \psi_{sc}(r;E) = S_{0}G(r,r';E) \), is then obtained in the final step. We need to take into account the term \( W_{ad}(r) \) in Eq. (10):

\[ W_{ad}(r) = \sum_{j=1}^{N} W_{ad}(r_{j}), \]

where \( W_{ad}(r) \) represents the potential of the adsorbed atoms. To this end, STM models generally invoke the Dyson equation, which connects \( G_{2D}^{a}(r',r';E) \) to the full Green function:

\[ G(r,r';E) = G_{2D}^{a}(r,r';E) \]
\[ + \int d^{3}r''G(r,r'';E)W_{ad}(r'')G_{3D}^{a}(r'',r';E). \]

(19)

The Dyson equation (19) is an integral equation, which is largely intractable but for short-range scattering. \cite{38,39} \( W_{ad}(r_{j},r_{j}) = u_{j}D(r_{j},r_{j}) \), reduces to an algebraic equation that can be easily solved. Here the \( u_{j} \) denote the interaction strength between the transmitted electron and the \( j \)-th adatom at \( r = r_{j} \). The function \( D(r) \) represents the regularized \( \delta \) function in three dimensions. We may then write Eq. (19) in the form

\[ G(r,r';E) = G_{2D}^{a}(r,r';E) \]
\[ + \sum_{j,k=1}^{N} G_{2D}^{a}(r_{j},r_{k};E)T_{jk}(E)G_{3D}^{a}(r_{k},r';E), \]

(20)

where the \( T \) matrix takes care of all multiple scattering events among the \( N \) adatoms, that is, sums over all possible orbits. Details can be found in Appendix D.

The imaginary part of the Green function, which is required to calculate the conductivity \( \sigma_{0}(r',E) \) of the tunneling junction according to Eq. (11), assumes a particularly simple form if there is only a single adatom \( (N=1) \) at \( r = r_{1} \).

\[ \text{Im}[G(r',r';E)] = \text{Im}[G_{3D}^{a}(r',r';E)] \]
\[ = |T_{11}| \text{Im}[G_{3D}^{a}(r_{1},r_{1};E)]^{2} \exp(i\Phi), \]

(21)

where \( \Phi \) is the phase of \( T_{11} \). We also have made use of the symmetry property \( G_{3D}^{a}(r',r_{1};E) = G_{3D}^{a}(r_{1},r';E) \). Note that only the second term in Eq. (21) varies during a STM scan for which the tip changes its position \( r' \), thus giving rise to corrugation observed either in the current during a constant height scan \((z' = \) constant) or in the tip-surface distance for a constant current scan \([\sigma_{0}(r',E) = \) constant].

IV. ELECTRON RESONANCES, SURFACE STATES, AND THE “BOUNCING BALL PROBLEM”

An electron surface state can be observed by a STM if the scattered electron stays long enough in the surface region. When the electron leaves the tunnel at \( z = 0 \) (for convenience, we set \( E = 0 \)), we may picture it as bouncing back and forth between the tunnel exit and the surface barrier \((0 < z < z_{w})\).

Eventually, the electron penetrates the surface barrier that hinders the electron from entering the solid \((z > z_{w}) \) (see Fig. 2). A particle moving in the potential given by Eq. (15) will never leave the surface if the barrier strength \( \alpha \) goes to infinity. In this limit the current is restricted to the surface layer. The bouncing-ball problem then can be solved without approximation. \cite{40} In recent years the dynamics of such a quantum bouncer has been of considerable interest. \cite{41-45} The semiclassical Wentzel–Kramers–Brillouin (WKB) solution agrees very well with the exact bound-state spectrum \( E_{n}(\nu) = 0, 1, 2, \ldots, \).

For finite values of \( \alpha \), these bound states become resonances, meaning that the electron can penetrate the barrier at \( z = z_{w} \) after a finite number of reflections. Multiple reflections couple the electron states of the tip and surface. \cite{46}

The resonances are characterized by complex energy values, with the real parts close to the corresponding bound-state energies. We evaluate the background Green function \( G_{3D}^{a}(r,r';E) \) in the resonance approximation (see Appendix C) and obtain:
\[ G_{3D}^{\sigma}(r, r'; E) = \frac{m}{2i\hbar^2} \sum_{n=0}^{\infty} \psi_n(z) \psi_n(z') H_0^{(1)}(k_{\Delta \rho}). \]  

Here \( \psi_n(z) \) denotes the normalized resonant wave function in the potential \( \tilde{W}(z) \) given in Eq. (15), \( k^2_{\rho} = 2m(E - E_\rho) / \hbar^2 \) is the lateral wave number, and

\[ H_0^{(1)}(u) = J_0(u) + iY_0(u) \]

is an outgoing wave Hankel function. For the closed channels with \( E_\rho = E \) the wave number \( k_\rho \) becomes almost purely imaginary. In this case, the relation \( \pi H_0^{(1)}(u) = -2iK_0(u) \) [where \( K_0(u) \) is a modified Bessel function] shows that these contributions are almost real; they also will drop off exponentially with increasing lateral distance \( \Delta \rho \). The sum in Eq. (22) becomes ill-conditioned, however, as \( \Delta \rho \to 0 \).

