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# Tunnel current and generalized Ehrenfest theorem

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**Abstract.** The interrelation between two different theoretical formulations of the theory of scanning tunnelling microscopy (STM) is investigated. The mathematical equivalence of the current density formulation of STM theory and the generalized Ehrenfest theorem (GET) is demonstrated. The GET is of practical importance, because it facilitates the numerical evaluation of the tunnel current and provides additional physical insight. Using formal scattering theory, the integration of the current density over a plane parallel to the sample electrode yields half the value of the total tunnel current as obtained from the generalized Ehrenfest theorem. This discrepancy is removed if an adequate normalization of the wavefunction in the current density formulation is chosen. The proof includes a generalization of Bardeen's transfer Hamiltonian expression for the transition matrix element.

## 1. Introduction

The intuitive approach to calculating the current in STM theory is to first evaluate the current density in position space and then to integrate it over an interface parallel to the electrodes (Lucas *et al* 1988, Vigneron *et al* 1990, Derycke *et al* 1991). An apparently completely different approach starts from the transfer Hamiltonian formulation given by Bardeen (1961). This is a perturbative theory that agrees with exact methods (e.g. the wavefunction matching method (Garcia *et al* 1983, Stoll *et al* 1985)) in the limit in which the overlap is small. Problems connected with the derivation of Bardeen's result have been discussed in the literature (Prange 1963, Duke 1969). Feuchtwang and Cutler (1987) emphasized the importance of these unsolved problems for STM theory.

Several three-dimensional approaches to the theory of STM have been formulated which do not rely on Bardeen's perturbation approach (see e.g. Lang (1987) and Noguerra (1989)). Numerically exact solutions of the STM current have been sought mainly via a current density formulation (Pendry *et al* 1991, Lucas *et al* 1988, Vigneron *et al* 1990, Derycke *et al* 1991). The connection between the current density formulation and the transfer Hamiltonian approach has, however, remained unclear and this needs to be established in order to obtain a sound foundation of STM theory. Pendry *et al* (1991) addressed this problem by starting from the current density point of view and deriving Bardeen's transfer Hamiltonian expression in the perturbation limit. The idea behind the transfer Hamiltonian approach can be generalized to an exact treatment of STM theory by using the generalized Ehrenfest theorem (GET) (Doyen 1993).

The current density itself is not an observable as it implies simultaneous sharp measurements of position and momentum (Schiff 1968). It is usually maintained that integration over an interface yields the observable 'total current'. The primary aim of this paper is to prove the equivalence of the current density formulation and the GET. It has

already been demonstrated that the GET has relevance in real calculations, because it offers several advantages (Doyen 1992). The current density formulation requires integration in the position space of an oscillating function. The summation over the initial states involves the evaluation of many different current densities. This is time consuming and of limited accuracy. The calculation of the Green operator in the local environment of the tip also requires a summation over many states. With the help of the GET the total current can be obtained directly from quantities which become available when constructing the local Green operator. The additional steps necessary for evaluating the current density distribution can then be omitted. The GET also provides additional physical insight, because it allows the definition of the tip-projected local density (TIP-LOD) and capacitor-projected local density (CAP-LOD) which are helpful in the interpretation of the numerical results. The total tunnel current factorizes in TIP-LOD, CAP-LOD and the square of an effective tip-induced potential, which permits us to separate the influence of the tip-sample interaction on the tunnel current in a unique way (Doyen 1993).

The problem is stated in its mathematical form in section 2. A generalization of Bardeen's formula which applies to the exact transition matrix element is derived in section 3. This generalized Bardeen formula is an essential step in the proof of the equivalence of the two approaches. The expansion coefficients of the exact scattering wavefunction in a plane-wave basis are calculated in section 4. The normalization of the scattering wavefunction is discussed in section 5.

