Tunneling theory without the transfer-Hamiltonian formalism. IV. The abrupt (zero-width) three-dimensional junction

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A general three-dimensional many-body theory of tunneling across an abrupt junction was developed independently of the transfer-Hamiltonian formalism. The theory is based on Keldysh's perturbation theory for nonequilibrium processes. The extension of our previously published one-dimensional theory to three dimensions produced significant new insight. It was demonstrated that a "transfer-Hamiltonian-like" expression for the (energy density of the) tunneling current can be derived. However, this expression depends on a "transmissivity" weighted-average product of the spectral densities of the "uncoupled" subsystems (electrodes) over the interface, rather than on the product of their local energy densities of state at the interface. This qualitative agreement with Appelbaum and Brinkman's theory was shown to reflect the fact that Appelbaum and Brinkman's tunneling theory may be derived from our theory if it is linearized in the (pseudo) transfer Hamiltonian $\mathcal{H}'(\vec{r})$ defined by us. Thus, several conjectures concerning the transfer-Hamiltonian formalism were confirmed. Namely, it is a "thick-barrier approximation" involving a (pseudo) perturbing potential which is correct to first order in this pseudo-operator. The general theory is complemented by a brief examination of the translationally invariant and of the ordered planar junctions. The important consequences of the convention used in defining the spectral densities, and Green's functions for the uncoupled electrodes were further elucidated. An examination of the "surface Green's function" introduced by Garcia-Moliner and Rubio indicates that our formalism explicitly accounts for the contribution of interfacial states to the tunneling. Though cast into a many-body formalism, the present results were derived for a noninteracting system. The effects of a nontrivial interaction are currently investigated and will be reported in a subsequent publication.

I. INTRODUCTION

This is the fourth publication in a series of several papers in which we develop a new many-body theory of electron tunneling which does not involve the formalism of the transfer Hamiltonian.[1] The theory is based on a perturbation theory for nonequilibrium processes developed by Keldysh.[2] The basic motivation for our work, and the general approach to be followed were discussed at length in Paper I. In the present paper we concentrate on the modifications of the simple one-dimensional version of our theory, developed in Papers I–III, when it is extended to a full three-dimensional theory. Our experience in treating the finite junction in II suggested that short of such obvious barrier effects as resonant and inelastic tunneling, the abrupt junctions include essentially all of the physics of tunneling. Hence, we decided to avoid some of the cumbersome algebra by restricting our analysis to the abrupt junction. We also continue to restrict ourselves to a noninteracting (many electron) system. This last restriction will be dropped in a future publication of this series.

Our purpose in developing a detailed three-dimensional theory is twofold: First we wish to demonstrate the versatility of the formalism which was developed in I and II, and the relative ease with which it can be applied to more realistic problems. Second, and more significant in our opinion, is the need to obtain a detailed check on the reliability of the several current three-dimensional tunneling theories based on the transfer-Hamiltonian formalism. Here we refer in particular to the theory of Appelbaum and Brinkman,[3] and to its adaptation by Penn, Gomer, and Cohen.[4] These theories, like all tunneling theories based on the transfer-Hamiltonian formalism,[5–10] do not seem to depend on the dimensionality of the problem. On the other hand, a strictly one-dimensional analysis in I, led to the "transfer-Hamiltonian-like" expression for the tunneling current,

$$\langle J\rangle = \frac{2e}{\hbar}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(2\pi)^2[f_L(\omega)-f_R(\omega)] \times|\Lambda^r(\omega)|^2\rho_L(0;\omega)\rho_R(0;\omega)\,, \tag{1.1}$$

where, in contrast to the actual transfer-Hamiltonian formalism, $|\Lambda^r(\omega)|$ is not a "matrix element" but a simple expression involving appropriate Green's functions of the uncoupled electrodes. Furthermore, $\rho_{L,R}$ are *local* energy densities of states (evaluated at the interface) rather than the *bulk*, i.e., position-independent densities entering the conventional formulation. Thus there was reasonable doubt that even such a limited agreement with the transfer-Hamiltonian theories as was achieved in I could be established for a three-dimensional formulation of our theory. This suspicion was indeed corroborated. Our results con-

firm the expression quoted by Caroli *et al.*[11] for the field emitted current from a planar electrode, based on an alternative version of our formalism. The tunneling current energy density $\langle J(\omega)\rangle$ depends on a weighted average of spectral densities (rather than of the local energy densities of states), over the interface of the abrupt junction. This result agrees qualitatively with one formulation of the tunneling theory of Appelbaum and Brinkman.[11a] In fact, we can demonstrate that the latter theory represents an approximation of our theory formally valid to first order in the pseudo (transfer) Hamiltonian $\mathcal{H}'(\vec{r})$. This is a most interesting result since it provides a rather complete insight into the significance of this formalism. We also briefly discuss our representation of Garcia-Moliner *et al*'s.[12] "surface Green's function" and indicate that our tunneling current explicitly includes the contribution of interfacial states localized at the interface of the abrupt junction. Readers who wish to avoid the detailed algebra may find the notation introduced in Secs. II A and II C adequate to understand the main results stated in Sec. III C and their discussion in Sec. IV.

The formal analysis, while somewhat lengthy, is fairly transparent. This analysis, presented in Secs. II and III is essentially self-contained. However, to avoid duplication of the extensive discussion in I, verbal arguments are kept to a minimum.