According to Eq. (11), the conductivity of the STM junction, \( \sigma_\rho^{(2)}(r^2; E) \), depends only on the imaginary part of the Green function at the position of the tip \( r^2 \). In our case study, only the ground state \( (\nu=0) \) will effectively contribute to the STM image (see Fig. 2). If we neglect all higher terms in Eq. (22), we find an approximate analytic expression for the corrugation in a constant-height scan \( (z'=\text{constant}) \). If we ignore the off-diagonal elements of the \( T \) matrix (diagonal resonance approximation), that is, treat all adatoms as isolated scatterers, Eq. (20) yields:

\[ \text{Im} \left[ G(r', r; E) \right] = A + A^2 \sum_{j=1}^{N} \text{Im} \left[ T_{j,j}(E) H_0^{(1)}(k_{\Delta \rho}) \right], \]

where \( \Delta \rho_j = [(x_j-x)^2 + (y_j-y)^2]^{1/2} \) is the lateral distance between the tip and atom number \( j \). The constant \( A = -m/\left[ \psi(z')^2 \hbar^2 \right] \) can be found from Eq. (22); it depends only on the transmission coefficient \( T(E) \) of the potential barrier \( \tilde{W}(z) \) between the tip and surface. We remark that the corrugative part of the conductivity in Eq. (24) is proportional to \( T(E)^2 \) and thus decays twice as fast with increasing separation \( z' \). For a first comparison with experimental results, the constants \( A \) and \( T_{j,j}(E) \) can be regarded as fit parameters. The neglect of the nondiagonal matrix elements of the \( T \) matrix will be shown to be a reasonably good approximation (see also Fig. 4).

We remark that the Hankel function \( H_0^{(1)}(k_{\Delta \rho}) \) is the Green function of a free particle moving in a plane (see Appendix C). Equation (22) therefore explains why the two-dimensional, freely propagating model discussed in Refs. 46 and 47 can reproduce the experimentally observed corruga-

\[ \text{tion in corral structures.}^{13} \]

V. NUMERICAL EVALUATION

We now can calculate the current profile. At constant current (and fixed voltage), the task is to determine a surface of constant conductivity. In this case the position \( r' \) of the tip is varied with the constraint \( \sigma_{\rho}(r', E) = \text{constant} \) [see Eqs. (11) and (12)]. A zero-temperature corrugation plot obtained from such a calculation (which typically takes a few minutes on a personal computer) is shown in Fig. 3. When the bias voltage has the appropriate sign, electrons will move from an occupied tip state to an unoccupied surface state in the presence of a quantum corral. In this case the square brackets in Eq. (14) can be replaced by unity.

![Fig. 3. Model calculation of a corrugation plot at constant conductivity \( \sigma_\rho \). The structure of the circular ripples both inside and outside the corral can be related to the quantum boundary problem illustrated in Fig. 2 and discussed in the text. For comparison with experimental results (Refs. 4 and 5) using Fe adatoms placed on a Cu(111) surface, we show a similar setup with a single scatterer on a reflecting surface (upper panel) and a quantum corral consisting of 48 atoms on a circle with radius 71.3 Å. The corrugation of the adatoms is 0.5 Å and corresponds to the conductivity \( \sigma_\rho = 2.7 \times 10^{-4} \text{A/\text{V}} \). All other parameters are given in the text. Note that there is no adatom at the center of the corral.]

The following parameters were used for our model calculation: The binding energy of the tip \( s \)-orbital is fixed at \( E_{\text{bind}} = 4.3 \text{ eV} \) (see Fig. 2). The strength of the electric field is \( F = 1 \text{ eV/Å} \). The electron exits the tunnel at \( z = 0.3 \text{ Å} \), that is, \( E = -0.3 \text{ eV} \). The adatoms are located in the plane \( z = 0 \), and the strength of the reflecting surface barrier at \( z = 4 \text{ Å} \) is \( \alpha = 60 \text{ eV/Å} \). The average distance between tip and adatoms is chosen to be \( 4 \text{ Å} \). The atomic potential strength \( U_j = 27.6 \text{ eV}^3 \) corresponds to an \( s \)-wave scattering length \( g^{-1} = 0.57 \text{ Å} \) (see Appendix D). We used \( k_{\rho} = 1.5 \text{ Å}^{-1} \) as a typical value for the Fermi wave number of a \( s \) (metallic) tip.