## 2. The problem

The exact formulation in scattering theory is to calculate the total current of the scattering wavefunction  $|\hat{i}+\rangle$  from the generalized Ehrenfest theorem (GET) (Lippmann 1965):

$$J(\hat{i}) = \frac{2\pi e}{\hbar} \sum_f |\langle f | V_{\text{tip}} + V_{\text{sample}} | \hat{i}+\rangle|^2 \delta(E_f - E_i) \quad (1)$$

where  $|f\rangle$  is a current-carrying state in the sample metal (the states are labelled by the incident momentum  $\hat{i}$  and the final momentum  $f$ , respectively). The meaning of the scattering potentials is explained below. Equation (1) describes the scattering of a single electron. To obtain total tunnel currents as measured in experiment, the contributions due to all incoming electrons have to be summed. In this paper only the current induced by a single electron is calculated.

As Bardeen's expression can be derived from the generalized Ehrenfest theorem in first-order perturbation theory (by replacing  $|\hat{i}+\rangle$  by the unperturbed tip wavefunction  $|\hat{i}\rangle$ ), the work of Pendry *et al* (1991) can be taken as having demonstrated that in the perturbation limit the current density formulation and the GET reduce to the same expression. However, this does not prove the equivalence to the GET for strong coupling and hence does not establish the connection to the exact formulation of scattering theory. The current density of the scattering wavefunction  $|\hat{i}+\rangle$  is defined by

$$\mathbf{j}(\mathbf{r}) = \frac{e\hbar}{m} \text{Im}(\psi_{i+}^* \nabla \psi_{i+}) = \frac{e\hbar}{2im} (\psi_{i+}^* \nabla \psi_{i+} - (\nabla \psi_{i+}^*) \psi_{i+}). \quad (2)$$

We make the connection between formal scattering theory and the position space representation of the scattering wavefunction by means of the relationship:

$$\psi_{i+}(\mathbf{r}) = \langle \mathbf{r} | \hat{i}+\rangle = \sum_k \langle \mathbf{r} | \mathbf{k}\rangle \langle \mathbf{k} | \hat{i}+\rangle$$

where  $|\mathbf{k}\rangle$  is a generalized eigenvector of the momentum operator and

$$\langle \mathbf{r} | \mathbf{k} \rangle = (2\pi\hbar)^{-1/2} e^{i\mathbf{k}\mathbf{r}/\hbar}.$$

The definition of the total current is the surface integral of the current density:

$$\begin{aligned} J_{\partial G}(\mathbf{i}) &= (e\hbar/m) \int_{\partial G} \text{Im}(\psi_{i+}^* \nabla \psi_{i+}) d\mathbf{F} \\ &= (e\hbar/m) \text{Im}\langle \mathbf{i}+ | \nabla \mathbf{i}+ \rangle_{\partial G}. \end{aligned} \quad (3)$$

The second line is a short-hand notation for the surface integral. As we use an exact description of the one-electron scattering process, the boundary surface  $\partial G$  can be any interface parallel to the sample electrodes, because total current is conserved. In particular,  $\partial G$  can be assumed to be far inside the sample metal. Inserting the expansion (cf section 4)

$$|\mathbf{i}+\rangle = \sum_f \langle \mathbf{f} | \mathbf{i}+\rangle |\mathbf{f}\rangle \quad (4)$$

in the expression equation (3) for the total current yields, with the notation defined in equation (3),

$$J_{\partial G}(\mathbf{i}) = \frac{e\hbar}{2im} \sum_f \langle \mathbf{i}+ | \mathbf{f} \rangle [\langle \nabla \mathbf{f} | \mathbf{i}+ \rangle_{\partial G} - \langle \mathbf{f} | \nabla \mathbf{i}+ \rangle_{\partial G}]. \quad (5)$$

We shall prove that the following relationship holds in general:

$$\begin{aligned} J_{\partial G}(\mathbf{i}) &= \frac{e\hbar}{2im} [\langle \mathbf{i}+ | \nabla \mathbf{i}+ \rangle_{\partial G} - \langle \nabla \mathbf{i}+ | \mathbf{i}+ \rangle_{\partial G}] \\ &= \frac{\pi e}{\hbar} \sum_f |\langle \mathbf{f} | V_{\text{tip}} + V_{\text{sample}} | \mathbf{i}+ \rangle|^2 \delta(E_f - E_i). \end{aligned} \quad (6)$$

