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Reprint of : Scattering approach to scanning gate microscopy

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ABSTRACT

We present a perturbative approach to the conductance change caused by a weakly invasive scattering potential in a two-dimensional electron gas. The resulting expressions are used to investigate the relationship between the conductance change measured in scanning gate microscopy as a function of the position of a scattering tip and local electronic quantities like the current density. We use a semiclassical approach to treat the case of a strong hard-wall scatterer in a half-plane facing a reflectionless channel. The resulting conductance change is consistent with the numerically calculated quantum conductance.

1. Introduction

The scanning gate microscopy (SGM) is an experimental technique detecting the change in the conductance of a nanostructure while the charged tip of an atomic force microscope is scanned over the surface of the device [1–9]. The interpretation of what are the physical properties actually probed with the SGM technique is still a point of debate (for a review see Ref. [10]).

Our first contribution to this intriguing physical problem [11] was quickly greeted by a short note from Markus Büttiker saying "*Dear Rodolfo, dear Dietmar : You clearly wrote a paper that needed to be written! Since the conductance is proportional to the transmission probability, the change of conductance is the change of the transmission probability due to the variation in the potential. Many years ago, in a paper which I have enclosed, we looked at this quantity.*" And he went on in his scholar style discussing what should be done in order to get his approach [12] to agree with ours in their common regime of applicability (which we could soon establish). Kind notes as this one, that many colleagues frequently received from our tireless role-model, shaped the evolution of Mesocopic Physics since the eighties and gave rise to important developments.

In this article we first review the progressive understanding achieved through our contributions to SGM in the limit of a weakly perturbing tip. The linear-response regime of small bias voltages [11,13] as well as the weakly non-linear case [14] is presented. In an attempt to connect with other theoretical and experimental work, we go beyond the perturbative regime and study SGM setups by means of semi-classical approximations and numerical calculations. Since SGM is a cornerstone of Mesoscopic Physics, it is noticeable how many of the concepts encountered are connected with the seminal contributions of Markus Büttiker to the field.

2. The scattering approach

Conductance is transmission in the scattering approach to quantum transport that was put forward by Landauer and Büttiker. The two-probe dimensionless conductance g (in units of $2e^2/h$) is given in linear response to the applied bias voltage by [15]

$$g = \mathrm{Tr}[t^\dagger t] = \sum_{m=1}^{N} \mathcal{T}_m^2, \tag{1}$$

where t is the matrix of transmission amplitudes between the left and right leads (evaluated at the Fermi energy ε_F of the reservoirs). The trace is taken over the N incoming, right-moving modes. In the basis of the scattering eigenmodes (eigenvectors of the matrix $t^\dagger t$) the trace takes the simple form of a sum over the squares of the transmission eigenvalues $\mathcal{T}_m$. The transmission matrix constitutes one of the blocks of the scattering matrix

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}. \tag{2}$$

The other blocks r, r', and t' characterize the complementary reflection and transmission amplitudes (primes are used to indicate

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scattering amplitudes with incident modes impinging from the right lead). Current conservation dictates the unitarity of the scattering matrix ($SS^{\dagger}=I$). In the absence of magnetic fields, time-reversal symmetry implies that S is a symmetric matrix ($S^{\mathrm{T}}=S$).

The transmission and reflection amplitudes determine the asymptotic behavior of the scattering wave-functions. For instance, the incoming mode from the left lead ($l=1$) in the ath channel, $\varphi^{(-)}_{1,\varepsilon,a}(\mathbf{r})=(c/\sqrt{k_a})\exp[ik_a^{-}x]\phi_a(y)$ defines the outgoing scattering state $\Psi_{1,\varepsilon,a}(\mathbf{r})$ given, respectively, in the left and right leads by

$$\Psi_{1,\varepsilon,a}(\mathbf{r})=\begin{cases}\varphi^{(-)}_{1,\varepsilon,a}(\mathbf{r})+\sum_{b=1}^{N} r_{ba}\varphi^{(+)}_{1,\varepsilon,b}(\mathbf{r}),\\ \sum_{b=1}^{N} t_{ba}\varphi^{(+)}_{2,\varepsilon,b}(\mathbf{r}).\end{cases} \tag{3}$$

We note $c=(M_{\mathrm{e}}/2\pi\hbar^2)^{1/2}$, M_{e} the effective electron mass, k_a the longitudinal wave-vector, and $v_a=\hbar k_a/M_{\mathrm{e}}$ the longitudinal velocity. The index of the wave-vector stands for an infinitesimal imaginary part needed to ensure the proper time-ordering in the incoming ($-$) and ($+$) outgoing modes. $\phi_a(y)$ represents the transverse wave-function of the ath channel.