As we have explained, the term \( G_{3D}^{s}(r, r'; E)G_{3D}^{s}(E) \) in Eq. (20) accounts for the observed surface roughness. The \( T \) matrix plays an essential role for surface electron scattering.\(^{46,49,50}\) The analytical model presented here clearly bears this out. For a single adsorbed atom \( (N = 1) \), the \( T \) matrix reduces to a \( r \)-number. Its absolute value will become large for \( \nu = -\text{Re}(C(E)) \) (Appendix D). Such a situation leads to an amplification of atomic corrugation and resolution.

It is useful to explore the resonance approximation (22) to the Green function \( G_{3D}^{s}(r, r'; E) \) in more detail because this quantity controls the current profile. In the example under consideration the first resonance occurs at \( E_\rho = -0.411 \text{ eV} \) \((-0.376 \text{ eV in the WKB approximation}) \) and dominates the current. As can be seen from Fig. 2, higher resonances \( (\nu > 0) \) with energies \( E_\rho < E \) are classically forbidden and can
Fig. 4. Conductivity profile of a quantum corral for a constant-height scan. The conductivity is evaluated in various approximations. The full line represents the result from the T-matrix calculation (20). Also shown are the diagonal resonance approximation neglecting the off-diagonal elements of the T matrix in the sum in Eq. (20), and the approximation (24), where the Green function expansion (22) has been truncated after the leading term ($n=0$). To achieve quantitative agreement with experiment (Ref. 5), an admixture of several Hankel functions (instead of one) is required.

be omitted. In this approximation we therefore have an outgoing cylindrical surface wave with asymptotic wave number $k_0=(2mE_1/\hbar)^{1/2}$ which results from energy conservation, $E_1=E-E_0=0.111$ eV.

The Hankel function $H_0^{(1)}(k_0\rho)$ oscillates in the $\rho$ direction with spatial periodicity $\Lambda_0=2\pi/k_0=36.81\ \AA$. Because of the second term in Eq. (19), the contribution responsible for the corrugation $G_{5D}^{3D}T_{5D}^{3D}$ will asymptotically exhibit oscillations with half the wavelength $18.41\ \AA$, in perfect agreement with the results shown in Fig. 3. (The small imaginary part, $\text{Im}E_0=-3.9$ meV, causes the decay of the cylindrical surface wave into the sample bulk on a lateral length scale $\xi=410\ \AA$, which does not affect our interpretation of Fig. 3.) The quantum corral shown in Fig. 3 is indeed leaky, and the electrons are therefore not confined to the corral.

Figure 4 shows the conductivity profile observed in the quantum corral of Fig. 3 where the distance between the tip and surface-adatom is kept constant at $z=4\ \AA$. The distance between the tip and surface barrier is twice as large. It is interesting that the approximation (24), despite its simplicity, yields a fast and reliable means of simulating the quantum corral apart from the vicinity of the adatoms where the single-resonance approximation is not adequate, as we have discussed. Because $H_0^{(1)}(u) \sim 2i\ln u/\pi$ as $u \to 0$, this approximation diverges logarithmically at the positions of the adatoms.

The theoretical method presented here is not confined to adatoms on a circle. An example of another simple structure is shown in Fig. 5 where the adatoms are lined up on a parabola. As in the case of the circular quantum corrals, elastic scattering from the adatoms and the subsequent interference of the scattered electron waves will result in an oscillatory electronic density pattern.

VI. CONCLUSION

Our intention has been to demonstrate that "quantum corrals are the beautiful result of a marriage between technology and basic science." By utilizing the idea of quantum sources, we have presented a case study of the STM where both the tip and sample were included in a nonperturbative fashion. We regarded the tip as a quantum source for the electrons and used a few model parameters to calculate the current profile of simple atomic surface structures analytically, apart from the inversion of a matrix and the evaluation of the integral in Eq. (17). The conditions that favor the detection of single atoms and electron surface states were worked out in detail.

The use of localized particle sources is not restricted to tunneling sources. Recent examples of spatially-extended or time-dependent sources are given in Refs. 51, 24, 52, and 53. In addition, the source formalism does not depend on simple model potentials such as the one given by Eq. (10), but can be combined with more elaborate field configurations and scattering amplitudes that are taken from ab initio calculations. We note that the Green function formalism gives access to the full electronic wave function (20) rather than just the density of states (21) used in the STM calculations. This advantage could render the source formalism an important tool in problems such as mesoscopic transport, quantum chaos, and order–disorder transitions.