As we need an expression for  $\langle \mathbf{i}+ | \mathbf{f} \rangle$  and the square bracket in equation (5), the proof of equation (6) obviously involves the conversion of a surface integral to a sum over volume integrals. In his perturbation theory Bardeen provided a relationship between a transition matrix element and a surface integral over a current density expression. His treatment (published before Lippmann derived the GET) is, however, only valid in the perturbation limit. We need a corresponding expression for the exact transition matrix element in equation (1). Therefore we derive in the next section a generalization of Bardeen's formula. The expression of equation (6) differs by a factor of 2 from the GET of equation (1). This is connected with the normalization of the scattering wavefunction and will be explained in section 5. For the remainder of this paper we use atomic units ( $e = m = \hbar = 1$ ).

### 3. Generalization of Bardeen's formula

#### 3.1. Partitioning of the Hamiltonian and the measuring state

The total Hamiltonian can be partitioned in various ways:

$$\begin{aligned} H &= H_0 + V_{\text{tip-sample}} \\ &= H_0 + V_{\text{tip}} + V_{\text{sample}} \\ &= H_{\text{tip}} + H_{\text{sample}} + V_{\text{tip}} \\ &= -\frac{1}{2}\nabla^2 + V_{\text{sample}} + V_{\text{tip}} + V_{\text{base}} \end{aligned} \quad (7)$$

where  $H_{\text{tip}}$  and  $H_{\text{sample}}$  are the Hamiltonians of the isolated tip and sample, respectively.  $H_0$  describes two separated electrodes without the potential provided by the atoms in the sample leading to multiple scattering.  $V_{\text{tip}}$  is the interaction potential between tip and sample surface.  $V_{\text{sample}}$  is the scattering potential of the atoms in the sample:  $V_{\text{tip-sample}} = V_{\text{tip}} + V_{\text{sample}}$ .

In the following it is always assumed that the current flows from the tip to the sample. The measuring state  $|f\rangle$  is defined as an eigenstate of the kinetic energy operator:

$$-\frac{1}{2}\nabla^2|f\rangle = E_f|f\rangle. \quad (8)$$

The measurement might be thought of as detecting the electron in the state  $|f\rangle$  in a region of flat potential after it has passed through the tunnel junction and the sample electrode. In this paper scattering states are considered as generalized eigenvectors with  $\delta$ -function normalization (Böhm 1979).

### 3.2. The transition matrix element

The transition matrix element in the GET equation (1) can be manipulated in the following way:

$$\begin{aligned} T_{fi} &= \langle f|V_{\text{tip-sample}}|\dot{i}+\rangle \\ &= \langle f|H - H_0|\dot{i}+\rangle \\ &= \langle f|H - H_0|\dot{i}+\rangle + \langle (H_0 - E_f)f|\dot{i}+\rangle \\ &= \langle f|H|\dot{i}+\rangle - \langle f|H_0|\dot{i}+\rangle - E_f\langle f|\dot{i}+\rangle + \langle H_0f|\dot{i}+\rangle \\ &= \langle f|(H - E_f)\dot{i}+\rangle + \langle H_0f|\dot{i}+\rangle - \langle f|H_0\dot{i}+\rangle. \end{aligned} \quad (9)$$

The bra-ket notation implies integration over all space. The first term in the last line of equation (9) is zero, because we consider elastic scattering with  $E_i = E_f$ . Concerning the operation on the measuring state  $|f\rangle$ ,  $H_0$  is the kinetic energy operator (cf equation (8)):

$$\langle f|V_{\text{tip-sample}}|\dot{i}+\rangle = \langle \frac{1}{2}\nabla^2 f|\dot{i}+\rangle - \langle f|\frac{1}{2}\nabla^2|\dot{i}+\rangle. \quad (10)$$