In Sec. II, we determine the single-particle, thermal-equilibrium Green's function for the abrupt junction G in terms of the thermal-equilibrium "uncoupled" Green's functions for the two uncoupled subregions or electrodes g_δ. The pseudo Hamiltonian which "couples" the subregions and hence determines G, in terms of the g_δ's, is also derived. We treat separately the interesting, special, case of a planar ordered junction which allows a more explicit solution than is possible for the general junction.

In Sec. III, the tunneling current is expressed in terms of the correlation function G^+ which has to satisfy Keldysh's (matrix) Dyson equation relating it to the several uncoupled Green's and correlation functions g^ν_δ.[2] The theory is developed in a way to permit ready comparison with the corresponding results for the one-dimensional junction, obtained in I.

In Sec. IV, we present a reasonably extensive discussion of our results and their relation to Appelbaum and Brinkman's theory.

II. EQUILIBRIUM GREEN'S FUNCTION

In this section we compute the Green's function for an abrupt three-dimensional junction, in the absence of an external potential, in terms of the (uncoupled) Green's functions of the uncoupled electrodes. The general (abrupt) junction is discussed first, and then more explicit results are derived for the planar junction. All of these results are directly applicable to the nonequilibrium Green's functions $G^{r,a}$, to be introduced in Sec. III.

A. Definitions

We consider

$$\mathcal{H}=\Theta_2\mathcal{H}_2+\Theta_1\mathcal{H}_1\ , \tag{2.1}$$

where Θ_δ is the characteristic function of the δth region; $\delta=1,2$ corresponds either to the left, right half-spaces $z\gtrless 0$, or to the inside, outside regions. The uncoupled Green's functions are required to satisfy the following equations:

$$[\omega-\mathcal{H}_\delta(\vec{r})]g_\delta(\vec{r},\vec{r}';\omega)=\delta(\vec{r}-\vec{r}')\ , \tag{2.2}$$

and the general homogenous boundary conditions[13]

$$\alpha(\vec{r})g_\delta(\vec{r}\in B,\vec{r}'\in D_\delta;\omega)+\beta(\vec{r})\frac{\partial g_\delta}{\partial n}(\vec{r}\in B,\vec{r}'\in D_\delta;\omega)=0, \tag{2.3}$$

$$\alpha(\vec{r}')g_\delta(\vec{r}\in D_\delta,\vec{r}'\in B;\omega+\beta(\vec{r})\frac{\partial g_\delta}{\partial n'}(\vec{r}\in D_\delta,\vec{r}'\in B;\omega)=0.$$

Here, α and β are real functions and B is the boundary surface separating the full region of (physical) interest into the two regions whose interiors are denoted D_δ.[14] At the other boundaries of $D_1\cup D_2$ we impose appropriate (homogeneous) boundary conditions.[15] These are identical to those imposed on the full Green's function G and do not have to be spelled out in further detail.[16] The Green's functions all display a characteristic singularity which is a consequence of Eq. (2.2). It can be conveniently written in the following form, adapted from the standard, one-dimensional theory:

$$\Delta_s\frac{\partial}{\partial n}g(\vec{r},\vec{r}_s';\omega)=\frac{2m}{\hbar^2}\delta^{(2)}(\vec{r}_s-\vec{r}_s')\ . \tag{2.4}$$

Here, the subscript s denotes a vector whose tip lies on the surface S. $\partial/\partial n$ is the derivative along the positive normal to S. Δ_s denotes the difference in the function evaluated with $\vec{r}$ tending to the positive (negative) side of S. $\delta^{(2)}$ is a two-dimensional Dirac δ function.[17]

On combining Eq. (2.4) with the homogeneous boundary conditions imposed on the uncoupled Green's functions, Eqs. (2.3), we obtain the following discontinuity conditions imposed on g_δ at the boundary B: When $\beta\neq 0$,

$$\frac{\hbar^2}{2m}\lim_{\vec{r}\to B_\delta(\text{in})}\left(\frac{\alpha(\vec{r})}{\beta(\vec{r})}+\frac{\partial}{\partial n}\right)g_\delta(\vec{r},\vec{r}';\omega)\Big|_{\vec{r}'\in B}$$

$$=-(-1)^\delta\delta^{(2)}(\vec{r}_B-\vec{r}_B') \tag{2.5}$$

$$=\frac{\hbar^2}{2m}\lim_{\vec{r}'\to B_\delta(\text{in})}\left(\frac{\alpha(\vec{r}')}{\beta(\vec{r}')}+\frac{\partial}{\partial n'}\right)g_\delta(\vec{r},\vec{r}';\omega)\Big|_{\vec{r}\in B}\ ; \tag{2.5'}$$

and if $\alpha \neq 0$,

$$\frac{\hbar^2}{2m}\lim_{\vec{r}\to B_\delta(\mathrm{in})}\left(1+\frac{\beta(\vec{r})}{\alpha(\vec{r})}\frac{\partial}{\partial n}\right)\frac{\partial}{\partial n'}g_\delta(\vec{r},\vec{r}';\omega)\Big|_{\vec{r}'\in B}$$

$$=(-1)^\delta\delta^{(2)}(\vec{r}_B-\vec{r}'_B)\ , \tag{2.6}$$

$$=\frac{\hbar^2}{2m}\lim_{\vec{r}'\to B_\delta(\mathrm{in})}\left(1+\frac{\beta(\vec{r}')}{\alpha(\vec{r}')}\frac{\partial}{\partial n'}\right)\frac{\partial}{\partial n}g_\delta(\vec{r},\vec{r}';\omega)\Big|_{\vec{r}\in B}\ . \tag{2.6'}$$