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APPENDIX A: TRANSPORT PROPERTIES OF A QUANTUM SOURCE

In the presence of the source term $S(r;E) = W(r)\psi_{spec}(r;E)$ given in Eq. (4), solutions to the stationary Schrödinger equation (5) may carry a persistent current generated in the source region. The current density $j(r)$ is given by the usual expression
\[ j(r;E) = \frac{\hbar}{2im} [\psi_{sc}^* \nabla \psi_{sc} - \psi_{sc} \nabla \psi_{sc}^*] , \]  
(A1)

with \( \psi_{sc}(r;E) \) satisfying Eq. (5). By differentiation and comparison with Eq. (5), we infer that the source generates particles at the local rate:

\[ \text{div} \, j(r;E) = \frac{i}{\hbar} [S^* \psi_{sc} - \psi_{sc} S] = -\frac{2}{\hbar} \text{Im}[S^*(r;E)\psi_{sc}(r;E)]. \]  
(A2)

Note that this rate depends on the wave function \( \psi_{sc}(r;E) \), which lets us incorporate the boundary conditions into Eq. (A2). The total particle current \( J(E) \) sustained by the source is obtained by integration over a surface \( \partial \Omega \) enclosing the source region \( \Omega \):

\[ J(E) = \oint_{\partial \Omega} d\Omega j(r;E) \cdot \mathbf{n}(r) = \int_{\Omega} d^3r \text{div} \, j(r;E). \]  
(A3)

In view of Eq. (A2), Eq. (A3) yields

\[ J(E) = \frac{2}{\hbar} \text{Im} \left[ \int d^3r S^*(r;E) \psi_{sc}(r;E) \right]. \]  
(A4)

We express the scattering wave \( \psi_{sc}(r;E) \) in terms of the energy Green function \( G(r,r';E) \) in Eq. (6) and obtain a bilinear expression for the total current \( J(E) \):

\[ J(E) = \frac{2}{\hbar} \text{Im} \left[ \int d^3r_1 d^3r_2 S^*(r_1;E) G(r_1,r_2;E) S(r_2;E) \right]. \]  
(A5)

For orthonormalized basis states,

\[ \int d^3r \psi_{hga}(r;E)^* \psi_{hgb}(r;E') = \delta(E - E'), \]  
(A6)

it is easily verified that the term in square brackets in Eq. (A5), and therefore the product \( \hbar J(E) \), is dimensionless. In other words, \( J(E) \) is the particle number current per energy, and we may write

\[ J(E) = \frac{dN}{dE}. \]  
(A7)

The differential conductivity \( \sigma_d = dI/dU \) is obtained from Eqs. (A8) and (A7) by realizing that the variation \( dU \) in the applied bias voltage leads to the change \( dE = -\hbar \alpha > 0 \) in the electron energy, while the particle number current \( dN \) is equivalent to an electric current \( J = -e dN \). Hence, the intrinsic conductivity is \( \sigma_d = e^2 J(E) \).

For the isotropic point source \( S(r) = S_0(E) \delta(r - r') \) in Eq. (8), Eq. (A5) yields

\[ J(E) = \frac{\hbar^2}{2m} [k^2 + \Delta] \psi_{sc}(r;E) S_0(E) \delta(r - r'). \]  
(A9)

The retarded solution \( \psi_{sc}(r;E) \) of the free-particle Green function,

\[ G_{\text{free}}(r,r';E) = -\frac{m}{2\pi\hbar^2} \frac{e^{i|r-r'|}}{|r-r'|}, \]  
(A10)

is an outgoing spherical wave. The maximum strength \( S_0(E) \) of the free-particle source can be found from Pauli's principle—only one electron is allowed to occupy each scattering state. This constraint relates to the normalization of the wave functions \( \psi_{sc}(r;E) \). If we use Eq. (A10), we find

\[ \int d^3r \psi_{sc}(r;E)^* \psi_{sc}(r;E') - \frac{mk}{\hbar^2} S_0(E)^2 \delta(E - E'), \]  
(A11)

and hence we obtain a physical limit for the emission strength \( S_0(E) \) for asymptotically free electrons:

\[ |S_0(E)|^2 = \frac{\hbar^2}{mk}. \]  
(A12)

The conductivity of the free s-wave point source is therefore quantized, \( \sigma_{\text{free}} = e^2 / \pi \hbar \), as expected for a mesoscopic conductor. To establish the connection with the STM, we assume that the tip essentially acts as a point source of free electrons whose initial energy is determined by the Fermi energy \( E_F \) of the tip metal. Equation (A8) presents a natural extension of the familiar Landauer formulae \( \sigma_{ij} = e^2 |t_{ij}|^2 / \hbar \) describing the conductivity of the three-dimensional STM junction.