The transmission and reflection amplitudes between modes a and b can be obtained, respectively, from the retarded Green function $\mathcal{G}(\mathbf{r},\bar{\mathbf{r}},\varepsilon)$ associated to the Hamiltonian that defines the structure [16]

$$t_{ba}=i\hbar(v_a v_b)^{1/2}\exp\left[-i(k_b^{+}x-k_a^{+}\bar{x})\right]\int_{\mathcal{S}_x}\mathrm{d}y\int_{\mathcal{S}_{\bar{x}}}\mathrm{d}\bar{y}\,\phi_b^{*}(y)\mathcal{G}(\mathbf{r},\bar{\mathbf{r}},\varepsilon)\,\phi_a(\bar{y}), \tag{4}$$

$$r_{ba}=-\delta_{ab}\exp\left[i(k_b^{+}x+k_a^{+}\bar{x})\right]\exp\left[ik_b^{+}|x-\bar{x}|\right]+i\hbar(v_a v_b)^{1/2}\exp\left[-i(k_b^{+}x+k_a^{+}\bar{x})\right]\int_{\mathcal{S}_x}\mathrm{d}y\int_{\mathcal{S}_{\bar{x}}}\mathrm{d}\bar{y}\,\phi_b^{*}(y)\,\mathcal{G}(\mathbf{r},\bar{\mathbf{r}},\varepsilon)\phi_a(\bar{y}). \tag{5}$$

The integrations take place at the transverse cross-sections $\mathcal{S}_{\bar{x}}$ on the left lead and $\mathcal{S}_x$ on the right (left) lead for the transmission (reflection) amplitudes.

The expressions (4), (5) have a clear physical interpretation highlighting the quantum propagation through the structure, and are extremely useful for numerical and analytical calculations. Among the latter, approximations to the Green function by perturbation theory or semi-classical expansions are particularly useful, and have be thoroughly used in the present context.

3. Perturbation by the tip potential

The scattering approach sketched in the previous section is applicable to any phase-coherent two-lead setup. We are interested in testing the response of a given nanostructure to a capacitively coupled scanning gate microscope. Therefore, we take the total Hamiltonian as

$$H_{\mathrm{T}}=H+V_{\mathrm{T}}, \tag{6}$$

where H represents the unperturbed structure to be characterized and V_{T}, intended to act as a probe, is the electrostatic energy of an electron in the potential generated by the perturbing tip. While most of the analysis is developed for an arbitrary H, the case of a quantum point contact (QPC) is treated in detail. Similarly, general results for a non-specified V_{T} are established, and then the case of local spatial perturbations will be the focus.

In Refs. [11,13] V_{T} was included within a Lippmann–Schwinger scheme, working up to second order in perturbation theory of the scattering wave-functions, and an equivalent alternative path based on the perturbative expansion of the Green function was outlined. In the sequel we develop this second approach, highlighting the use of Green functions beyond perturbation theory.

The Green function $\mathcal{G}_{\mathrm{T}}$ of the perturbed system is related with that of the unperturbed case $\mathcal{G}$ through Dyson's equation

$$\mathcal{G}_{\mathrm{T}}(\mathbf{r},\bar{\mathbf{r}},\varepsilon)=\mathcal{G}(\mathbf{r},\bar{\mathbf{r}},\varepsilon)+\int\mathrm{d}\bar{\bar{\mathbf{r}}}\mathcal{G}(\mathbf{r},\bar{\bar{\mathbf{r}}},\varepsilon)V_{\mathrm{T}}(\bar{\bar{\mathbf{r}}})\mathcal{G}_{\mathrm{T}}(\bar{\bar{\mathbf{r}}},\bar{\mathbf{r}},\varepsilon) \tag{7}$$

The second-order correction of the reflection amplitude $\delta r=\delta r^{(1)}+\delta r^{(2)}$ determines, through the Landauer–Büttiker Eq. (1) for the perturbed problem, the change of the conductance due to the presence of the tip

$$\delta g^{(1)}=-2\,\mathrm{Re}\left\{\mathrm{Tr}\left[r^{\dagger}\delta r^{(1)}\right]\right\}, \tag{8}$$

$$\delta g^{(2)}=\delta g^{(2)\alpha}+\delta g^{(2)\beta}, \tag{9}$$

with

$$\delta g^{(2)\alpha}=-2\,\mathrm{Re}\left\{\mathrm{Tr}\left[r^{\dagger}\delta r^{(2)}\right]\right\}, \tag{10}$$

$$\delta g^{(2)\beta}=-\mathrm{Re}\left\{\mathrm{Tr}\left[\delta r^{(1)\dagger}\delta r^{(1)}\right]\right\}, \tag{11}$$

where the traces are taken over the right-moving modes and the energy arguments are set at ε_{F}.