Here, we denote with the subscript B any position vector $\vec{r}$ whose tip lies on the boundary (interface) surface B. $B_\delta(\mathrm{in})$ denotes the side of B facing the interior of D_δ. Finally, $\delta = 1(2)$ denotes either the left (right) or the inside (outside) electrode.[18,19]

The full Green's function G satisfies the equation

$$[\omega-\mathcal{H}(\vec{r})]\,G[\vec{r},\vec{r}';\omega]=\delta(\vec{r}-\vec{r}')\ , \tag{2.7}$$

and at infinity it satisfies the same (homogenous) boundary conditions as imposed on the uncoupled Green's functions g_δ.

B. Determination of full (equilibrium) Green's function G

Applying Green's theorem, we can deduce the three-dimensional version[20] of Eqs. (I2.12) and (I2.15):

$$\Theta_\delta(\vec{r})G(\vec{r},\vec{r}';\omega)=g_\delta(\vec{r},\vec{r}';\omega)\Theta_\delta(\vec{r}')+\frac{\hbar^2}{2m}\int_B[\nabla_{r_1}(g_\delta(\vec{r},\vec{r}_1;\omega))G(\vec{r}_1,\vec{r}';\omega)-g_\delta(\vec{r},\vec{r}_1;\omega)\nabla_{r_1}G(\vec{r}_1,\vec{r}';\omega)]\,ds_1\ . \tag{2.8}$$

Here it should be noted that Eq. (2.8) explicitly includes the fact that over the remainder of the boundary, B_δ, of D_δ, g_δ and G satisfy the same boundary conditions. These equations can be recast in the form of a three-dimensional integral equation,

$$G(\vec{r},\vec{r}';\omega)=g(\vec{r},\vec{r}';\omega)+\int_{\text{all space}}g(\vec{r},\vec{r}_1;\omega)\times\mathcal{H}'(\vec{r}_1)G(\vec{r}_1,\vec{r}';\omega)\,d^3r_1\ , \tag{2.9}$$

where

$$g(\vec{r},\vec{r}';\omega)=\sum_\delta\Theta_\delta(\vec{r})\Theta_\delta(\vec{r}')g_\delta(\vec{r},\vec{r}';\omega)\ . \tag{2.10}$$

Here we defined, in analogy to Eq. (I2.21), the pseudo Hamiltonian or perturbing pseudopotential

$$\mathcal{H}'(\vec{r})=-\frac{\hbar^2}{2m}\sum_\delta\left(\delta^{(1)}(\vec{r}-\vec{r}'_{B_\delta(\mathrm{in})})\ ,\ \frac{\partial}{\partial n_\delta}\right)_+=-[\mathcal{H}'(\vec{r})]^\dagger\ , \tag{2.11}$$

with $\partial/\partial n_\delta$ equal to the derivative along the outward normal to the boundary of D_δ (i.e., B_δ). The one-dimensional δ function $\delta^{(1)}$ is defined by the relation

$$\int_{D_\delta}\delta^{(1)}(\vec{r}-\vec{r}_{B_\delta(\mathrm{in})})f(\vec{r})\,d^3r=\int_B f(\vec{r})\,ds \tag{2.12}$$

or, alternatively,

$$\int_B\delta(\vec{r}-\vec{r}')\,ds'=\delta^{(1)}(\vec{r}-\vec{r}_{B_\delta(\mathrm{in})})\ . \tag{2.13}$$

It should be noted that Eqs. (2.5) and (2.5′) assure the consistency of Eqs. (2.8) (and of their transpose) in the limits $\vec{r}\to\vec{r}_{B_\delta(\mathrm{in})}(\vec{r}'\to\vec{r}_{B_\delta(\mathrm{in})})$. It is easily verified that besides Eq. (2.8) also the following (transposed) equation applies:

$$\Theta_\delta(\vec{r}')G(\vec{r},\vec{r}';\omega)=g_\delta(\vec{r},\vec{r}';\omega)\Theta_\delta(\vec{r})+\frac{\hbar^2}{2m}\int_B[G(\vec{r},\vec{r}_1;\omega)\nabla_{r_1}g_\delta(\vec{r}_1,\vec{r}';\omega)-\nabla_{r_1}G(\vec{r},\vec{r}_1;\omega)g_\delta(\vec{r}_1,\vec{r}';\omega)]\,ds_1\ . \tag{2.8'}$$