Classically, the imaginary part of \( G(r',r';E) \) contains information about all closed orbits that begin and end at the position \( r = r' \) of the electron source. Quantum mechanically, the imaginary part of the Green function can be related to the local density of states

\[ n(r;E) = \sum_{\{k\}} |\psi_k(r)|^2 \delta(E - E_k), \]  
(A13)

where the symbolic sum runs over the complete and normalized set \( \{k\} \) of bound and continuous eigenstates \( \psi_k(r) \) with eigenenergy \( E_k \). The connection is established by writing the (retarded) Green function in the form

\[ G(r,r';E) = \sum_{\{k\}} \frac{\psi_k(r) \psi_k(r')^*}{E - E_k + i\eta}, \]  
(A14)

with \( \eta \to 0^+ \) and using the fact that \( \text{Im}[E - E_k + i\eta]^{-1} = -\pi \delta(E - E_k) \). From Eqs. (A13) and (A14) we have the identity

\[ n(r;E) = -\frac{1}{\pi} \text{Im}[G(r,r;E)]. \]  
(A15)

which connects the source formalism to the approach in Refs. 2 and 3.

**APPENDIX B: THREE-DIMENSIONAL TUNNELING PROPERTIES**

In the notation of Eq. (15), the retarded Green function of the one-dimensional ballistic problem is the solution of
that behaves like an outgoing wave as $z \rightarrow \infty$. It is not difficult to verify that,

$$G_{1D}^0(z, z'; E) = -4\pi\Delta F^2 C_i(u_+)|A_i(u_-)|,$$  \hspace{1cm} (B2)

with

$$u_+(z, z') = -\mathcal{B}[2E F(z + z') + F|z - z'|],$$  \hspace{1cm} (B3)

and $\mathcal{B} = [m/(4\hbar^2 F^2)]^{1/3}$. Here, $A_i(u)$ denotes the Airy function, and $C_i(u)$ is a Hankel-type outgoing wave solution to the Airy differential equation. In three dimensions, with the substitutions $F \rightarrow F^3 r$ and $d^2/dz^2 - V^2$ we find for the Green function of a uniform force field

$$G_{3D}^0(r, r'; E) = \frac{m}{2\hbar^2} \frac{1}{|r - r'|} [C_i(u_+)|A'_i(u_-)| - C'_i(u_+)|A_i(u_-)|],$$  \hspace{1cm} (B4)

where

$$u_+ = -\mathcal{B}[2E F \cdot (r + r') + F|r - r'|].$$  \hspace{1cm} (B5)

The primes denote derivatives of the Airy functions with respect to their arguments. This result can be derived by evaluating Eq. (21) with $\alpha = 0$ or, more easily, by means of parametric differentiation of an integral representation of $G_{1D}^0(z, z'; E)$.\textsuperscript{31,34}

Tunneling in three dimensions gives rise to effects that are absent in the usual textbook treatment of one-dimensional tunneling problems. For example, starting from a point-like source in the tunnel (circle in Fig. 6), the particle wave is free to spread in the lateral directions parallel to the surface as it moves through the tunneling region. At the end of the tunnel ($z = 0$), the emerging particle current [see Eq. (A1)] forms a circular current "spot." As can be inferred from Fig. 7, the shape of the tunneling spot is almost independent of the shape of the barrier. This independence might come as a surprise because the absolute tunneling probability (and thus the conductivity of the STM junction) strongly depends on the permeability of the barrier. Ultimately, the lateral width of the tunneling current spot determines the spatial resolution of the STM.\textsuperscript{99} The results shown in Fig. 7 explain why an apparently poor choice for the potential barrier in the junction, such as the linear potential $\mathcal{W}(z)$ used in Eq. (10), is able to give realistic simulations of STM images. We also note that the width of the current distribution always greatly exceeds the size of the emitting atom, justifying the idealized point source approach put forward in Sec. II.

A heuristic argument shows that irrespective of the details of the barrier potential, the current distribution at the surface will invariably be approximately Gaussian in shape. Deviations from the ideal escape path both in space (because the path then dells further into the tunneling sector) and in momentum space (where the kinetic energy bound in lateral motion must be compensated by an energy loss for the motion in the $z$ direction, effectively raising the tunneling barrier) carry a large penalty and are exponentially suppressed. These constraints squeeze the lateral uncertainties $\Delta \rho$ and $\Delta \rho_\rho$ of the scattering wave function $\psi_\rho(r; E)$, and therefore their product tends toward its minimum value, $\Delta \rho \Delta \rho_\rho = \hbar$. But minimum uncertainty states are always Gaussian.\textsuperscript{99} In addition, the width of the Gaussian spot is fixed by the ratio of the average lateral spreads $\Delta \rho$ and $\Delta \rho_\rho$, which in turn is a measure of the time an electron spends in the tunneling barrier. For the linear potential, this time is approximated roughly by the semiclassical bounce (or instanton) time scale\textsuperscript{31}

$$\tau_b(E_A) = m\Delta \rho/\Delta \rho_\rho = \hbar \xi F,$$  \hspace{1cm} (B6)

where $\xi = \sqrt{-2mE_A}/\hbar$ and $E_A$ is the initial binding energy in the barrier ($E_A = 3.2$ eV in Fig. 6). We point out that oriented "multipole" point sources with higher orbital character ($l > 0$), such as $p_x$ and $d_{z^2}$-tip states,\textsuperscript{26} generate increasingly narrow tunneling spots. These tip states were invoked by Chen to explain the resolution capability of the STM.\textsuperscript{21,23}
APPENDIX C: SEPARABLE POTENTIALS