Hence we recover the one-particle version of the equation which is found in Bardeen's paper (Bardeen 1961). Applying the product rule for differentiation

$$\begin{aligned} \nabla\langle \nabla f|\dot{i}+\rangle &= \langle \nabla f|\nabla\dot{i}+\rangle + \langle \nabla^2 f|\dot{i}+\rangle \\ \nabla\langle f|\nabla\dot{i}+\rangle &= \langle \nabla f|\nabla\dot{i}+\rangle + \langle f|\nabla^2\dot{i}+\rangle \end{aligned}$$

the transition matrix element can be cast in the form

$$\langle f|V_{\text{tip-sample}}|\dot{i}+\rangle = \frac{1}{2}\nabla[\langle \nabla f|\dot{i}+\rangle - \langle f|\nabla\dot{i}+\rangle] \quad (11)$$

which, explicitly written as an integral, yields

$$\langle f|V_{\text{tip-sample}}|\dot{i}+\rangle = \frac{1}{2}\int d\mathbf{r}^3\nabla[\psi_{i+}\nabla\psi_f^* - \psi_f^*\nabla\psi_{i+}]. \quad (12)$$

The integration can be restricted to a finite region  $G$  in space, if the integrand  $\psi_f^*(\mathbf{r})V_{\text{tip-sample}}(\mathbf{r})\psi_{i+}(\mathbf{r})$  decays exponentially away from the tunnel junction. In this case,

Gauss' theorem can be used to rewrite the transition matrix element as a surface integral over the boundary  $\partial G$  of  $G$ :

$$\begin{aligned} \langle f | V_{\text{tip-sample}} | i+ \rangle &= \frac{1}{2} \int_{\partial G} [\psi_{i+} \nabla \psi_f^* - \psi_f^* \nabla \psi_{i+}] dF \\ &= \frac{1}{2} [\langle \nabla f | i+ \rangle_{\partial G} - \langle f | \nabla i+ \rangle_{\partial G}]. \end{aligned} \quad (13)$$

We refer to this relationship as the generalized Bardeen formula. It is important, because it converts the *exact* transition matrix element to a surface integral. Up to now this conversion has only been demonstrated to be valid in perturbation theory under additional assumptions for the wavefunctions as discussed by Bardeen. The treatment is exact, but it is valid only for a plane-wave final state. The question is whether such an expression also holds for an eigenstate of  $H_{\text{sample}}$  as final state. This is indeed the case as will be proved in the next section by means of Gell-Mann and Goldberger's theorem (Gell-Mann and Goldberger 1953, Goldberger and Watson 1964).

### 3.3. Using exact sample states: elimination of $V_{\text{sample}}$

In practical calculations, the wavefunctions of the unperturbed sample electrode are commonly evaluated before the tip is introduced. It is therefore useful to have an expression for the transition matrix element where, instead of plane waves, these eigenstates of  $H_{\text{sample}}$  appear as final states. These eigenstates already contain the scattering effects of the potential inside the sample and therefore  $V_{\text{sample}}$  can be eliminated from the transition matrix element as will be shown in the following.

We write the Hamiltonian in the form:

$$H = -\frac{1}{2}\nabla^2 + V_{\text{sample}} + V_{\text{tip-sample}} + V_{\text{base}}.$$

The state  $|f\rangle$  still denotes an eigenstate of the kinetic energy operator (cf equation (8)). We define eigenstates of  $H_{\text{sample}}$ :

$$H_{\text{sample}} |f\pm\rangle = E_f |f\pm\rangle. \quad (14)$$

According to Gell-Mann and Goldberger (1953) the transition matrix element can be written in the form

$$\langle f | V_{\text{tip-sample}} | i+ \rangle = \langle f | V_{\text{sample}} | f+ \rangle + \langle f - | V_{\text{tip}} | i+ \rangle. \quad (15)$$

The first term on the right-hand side does not contribute to the tunnel current, because it describes pure forward scattering of electrons in the sample metal:

$$\begin{aligned} \langle f | V_{\text{sample}} | f+ \rangle &= \langle f | H_{\text{sample}} | f+ \rangle - \langle f | -\frac{1}{2}\nabla^2 | f+ \rangle \\ &= E_f \langle f | f+ \rangle - E_f \langle f | f+ \rangle = 0. \end{aligned}$$