Using Eq. (2.8′) to express $G(\vec{r}_1,\vec{r}';\omega)$ and $\nabla_{r_1}G(\vec{r}_1,\vec{r}';\omega)$ in Eq. (2.8), we recognize that the latter equation determines the Green's function G in terms of its "boundary values" at B

$$G(\vec{r}_B,\vec{r}'_B;\omega)\ ,\ \frac{\partial}{\partial n}G(\vec{r},\vec{r}';\omega)\Big|_{\substack{\vec{r}\to B_2(\mathrm{in})\\ \vec{r}'\to B_1(\mathrm{in})}}\ ,$$

$$\frac{\partial}{\partial n'}G(\vec{r},\vec{r}';\omega)\Big|_{\substack{\vec{r}\to B_2(\mathrm{in})\\ \vec{r}'\to B_1(\mathrm{in})}}\ ,$$

and

$$\frac{\partial^2}{\partial n\partial n'}G(\vec{r},\vec{r}';\omega)\Big|_{\substack{\vec{r}\to B_2(\mathrm{in})\\ \vec{r}'\to B_1(\mathrm{in})}}\ . \tag{2.14}$$

These functions are determined by a set of two-dimensional integral equations which express the consistency of Eqs. (2.8) and (2.8′). Thus, the characteristic singularity of g_δ enables us to deduce from Eqs. (2.8) and (2.8′) several relations of the form

$$\lim_{\substack{\vec{r}\to B_1(\mathrm{in})\\ \vec{r}'\in D_1}}\int_B\frac{\partial}{\partial n_1}[g_2(\vec{r},\vec{r}_1;\omega)]G(\vec{r}_1,\vec{r}';\omega)\,ds_1$$

$$=\lim_{\substack{\vec{r}\to B_2(\mathrm{in})\\ \vec{r}'\in D_1}}\int_B g_2(\vec{r},\vec{r}_1;\omega)\frac{\partial}{\partial n_1}G(\vec{r}_1,\vec{r}';\omega)\,ds_1 \tag{2.15}$$

and

$$\lim_{\substack{\vec{r}\to B_2(\mathrm{in})\\ \vec{r}'\in D_2}}\int_B\frac{\partial}{\partial n_1}[g_1(\vec{r},\vec{r}_1;\omega)]G(\vec{r}_1,\vec{r}';\omega)\,ds_1$$

$$=\lim_{\substack{\vec{r}\to B_1(\mathrm{in})\\ \vec{r}'\in D_2}}\int_B g_1(\vec{r},\vec{r}_1;\omega)\frac{\partial}{\partial n_1}G(\vec{r}_1,\vec{r}';\omega)\,ds_1\ . \tag{2.16}$$

The analogy of these equations to the one-dimensional algebraic equations leading to Eqs. (I2.18) and (I2.18′) is evident, and suggests that they might yield a corresponding set of algebraic equa-

tions which could be solved by an obvious generalization of the one-dimensional procedures followed in I. This is indeed the case for a planar configuration, provided the two semi-infinite electrodes are crystalline and have commensurate unit meshes in the planes parallel to the interface B.[21] In the following we shall restrict ourselves to this particular class of junctions. However, before we proceed, we shall indicate the particular form of Eq. (2.8) for a planar geometry when we impose on the uncoupled Green's function's g_δ Neumann conditions at the plane boundary B [$\alpha \equiv 0$ in Eq. (2.3)]:

$$G(\vec{r},\vec{r}';\omega)\Theta_\delta(z)=\left[g_\delta(\vec{r},\vec{r}';\omega)+\left(\frac{\hbar^2}{2m}\right)^2\int\int_B\left(g_\delta(\vec{r},\vec{r}_1;\omega)\frac{\partial^2}{\partial z_1\partial z_2}[G(\vec{r}_1,\vec{r}_2;\omega)]g_{\delta'}(\vec{r}_2,\vec{r}';\omega)\right)ds_1ds_2\right]\Theta_\delta(z')$$
$$-\left(\frac{\hbar^2}{2m}\right)^2\int\int_B\left(g_\delta(\vec{r},\vec{r}_1;\omega)\frac{\partial^2}{\partial z_1\partial z_2}[G(\vec{r}_1,\vec{r}_2;\omega)]g_{\delta'}(\vec{r}_2,\vec{r}';\omega)\right)ds_1ds_2[1-\Theta_\delta(z')]\,, \tag{2.17}$$

where, $\delta\neq\delta'$; the interface B is the plane $z=0$; the z component of $\vec{r}_1$ and $\vec{r}_2$ vanishes (since these position vectors lie on B).

Similarly when the uncoupled Green's functions g_δ satisfy Dirichlet conditions at the plane $B, z=0$ (i.e., $\beta\equiv 0$), we have

$$G(\vec{r},\vec{r}';\omega)\Theta_\delta(z)=\left(g_\delta(\vec{r},\vec{r}';\omega)+\left(\frac{\hbar^2}{2m}\right)^2\int\int_B\frac{\partial}{\partial z_1}[g_\delta(\vec{r},\vec{r}_1;\omega)]G(\vec{r}_1,\vec{r}_2;\omega)\frac{\partial}{\partial z_2}g_{\delta'}(\vec{r}_2,\vec{r}';\omega)ds_1ds_2\right)\Theta_\delta(z')$$
$$-\left(\frac{\hbar^2}{2m}\right)^2\int\int_B\frac{\partial}{\partial z_1}[g_\delta(\vec{r},\vec{r}_1;\omega)]G(\vec{r}_1,\vec{r}_2;\omega)\frac{\partial}{\partial z_2}g_{\delta'}(\vec{r}_2,\vec{r}';\omega)ds_1ds_2[1-\Theta_\delta(z')]\,. \tag{2.18}$$

In Eqs. (2.18) or (2.17) we have still to determine the values of the full Green's function G or, respectively, of its mixed second normal derivative over the interface. In general, these are difficult to determine.[22] However, as we shall see, the formal analysis does not require the explicit solution of this problem, and Eqs. (2.19) and (2.20), respectively, suffice.