Closed-form expressions for the corresponding Green function \(G(r, r'; E)\) (7) are obtained for only a few threedimensional potentials \(W(r)\). Otherwise, we need to use numerical methods. Here, we sketch a technique that works for simple separable potentials.

Assume that the Hamiltonian \(H(r) = H_1(r_1) + H_2(r_2)\) may be written as a sum of two commuting parts, where \(H_1(r_1)\) depends only on the partial set of coordinates \(r_1\), while \(H_2(r_2)\) depends on the complementary set \(r_2\). We denote the (normalized) eigenfunctions and eigenenergies for the Hamiltonian \(H_2(r_2)\) by \(\chi_1^{(2)}(r_2)\) and \(E_2^{(2)}\), respectively. According to Eq. (A14), the retarded Green function \(G_r^S(r_1, r_1'; E)\) for the Hamiltonian \(H_1(r_1)\) in the space of reduced dimension \(\{r_1\}\), is a solution to

\[
[E - H_1(r_1)]G_r^S(r_1, r_1'; E) = \delta(r_1 - r_1'),
\]

and is given by the symbolic sum over its spectrum \(\{k_1\}\):

\[
G_r^S(r_1, r_1'; E) = \lim_{\eta \to 0^+} \frac{\chi_1^{(1)}(r_1)\chi_1^{(2)}(r_1')^*}{E - E_2^{(2)} + i\eta},
\]

The spectrum of the complete Hamiltonian \(H(r)\) is the product of the spectra of its parts, \(\{k\} = \{(k_1, k_2)\}\). Its eigenfunctions \(\psi_k(r) = \chi_1^{(1)}(r_1)\chi_2^{(2)}(r_2)\) are all possible products of the eigenfunctions of the constituent Hamiltonians, and the corresponding eigenvalues \(E_k = E_1^{(1)} + E_2^{(2)}\) are the sum of the partial eigenvalues. From Eq. (A14), the energy Green function associated with \(H(r)\) then reads:

\[
G(r, r'; E) = \lim_{\eta \to 0^+} \sum_{\{k\}} \frac{\chi_1^{(1)}(r_1)\chi_1^{(1)}(r_1')^*}{E - E_1^{(1)} + i\eta} \times \frac{\chi_2^{(2)}(r_2)\chi_2^{(2)}(r_2')^*}{E - E_2^{(2)} + i\eta},
\]

or by comparison with Eq. (C2),

\[
G(r, r'; E) = \sum_{\{k\}} \frac{\chi_1^{(1)}(r_1)\chi_1^{(1)}(r_1')^*G_2(r_2, r_2'; E - E_1^{(1)})}{E - E_1^{(1)}},
\]

thereby effectively reducing the number of dimensions in the determination of the Green function.

We used this technique when we calculated the background Green function \(G_3D^{\alpha}(r, r'; E)\) in Eq. (17) from its onedimensional counterpart, and also in the "resonance approximation" (22) which decomposes the Green function into contributions of discrete channels linked to the resonant states in the \(z\) direction. Note that the Hankel function \(H_1^{(0)}(kx)\) in \((u)\) represents the free-particle Green function in two dimensions:

\[
G_{2D}^{\alpha}(r_1, r_1'; E) = \frac{m}{2\hbar^2}H_1^{(0)}(k|r_1 - r_1'|).
\]

APPENDIX D: THE T MATRIX FOR SHORT-RANGE POTENTIALS

We iterate Eq. (22) and obtain the expansion

\[
G = G_3D^{\alpha} + G_3D^{\alpha}W_{ad}G_3D^{\alpha} + G_3D^{\alpha}W_{ad}G_3D^{\alpha}W_{ad}G_3D^{\alpha} + \cdots,
\]

which is commonly referred to as the Born or Neumann series for \(G\). If we introduce the transition operator (or \(T\) matrix)

\[
T = W_{ad} + W_{ad}G_3D^{\alpha}T,
\]

we can write Eq. (D1) as

\[
G = G_3D^{\alpha} + G_3D^{\alpha}TG_3D^{\alpha}.
\]

The formal solution of Eq. (D2) for \(T\) yields

\[
T = [1 - W_{ad}G_3D^{\alpha}]^{-1}W_{ad}.
\]