We now have a version of the generalized Bardeen formula where the transition matrix element is expressed using the tip-induced potential and exact sample states:

$$\langle f - | V_{\text{tip}} | i+ \rangle = \frac{1}{2} [\langle \nabla f | i+ \rangle_{\partial G} - \langle f | \nabla i+ \rangle_{\partial G}]. \quad (16)$$

With the help of equations (5) and (16) one obtains

$$J_{\partial G}(i) = -i \sum_f \langle i+ | f \rangle \langle f - | V_{\text{tip}} | i+ \rangle. \quad (17)$$

In order to demonstrate the equivalence of this expression to the GET one has to study the properties of the expansion coefficients  $\langle i+ | f \rangle$ .

#### 4. Expansion coefficients for the scattering wavefunction

Assume  $\partial G$  to be a plane parallel to the surface deep inside the sample solid. In this region  $|\dot{z}+\rangle$  represents a wave moving away from the surface. The scattering wavefunction  $|\dot{z}+\rangle$  can therefore be expanded in outgoing plane-wave states in the sample surface as described by equation (4). Using the Lippmann-Schwinger equation

$$|\dot{z}+\rangle = |\dot{z}\rangle + G_0^+(E_i)V_{\text{tip-sample}}|\dot{z}+\rangle$$

and the fact that initial and final states lie on the energy shell

$$\lim_{\eta \rightarrow 0} \langle f | G_0(E_i + i\eta = E_f) | \dot{z}+\rangle = -i\pi \delta(E_i - E_f)$$

one obtains

$$\begin{aligned} \langle f | \dot{z}+\rangle &= \langle f | \dot{z}\rangle - i\pi \langle f | V_{\text{tip-sample}} | \dot{z}+\rangle \delta(E_i - E_f) \\ &= \langle f | \dot{z}\rangle - i\pi \langle f - | V_{\text{tip-sample}} | \dot{z}+\rangle \delta(E_i - E_f). \end{aligned} \quad (18)$$

Here we have used the theorem of Gell-Mann and Goldberger. Inserting this expression for the expansion coefficient into equation (17) one obtains

$$J_{\partial G}(\dot{z}) = \pi \sum_f |\langle f - | V_{\text{tip-sample}} | \dot{z}+\rangle|^2 \delta(E_i - E_f). \quad (19)$$

This proves equation (6), which states that the surface integral of the current density over a surface deep inside the sample is identical to Ehrenfest's theorem up to a factor of 2.

#### 5. Normalization of wavefunctions

The relationship equation (6) can also be derived in a slightly different way which demonstrates more clearly the origin of the missing factor 2. We follow the first steps in deriving the generalized Ehrenfest theorem from the Heisenberg equation of motion. For any hermitian operator  $A$  that commutes with  $H_0$  one has

$$\begin{aligned} \frac{d}{dt} \langle \dot{z} + | A | \dot{z}+\rangle &= \frac{1}{i} \langle \dot{z} + | [A, H] | \dot{z}+\rangle \\ &= \frac{1}{i} \langle \dot{z} + | A V_{\text{tip-sample}} | \dot{z}+\rangle + \langle \dot{z} + | V_{\text{tip-sample}} A | \dot{z}+\rangle \\ &= 2 \text{Im} \langle \dot{z} + | A V | \dot{z}+\rangle \end{aligned}$$

where we used

$$[A, H_0 + V_{\text{tip-sample}}] = [A, V_{\text{tip-sample}}].$$

Specializing to the operator

$$A = \sum_f |f\rangle \langle f|$$

one obtains

$$J(\mathbf{i}) = \frac{d}{dt} |\langle \mathbf{f} | \mathbf{i} + \rangle|^2 = 2 \operatorname{Im} \sum_f \langle \mathbf{i} + | \mathbf{f} \rangle \langle \mathbf{f} | V_{\text{tip-sample}} | \mathbf{i} + \rangle.$$