Using Eqs. (2.17) [or (2.18)] to evaluate the left-hand side of Eq. (2.4), we deduce, upon applying the appropriate form of Eqs. (2.5) [or (2.6)], for $\alpha\equiv 0$

$$\frac{2m}{\hbar^2}\delta^{(2)}(\vec{r}_B-\vec{r}'_B)=-\frac{\hbar^2}{2m}\int_B\frac{\partial^2}{\partial z\,\partial z_1}G(\vec{r},\vec{r}_1;\omega)\Big|_{z=0=z_1}$$
$$\times[g_1(\vec{r}_1,\vec{r}';\omega)+g_2(\vec{r}_1,\vec{r}';\omega)]\,ds_1\,, \tag{2.19}$$

and for $\beta\equiv 0$

$$\frac{2m}{\hbar^2}\delta^{(2)}(\vec{r}_B-\vec{r}'_B)=-\frac{\hbar^2}{2m}\int_B G(\vec{r},\vec{r}_1;\omega)\frac{\partial^2}{\partial z_1\partial z'}$$
$$\times[g_1(\vec{r}_1,\vec{r}';\omega)+g_2(\vec{r}_1,\vec{r}';\omega)]\big|_{z_1=0=z'}ds_1. \tag{2.20}$$

In both equations the arguments (position vectors) $\vec{r}$ and $\vec{r}'$ are on the interface B. These equations are clearly the three-dimensional version of Eqs. (I2.24) and (I2.18'').

Combining Eqs. (2.17) and (2.18), we can now obtain an implicit expression for G on the interface. Writing $\vec{r}=\vec{1}_z z+\vec{\rho}$, we have for $\vec{\rho}\neq\vec{\rho}'$

$$G(z=0^-,\vec{\rho};z=0^+,\vec{\rho}';\omega)=G(z=0^+,\vec{\rho};z'=0^-,\vec{\rho}';\omega)$$
$$=G(z=0^+,\vec{\rho};z'=0^+,\vec{\rho}';\omega)=G(z=0^-,\vec{\rho};z=0^-,\vec{\rho}';\omega)=G(z=0,\vec{\rho};z'=0,\vec{\rho}';\omega)$$
$$=-\left(\frac{\hbar^2}{2m}\right)^2\int\int_B g_1(\vec{r},\vec{r}_1;\omega)\frac{\partial^2}{\partial z_1\partial z_2}[G(\vec{r}_1,\vec{r}_2;\omega)]g_2(\vec{r}_2,\vec{r}';\omega)\Big|_{z=0=z'}ds_1ds_2$$
$$=-\left(\frac{\hbar^2}{2m}\right)^2\int\int_B g_2(\vec{r},\vec{r}_1;\omega)\frac{\partial^2}{\partial z_1\partial z_2}[G(\vec{r}_1,\vec{r}_2;\omega)]g_1(\vec{r}_2,\vec{r}';\omega)\Big|_{z=0=z'}ds_1ds_2\,. \tag{2.21}$$

Below we shall obtain an explicit solution of this interesting equation for the case of an ordered planar junction.

C. Full Green's function for crystalline junction

In the following we shall specialize our discussion to an ordered planar junction. Here "order" refers to the fact that the entire junction is assumed to exhibit a periodicity in the plane of the interface B.[23]

1. Notation

We shall write the position vector

$$\mathbf{r}=\vec{\rho}+\vec{1}_z z\,,$$

where $\vec{\rho}$ is a two-dimensional vector in a plane parallel to B which is now defined by $z=0$. The junction is invariant under the two-dimensional translation group

$$\vec{\rho} \to \vec{\rho}' = \vec{\rho} + \vec{R}_{\vec{n}} ,$$

where the two-dimensional net $\{\vec{R}_{\vec{n}}\}$ is spanned by the basis $\{\vec{a}_1, \vec{a}_2\}$,

$$\vec{R}_{\vec{n}} = \vec{a}_1 n_1 + \vec{a}_2 n_2 , \quad n_i \text{ are integers, } i=1,2 .$$

The (two-dimensional) reciprocal net $\{\vec{K}_{\vec{m}}\}$ is spanned by the reciprocal basis $\{\vec{b}_1, \vec{b}_2\}$

$$\vec{K}_{\vec{m}} = 2\pi(\vec{b}_1 m_1 + \vec{b}_2 m_2) , \quad m_i \text{ are integers, } i=1,2 . \tag{2.22}$$