Before we continue with the evaluation of Eq. (D4) for short-range scattering potentials, we discuss their somewhat peculiar behavior in three dimensions. The three-dimensional analog of a one-dimensional zero-range potential (ZRP) is obtained by the substitution:

\[
0 \delta(z) \rightarrow u \delta(r)\partial_r,
\]

where \(V_0\) and \(u\) are constants, and \(r = |r|\) is the radial distance. The operator \(\partial_r\) is necessary to regularize the three-dimensional delta potential, which otherwise would have ill-defined scattering properties. The resulting point-like pseudopotential,

\[
W_{ZRP}(r) = uD(r) = u\delta(r)\partial_r,
\]

supports pure \(s\)-wave scattering, where the scattering solutions \(\psi_k(r)\) are given by

\[
\psi_k(r) \sim e^{ikr} - \frac{1}{ik + \xi} \frac{e^{ikr}}{r}.
\]

Here, \(\xi = 2\pi\hbar^2/mu\) denotes the inverse scattering length of the potential at energy \(E = 0\). Note that the cross section diverges when \(k = i\xi\); this divergence can only occur for \(u > 0\) and corresponds to a single bound \(s\)-state with energy

\[
E_b = -\hbar^2\xi^2/(2m).
\]

Its wave function reads:

\[
\psi_0(r) = \frac{\xi}{2\pi r}e^{-\xi r}.
\]

For continuum states and in the limit \(k \to 0\), \(W_{ZRP}(r)\) behaves attractively for \(u < 0\). Therefore we expect positive corrugation (see Fig. 3) for negative values of \(u\). We now model the adsorbate as a sum of zero-range potentials (D6) located at the positions of the \(N\) adatoms in Eq. (18):

\[
W_{ad}(r) = \sum_{j=1}^{N} W_{ad}(r, r_j) = \sum_{j=1}^{N} u_j D(r - r_j).
\]

Although Eq. (D1) in space presents an intractable integral equation in general, it is not difficult to see that with the choice (D9), the Neumann series reduces to an algebraic sum that involves only the matrix elements:
\[ C_{jk}(E) = \lim_{r \to r_j} \frac{\partial^2}{\partial r^2} [r - r_j] G^{\alpha}_{3D}(r, r_k; E). \] (D10)

If we introduce the diagonal matrix \( \mathbf{U} = \text{diag}(u_1, u_2, \ldots, u_N) \) with the scattering strengths \( u_1, \ldots, u_N \) of the \( N \) individual adatoms, a comparison with Eq. (D4) yields the \( T \) matrix of the system \( T(E) \) as the inverse of the \( N \times N \) matrix:

\[ T(E) = [\mathbf{1} - \mathbf{U}C(E)]^{-1} \mathbf{U} = [\mathbf{U}^{-1} - \mathbf{C}(E)]^{-1}. \] (D11)

Finally, according to Eq. (D3), we write the Green function of the full problem \( G(r, r'; E) \) as a matrix product involving the Green function of the background potential \( G^{\alpha}_{3D}(r, r'; E) \):

\[ G(r, r'; E) = G^{\alpha}_{3D}(r, r'; E) + \sum_{j,k=1}^{N} G^{\alpha}_{3D}(r, r_j; E) T_{jk}(E) G^{\alpha}_{3D}(r_k, r'). \] (D12)

This form of the Dyson equation forms the basis for the developments of Sec. III C.

It remains to determine the matrix elements \( C_{jk}(E) \) in Eq. (D10) from the background Green function. According to the theory of elliptic differential operators, the solution \( \psi_{\alpha}(r; E) \) of the inhomogeneous Schrödinger equation (S) will be an analytic function everywhere in space, except at those points where either the potential \( W(r) \) or the source inhomogeneity \( S(r) \) become singular. The Green function under consideration is therefore analytic if the potential \( W(r) \) in Eq. (15) is analytic, that is, \( \epsilon \neq \epsilon_0 \) holds, and if \( r \neq r' \) [because otherwise the point source \( S(r) = S_0 \delta(r-r') \) in Eq. (8) is manifestly singular]. Because we place all adatom centers \( r_j \) in the space between the tip and the reflecting potential layer, we may expand \( G^{\alpha}_{3D}(r, r_j; E) \) into a power series about \( r = r_j \), for \( r_j \neq r_k \) and immediately find for the off-diagonal elements of \( C(E) \):

\[ C_{jk}(E) = G^{\alpha}_{3D}(r_j, r_k; E) \quad (j \neq k). \] (D13)