We demonstrated above (cf equation (17)) that  $\sum_f \langle \mathbf{i} + | \mathbf{f} \rangle \langle \mathbf{f} | V_{\text{tip-sample}} | \mathbf{i} + \rangle$  is purely imaginary and therefore

$$\begin{aligned} \frac{d}{dt} |\langle \mathbf{f} | \mathbf{i} + \rangle|^2 &= -i \frac{2}{\hbar} \sum_f \langle \mathbf{i} + | \mathbf{f} \rangle \langle \mathbf{f} | V_{\text{tip-sample}} | \mathbf{i} + \rangle \\ &= 2 \operatorname{Im} \langle \mathbf{i} + | \nabla \mathbf{i} + \rangle_{\partial G} \\ &= 2J_{\partial G}(\mathbf{i}) \end{aligned}$$

This is equivalent to equation (6) and demonstrates on a very basic level that formal scattering theory will inevitably lead to twice the value for the tunnel current as the current density integration. The important point to notice is that we assumed all wavefunctions to be normalized as in formal scattering theory:

$$\langle \mathbf{i} + | \mathbf{i} + \rangle = \langle \mathbf{i} | \mathbf{i} \rangle.$$

STM theories (Lucas *et al* 1988, Vigneron *et al* 1990, Derycke *et al* 1991) which use the current density picture normalize differently, however, namely in such a way that the flux before and after the scattering process is conserved:

$$|\langle \mathbf{i} | \hat{J} | \mathbf{i} \rangle_{\partial G}| = |\langle \Delta \mathbf{i} | \hat{J} | \Delta \mathbf{i} \rangle_{\partial G}|.$$

Here we decomposed the total scattering wavefunction into an incoming plane wave  $|\mathbf{i}\rangle$  and a scattered wave  $|\Delta \mathbf{i}\rangle$ :

$$\begin{aligned} A|\mathbf{i} + \rangle &= |\mathbf{i}\rangle + |\Delta \mathbf{i}\rangle \\ \hat{J} &= \frac{1}{2}i(\overleftarrow{\nabla} - \overrightarrow{\nabla}). \end{aligned}$$

The factor  $A$  accounts for a different normalization. Expanding the scattered wave  $|\Delta \mathbf{i}\rangle$  in plane waves

$$|\Delta \mathbf{i}\rangle = \sum_f C_f |f\rangle$$

one obtains with a surface  $\partial G$  enclosing all scattering centres at asymptotically large distances:

$$|\langle \Delta \mathbf{i} | J | \Delta \mathbf{i} \rangle_{\partial G}| = \sum_f |f| C_f^2 = |f| \sum_f C_f^2.$$

The last equality sign is valid because summation is on the energy shell. This is the total outgoing flux which has to be equal to the incoming flux,  $|\mathbf{i}| = |f|$ , and therefore normalization has to be such that

$$\sum_f C_f^2 = 1.$$

This implies, however, that

$$\langle \Delta \mathbf{i} | \Delta \mathbf{i} \rangle = \langle f | f \rangle = \langle \mathbf{i} | \mathbf{i} \rangle$$

and hence

$$A^2 \langle \mathbf{i} + | \mathbf{i} + \rangle = \langle \mathbf{i} | \mathbf{i} \rangle + \langle \Delta \mathbf{i} | \Delta \mathbf{i} \rangle = 2 \langle \mathbf{i} + | \mathbf{i} + \rangle.$$

Hence the current density of  $(A|\mathbf{i} + \rangle)$  is twice that of  $|\mathbf{i} + \rangle$ . The conclusion is therefore that by using the standard normalization of the current density picture one obtains the same total current as with the generalized Ehrenfest theorem, where in the latter case one uses the normalization of formal scattering theory.



## 6. Conclusion

This paper has discussed the interrelation of two different methods to calculate the current in the scanning tunnelling microscope: the current density formulation and the generalized Ehrenfest theorem. This is of interest because the GET offers several advantages for real calculations. The equivalence of the two methods has been demonstrated.

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