Where the reciprocal basis is specified by the conditions

$$\vec{a}_i \cdot \vec{b}_j = \delta_{ij} , \quad i,j=1,2 .$$

Thus, in particular,

$$\vec{K}_{\vec{m}} \cdot \vec{R}_{\vec{n}} = 2\pi(m_1 n_1 + m_2 n_2) .$$

It is well known that for systems in variant under a two-dimensional (discrete) translation group, the Green's function can be expanded in a double series of the form[23,24]

$$G(\vec{r}, \vec{r}'; \omega) = \sum_{\vec{m},\vec{m}'} e^{i\vec{K}_{\vec{m}}\cdot\vec{\rho} - \vec{K}_{\vec{m}'}\cdot\vec{\rho}'} \frac{a_c}{(2\pi)^2} \int_{BZ} d^2k_\rho \times e^{i\vec{k}_\rho\cdot(\vec{\rho}-\vec{\rho}')} G(z,z';\vec{k}_\rho,\vec{m},\vec{m}';\omega) , \tag{2.23}$$

where $\vec{k}_\rho$ is a two-dimensional (reduced) wave vector ranging over the first Brillouin zone of the net reciprocal to the net spanned by $(\vec{a}_1, \vec{a}_2)$ denoted by BZ. a_c is the area of the unit mesh (i.e., the 2-dimensional unit cell). The symbol $\vec{m}$ is defined by Eq. (2.22), each individual sum in the double summation indicated is thus a two-dimensional sum (over all pairs of integers).

It is easily verified that the convolution theorem for Fourier transforms can be extended to double transforms such as Eq. (2.23). In particular, we can verify by direct substitution that (for periodic systems) Eqs. (2.8) reduce to the set of algebraic equations

$$G(z,z';\vec{k}_\rho,\vec{m},\vec{m}';\omega)\Theta_\delta(z) = g_\delta(z,z';\vec{k}_\rho,\vec{m},\vec{m}';\omega)\Theta_\delta(z') - (-1)^\delta \frac{\hbar^2}{2m}\Big(\sum_{\vec{m}_1} \frac{\partial}{\partial z_1} g_\delta(z,z_1;\vec{k}_\rho,\vec{m},\vec{m}_1;\omega) \times G(z_1,z';k_\rho,\vec{m}_1,\vec{m}';\omega) - g_\delta(z,z_1;\vec{k}_\rho,\vec{m},\vec{m}_1)\frac{\partial}{\partial z_1} G(z_1,z';\vec{k}_\rho;\vec{m}_1,\vec{m}';\omega)\Big) . \tag{2.24}$$

Introducing a matrix notation, we shall denote the matrix, whose $(\vec{m},\vec{m}')$ element is equal to $G(z,z';\vec{k}_\rho,\vec{m},\vec{m}';\omega)$ by $\underline{G}(z,z';\vec{k}_\rho;\omega)$ i.e.,[23]

$$[\underline{G}(z,z';\vec{k}_\rho;\omega)]_{\vec{m}\vec{m}'} \equiv G(z,z';\vec{k}_\rho,\vec{m},\vec{m}';\omega) . \tag{2.25}$$

2. *Calculation of Green's function*

Using Eqs. (2.23)–(2.25), we can reduce Eqs. (2.8) to a pair of matrix equations,

$$\underline{G}(z,z';\vec{k}_\rho)\Theta_\delta(z) = \underline{g}_\delta(z,z';\vec{k}_\rho)\Theta_\delta(z') - (-1)^\delta \frac{\hbar^2}{2m}\Big(\frac{\partial}{\partial z_1}\underline{g}_\delta(z,z_1;k_\rho)\underline{G}(z_1,z';k_\rho) - \underline{g}_\delta(z,z_1;k_\rho)\frac{\partial}{\partial z_1}\underline{G}(z_1,z';k_\rho)\Big)\Big|_{(-1)^\delta z_1 = 0^+} . \tag{2.26}$$

Similarly, Eqs. (2.8′) reduce to[23]

$$\underline{G}(z,z';\vec{k}_\rho)\Theta_\delta(z') = \underline{g}_\delta(z,z';\vec{k}_\rho)\Theta_\delta(z) - (-1)^\delta \frac{\hbar^2}{2m}\Big(\underline{G}(z,z_1;\vec{k}_\rho)\frac{\partial}{\partial z_1}\underline{g}_\delta(z_1,z';\vec{k}_\rho) - \frac{\partial}{\partial z_1}\underline{G}(z,z_1;\vec{k}_\rho)\underline{g}_\delta(z_1,z';\vec{k}_\rho)\Big)\Big|_{(-1)^\delta z_1 = 0^+} . \tag{2.26′}$$

Here, and in the following, we shall suppress the argument ω whenever this will not introduce ambiguities.

The characteristic singularity of the Green's functions, Eq. (2.4), can now be expressed by

$$\lim_{z\to 0}\Big(\frac{\partial}{\partial z}\underline{G}(z,0^-;\vec{k}_\rho) - \frac{\partial}{\partial z}\underline{G}(z,0^+;\vec{k}_\rho)\Big) = \frac{2m}{\hbar^2}\underline{I} , \tag{2.27}$$

where $\underline{I}$ is the unit matrix.