For \( r_j = r_k \), this line of reasoning fails, and the Green function is singular. A more elaborate argument\(^{36}\) shows that the singularity is weak in the sense that \( G^{\alpha}_{3D}(r, r_k; E) \) can be decomposed into a sum:

\[ G^{\alpha}_{3D}(r, r_k; E) = -\frac{m}{2\pi \hbar^2} \left[ f(r, r_k; E) + g(r, r_k; E) \right], \] (D14)

where \( f \) and \( g \) are analytic functions in \( r \), even as \( r \to r_k \). Furthermore, \( f(r, r_k; E) \) is a unique, real, and symmetric function that has the expansion:

\[ f(r, r_k; E) = 1 - \frac{1}{2} \frac{\xi^2}{(r - r_k)^2} + O((r - r_k)^3). \] (D15)

where \( \xi = 2M[E - \bar{W}(r_k)]/\hbar^2 \) is the initial wave number of the particle. As an example, we note that the free-particle Green function \( G_{\text{free}}(r, r_k; E) \) in Eq. (A10) fits this description with \( f_{\text{free}}(r, r_k; E) = \cos(\Delta r_{r_k}) \) and \( g_{\text{free}}(r, r_k; E) = -im \sin(\Delta r_{r_k})/(2\pi \hbar^2) \). In particular, for \( E = 0 \) we recover the Green function of potential theory:

\[ G_{\text{free}}(r, r_k; E = 0) = -\frac{m}{2\pi \hbar^2} \frac{1}{|r - r_k|} \int_0^\infty dk_z J_0(k_z \Delta \rho) \times \exp(-k_z |z - z_k|). \] (D16)

The integral representation follows from Eq. (17) after inserting the free-particle Green function in one dimension, \( G_{\text{free}}^{\alpha}(z, z_k; E < 0) = -me^{-i\kappa z}/(\hbar^2 \kappa) \), where \( E = -\hbar^2 \kappa^2/(2m) \).

For further reference, we remark that the decomposition (D14) yields \( f_{\text{free}}(r, r_k; E = 0) = 1 \) and \( g_{\text{free}}(r, r_k; E = 0) = 0 \).

We return to the coefficients \( C_{jk}(E) \), for \( j = k \) and now evaluate Eq. (D10) using the decomposition of the Green function (D14). Due to the special structure of the function \( f(r, r_k; E) \) in Eq. (D15), the derivative \( D(r - r_k) \) of the first term identically vanishes:

\[ \lim_{r \to r_k} \frac{\partial}{\partial r} \left[ \frac{f(r, r_k)}{|r - r_k|} \right] = \lim_{r \to r_k} \epsilon_{r_k} \cdot \nabla f(r, r_k) = 0. \] (D17)

It is now easy to verify that the diagonal matrix elements of \( C(E) \) depend only on the second function in Eq. (D14):

\[ C_{kk}(E) = g(r, r_k; E). \] (D18)

As a practical means of evaluating the function \( g(r, r_k; E) \), we note that the leading term of the singularity in the Green function at the source location can be removed by proper regularization. From Eqs. (D14)-(D16), it follows that

\[ \lim_{r \to r_k} [G^{\alpha}_{3D}(r, r_k; E) - G_{\text{free}}(r, r_k; E = 0)] = g(r, r_k; E). \] (D19)

We replace the Green functions in Eq. (D19) by their integral representations (17) and (D16), respectively, and obtain the relation:

\[ C_{kk}(E) = \frac{1}{2\pi} \int_0^\infty dk_z J_0(k_z \Delta \rho) G^{\alpha}_{1D}(z_k, z_k; E - E_\lambda) + \frac{m}{\hbar^2} \] (D20)

with \( E_\lambda = \hbar^2 k_z^2/(2m) \), which is useful for numerical evaluation of the \( T \) matrix. We finally remark that for the simple linear potential ramp considered in Appendix B, a direct evaluation\(^{36}\) of the Green function \( G^{\alpha}_{3D}(r, r_k; E) \) in Eq. (B4) yields

\[ C_{kk}(E) = \frac{m\beta}{\hbar^2} \left( \nu Ci(u)Ai(u) - Ci'(u)Ai'(u) \right). \] (D21)

where \( \nu = -2\beta(E + Fz_k) \), and \( \beta^2 = m/(2\hbar^2) \). Together with Eq. (B2), this result may be used to validate the numerical integration scheme applied in Eq. (D20).

\( ^{36}\)Electronic mail: mkleber@ph.tum.de


9 P. A. Tipler and G. Mosca, Physics for Scientists and Engineers (Freeman, New York, 2003), 5th ed.
11 A. Messiah, Quantum Mechanics (North-Holland, Amsterdam, 1962), Vol. II.
14 J. Schwinger, Particles, Sources and Fields (Addison-Wesley, Reading, MA, 1973), Vol. II.
32 M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1972).
35 R. G. Newton, Scattering Theory of Waves and Particles (Dover, New York, 2002), 2nd ed.
40 J. Sakurai, Modern Quantum Mechanics (Addison-Wesley, Reading, MA, 1985).