3.1. First-order perturbation in the tip potential

Using the first-order approximation of Eq. (7) and relationship (5) between the Green function and the reflection amplitude, one gets the first-order Born approximation

$$\delta r^{(1)}_{ba}=i\hbar(v_a v_b)^{1/2}\exp\left[-i(k_b^{+}x+k_a^{+}\bar{x})\right]\times\int_{\mathcal{S}_x}\mathrm{d}y\int_{\mathcal{S}_{\bar{x}}}\mathrm{d}\bar{y}\int\mathrm{d}\bar{\bar{\mathbf{r}}}\phi_b^{*}(y)\mathcal{G}(\mathbf{r},\bar{\bar{\mathbf{r}}},\varepsilon)V_{\mathrm{T}}(\bar{\bar{\mathbf{r}}})\mathcal{G}(\bar{\bar{\mathbf{r}}},\bar{\mathbf{r}},\varepsilon)\phi_a(\bar{y}). \tag{12}$$

From the spectral decomposition of $\mathcal{G}$ in the basis of scattering states $\Psi_{l,\varepsilon,a}$ resulting from an incoming wave in the left (right) lead $l=1(2)$, in channel a and at energy ε, and integrating over the transverse coordinates y and $\bar{y}$ we have

$$\begin{aligned}\delta r^{(1)}_{ba}=\frac{i\hbar(v_a v_b)^{1/2}}{2\pi}\exp\left[-i(k_b^{+}x+k_{\bar{a}}^{+}\bar{x})\right]\int_{\varepsilon_1^{(\mathrm{t})}}^{\infty}\frac{\mathrm{d}\bar{\varepsilon}}{\varepsilon^{+}-\bar{\varepsilon}}\int_{\varepsilon_1^{(\mathrm{t})}}^{\infty}\frac{\mathrm{d}\bar{\varepsilon}}{\varepsilon^{+}-\bar{\varepsilon}}\frac{1}{\left(\bar{v}_a\bar{v}_b\right)^{1/2}}\times\\ \sum_{\bar{a},\bar{\bar{a}}=1}^{N}\Big\{\Big(\delta_{a\bar{a}}\exp\left[-i\bar{k}_a^{+}\bar{x}\right]+\bar{r}^{*}_{a\bar{a}}\exp\left[i\bar{k}_a^{-}\bar{x}\right]\Big)\\ \times\Big(\delta_{b\bar{a}}\exp\left[i\bar{k}_b^{-}x\right]+\bar{r}_{b\bar{a}}\exp\left[-i\bar{k}_b^{+}x\right]\Big)\mathcal{V}^{11}_{\bar{a}\bar{a}}(\bar{\varepsilon},\bar{\bar{\varepsilon}})\\ +\Big(\delta_{a\bar{a}}\exp\left[-i\bar{\bar{k}}_a^{+}\bar{x}\right]+\bar{\bar{r}}^{*}_{a\bar{a}}\exp\left[i\bar{\bar{k}}_a^{-}\bar{x}\right]\Big)\bar{\bar{t}}_{b\bar{a}}\exp\left[-i\bar{\bar{k}}_b^{+}x\right]\mathcal{V}^{21}_{\bar{a}\bar{\bar{a}}}(\bar{\varepsilon},\bar{\bar{\varepsilon}})\\ +\bar{\bar{t}}'^{*}_{a\bar{\bar{a}}}\exp\left[i\bar{\bar{k}}_a^{-}\bar{x}\right]\Big(\delta_{b\bar{a}}\exp\left[i\bar{k}_b^{-}x\right]+\bar{r}_{b\bar{a}}\exp\left[-i\bar{k}_b^{+}x\right]\Big)\mathcal{V}^{12}_{\bar{a}\bar{\bar{a}}}(\bar{\varepsilon},\bar{\bar{\varepsilon}})\\ +\bar{\bar{t}}'^{*}_{a\bar{\bar{a}}}\exp\left[i\bar{\bar{k}}_a^{-}\bar{x}\right]\bar{\bar{t}}_{b\bar{a}}\exp\left[-i\bar{k}_b^{+}x\right]\mathcal{V}^{22}_{\bar{a}\bar{\bar{a}}}(\bar{\varepsilon},\bar{\bar{\varepsilon}})\Big\}.\end{aligned} \tag{13}$$

We have defined $\mathcal{V}^{\bar{l}l}_{\bar{a}a}$ as the $(\bar{a},a)$ matrix element of the $N\times N$ matrix $\mathcal{V}^{\bar{l}l}(\bar{\varepsilon},\varepsilon)$ of the perturbation in the basis of the scattering wave-functions; that is,

$$\mathcal{V}^{\bar{l}l}_{\bar{a}a}(\bar{\varepsilon},\varepsilon)=\int\mathrm{d}\mathbf{r}\Psi^{*}_{\bar{l},\bar{\varepsilon},\bar{a}}(\mathbf{r})V_{\mathrm{T}}(\mathbf{r})\Psi_{l,\varepsilon,a}(\mathbf{r}). \tag{14}$$

The bar and double-bar in the wave-vectors and scattering amplitudes indicate their energy argument. The integrations over $\bar{\bar{\varepsilon}}$ and $\bar{\varepsilon}$ can be easily performed by contour-integration for the case $x,\bar{x}<0$ (see Appendix A of Ref. [13]), yielding