Finally, we note that in the present discussion the function $\alpha(\vec{r})$, $\beta(\vec{r})$ entering the statement of the homogenous boundary conditions have to be periodic, with the unit mesh defined by $\{\vec{a}_1, \vec{a}_2\}$. Hence the boundary conditions, Eqs. (2.3), now reduce to

$$\underline{\alpha g}_\delta(z,z';\vec{k}_\rho) + \underline{\beta}\frac{\partial}{\partial z}\underline{g}_\delta(z,z';\vec{k}_\rho) = 0 ,$$

when

$$z=0 , \quad (-1)^\delta z' \geq 0 ,$$

and

$$\underline{g}_\delta(z, z'; \vec{k}_\rho)\underline{\alpha} + \frac{\partial}{\partial z'}\underline{g}_\delta(z, z'; \vec{k}_\rho)\underline{\beta} = 0 ,$$

when,

$$z' = 0 , \quad (-1)^\delta z \geq 0 . \tag{2.28}$$

In these equations the $(\vec{m}, \vec{m}')$ element of the matrix $\underline{\alpha}$

$$\alpha(\vec{m} - \vec{m}') = \int_B \alpha(\rho)\, e^{(i\vec{K}_{\vec{m}} - \vec{K}_{\vec{m}'})\cdot\vec{\rho}}\, ds . \tag{2.29}$$

The matrix $\underline{\beta}$ is defined by a similar relation, and furthermore the $(\vec{m}, \vec{m}')$ element of $(\underline{\beta})^{-1}\underline{\alpha}$ is

$$(\underline{\beta})^{-1}\underline{\alpha}(\vec{m} - \vec{m}') = \int_B \frac{\alpha(\rho)}{\beta(\rho)}\, e^{i(\vec{K}_{\vec{m}} - \vec{K}_{\vec{m}'})\cdot\vec{\rho}}\, ds . \tag{2.30}$$

It is now easily verified, either directly from Eqs. (2.26), (2.26′), and (2.27), or by transforming Eqs. (2.15) and (2.16), that

$$\frac{\partial}{\partial z_1}\underline{G}(z_1, 0^-; \vec{k}_\rho)\Big|_{z_1=0} = [\underline{g}_2(0^+, 0; \vec{k}_\rho)]^{-1}\frac{\partial}{\partial z_1} \times g_2(0^-, z_1; \vec{k}_\rho)\underline{G}(0, 0^-; \vec{k}_\rho)\Big|_{z_1=0} \tag{2.31}$$

and

$$\frac{\partial}{\partial z_1}\underline{G}(z_1, 0^+; \vec{k}_\rho)\Big|_{z_1=0} = [\underline{g}_1(0^-, 0; \vec{k}_\rho)]^{-1}\frac{\partial}{\partial z_1} \times \underline{g}_1(0^+, z_1; \vec{k}_\rho)\underline{G}(0, 0^+; \vec{k}_\rho)\Big|_{z_1=0} . \tag{2.32}$$

These two equations can be combined with Eq. (2.27) to yield

$$\frac{\hbar^2}{2m}\underline{G}(0, 0; \vec{k}_\rho) = [\underline{g}_2(0, 0; \vec{k}_\rho)]^{-1}\frac{\partial}{\partial z_1}\underline{g}_2(0^-, z_1; \vec{k}_\rho) - [\underline{g}_1(0, 0; \vec{k}_\rho)]^{-1}\frac{\partial}{\partial z_1}\underline{g}_1(0^+, z_1; \vec{k}_\rho) . \tag{2.33}$$

Here we explicitly use the fact that the matrix $\underline{g}(z, z'; \vec{k}_\rho)$ is continuous at $z = z'$. Equation (2.31) can be further simplified. When the characteristic singularity of the "uncoupled" Green's function [Eq. (2.27)] and the homogenous boundary conditions [Eq. (2.28)] are explicitly accounted for, we obtain a result strikingly similar to Eq. (I2.18),

$$\underline{G}(0, 0; \vec{k}_\rho) = \{[\underline{g}_1(0, 0; \vec{k}_\rho)]^{-1} + [\underline{g}_2(0, 0; \vec{k}_\rho)]^{-1}\}^{-1} = \underline{g}_1(0, 0; \vec{k}_\rho)[\underline{g}_1(0, 0; \vec{k}_\rho) + \underline{g}_2(0, 0; \vec{k}_\rho)]^{-1}\underline{g}_2(0, 0; \vec{k}_\rho) . \tag{2.34}$$

The preceding analysis illustrated the technique which yields the expressions for the several derivatives of $\underline{G}(z, z'; \vec{k}_\rho)$, evaluated at the interface, required to solve Eqs. (2.26). We shall not pursue this point any further except to note that when $\alpha \equiv 0$ (for Neumann boundary conditions at B)[25]

$$\frac{\partial^2}{\partial z\, \partial z_1}\underline{G}(z, z_1; \vec{k}_\rho)\Big|_{z=0=z_1} = -\left(\frac{2m}{\hbar^2}\right)^2 [\underline{g}_1(0, 0; \vec{k}_\rho) + \underline{g}_2(0, 0; \vec{k}_\rho)]^{-1} . \tag{2.35}$$

Substituting Eq. (2.35) into Eq. (2.34), we obtain the Fourier transform of Eq. (2.21), specialized for ordered junctions. Evidently, when the uncoupled Green's functions satisfy Neumann conditions at the interface ($z = 0$), then substitution of Eqs. (2.35) and (2.26′) into Eq. (2.26) yields a complete solution of that equation. A similar solution is obtained for the case where the uncoupled Green's functions satisfy Dirichlet conditions, when instead of Eq. (2.35), Eq. (2.36) is to be used,[26]

$$\underline{G}(0, 0; \vec{k}_\rho) = -\frac{2m}{\hbar^2}\left(\frac{\partial^2}{\partial z\, \partial z_1}[\underline{g}_1(z, z_1; \vec{k}_\rho) + \underline{g}_2(z, z_1; \vec{k}_\rho)]\Big|_{z=0=z_1}\right)^{-1} . \tag{2.36}$$

III. TUNNELING CURRENT

A. Introduction

In this section we shall derive the general (formal) expressions for the tunneling current (in an abrupt junction) and deduce a more explicit result for the ordered planar junction.

The formalism developed in Sec. III of I is easily extended to the three-dimensional setting. The ensemble-averaged current density can be written

$$\langle\vec{J}(\vec{r})\rangle = -\frac{e\hbar}{2m}\lim_{rt \to r't'}(\vec{\nabla}_r - \vec{\nabla}_{r'})G^+(\vec{r}, t; \vec{r}'t') . \tag{3.1}$$

Conservation of current implies that current across the junction is given by

$$\int_B \langle\vec{J}(\vec{r})\rangle \cdot d\vec{s} = B\langle\bar{J}\rangle = B\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\langle\bar{J}(\omega)\rangle = -\frac{e\hbar}{2m}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left(\int_B \lim_{\vec{r}\to\vec{r}'}(\nabla_r - \nabla_{r'}) \times G^+(\vec{r}, \vec{r}'; \omega)\cdot d\vec{s}\right), \tag{3.2}$$

where

$$G^+(\vec{r}, t; \vec{r}', t') = i\langle\psi^\dagger(\vec{r}', t')\psi(\vec{r}, t)\rangle \tag{3.3}$$

and

$B = \int_B ds$ is the area of the interface.

Here it should be emphasized that when the junction has planar geometry (subject to periodic boundary conditions on the x and y dependence), $\langle I\rangle = B\langle\bar{J}\rangle$ is the constant (position independent) current across any plane $z = \text{const}$. For any other geom-

etry B is in fact a *closed* surface (separating the inside from the outside electrode) and Eq. (3.2) is the familiar statement of current conservation. We shall see that while relatively simple expressions can be derived for $\langle\bar{J}(\omega)\rangle$, this is not the case for $\langle\vec{J}(\vec{r})\rangle$.

B. Calculation of tunneling current and current density

Keldysh's formalism which is summarized in Sec. II B of I is, in fact, a three-dimensional theory, and the transcription of the relevant equations in I is trivial. Thus we can write down directly the three-dimensional version of Eq. (I3.5):

$$G^{+}(\vec{r},\vec{r}';\omega)=g^{+}(\vec{r},\vec{r}';\omega)+\int d^3r_1[g^{+}(\vec{r},\vec{r}_1;\omega)\mathcal{K}'(\vec{r}_1)\times G^{a}(\vec{r}_1,\vec{r}';\omega)+g^{r}(\vec{r},\vec{r}_1;\omega)\mathcal{K}'(\vec{r}_1)G^{+}(\vec{r}_1,\vec{r}';\omega)], \tag{3.4}$$

and

$$G^{r,a}(\vec{r},\vec{r}';\omega)=g^{r,a}(\vec{r},\vec{r}';\omega)+\int d^3r_1\, g^{r,a}(\vec{r},\vec{r}_1;\omega)\mathcal{K}'(\vec{r}_1)G^{r,a}(\vec{r}_1,\vec{r}';\omega), \tag{3.4'}$$

where $\mathcal{K}'(r_1)$ is defined by Eq. (2.11). The Green's functions entering Eq. (3.4) are the time Fourier transforms of the functions

$$\begin{aligned}
&g^{+}(\vec{r},t;\vec{r}',t')=i\langle\psi^{\dagger}(\vec{r}',\omega')\psi(\vec{r},t)\rangle_0\,,\\
&g^{-}(\vec{r},t;\vec{r}'t')=-i\langle\psi(\vec{r},t)\psi^{\dagger}(\vec{r}',t')\rangle_0\,,\\
&g^{r,a}(\vec{r},t;\vec{r}',t')=\mp i\langle[\psi(\vec{r},t),\psi^{\dagger}(\mathrm{r}',t')]_{+}\rangle_0\Theta(\pm t\mp t)\,,\\
&g(\vec{r},t;\vec{r}',t')=-i\langle T\{\psi(\vec{r},t),\psi^{\dagger}(\vec{r}',t')\}\rangle_0\,.
\end{aligned} \tag{3.5}$$

Here, the subscript 0 denotes that the averaging of the products of field operators is to be taken with respect to the unperturbed (equilibrium) density matrix. The full Green's functions G involve instead of the equilibrium the full (nonequilibrium) density matrix. The following relations between the Fourier transforms of the several Green's functions are useful:

$$g^{+}(\vec{r},\vec{r}';\omega)=-2if(\omega)[-\tfrac{1}{2}\rho(\vec{r},\vec{r}';\omega)]\,, \tag{3.6}$$

$$g^{-}(\vec{r},\vec{r}';\omega)=2i[1-f(\omega)][-\tfrac{1}{2}\rho(\vec{r},\vec{r}';\omega)]\,, \tag{3.7}$$

$$g^{r}(\vec{r},\vec{r}';\omega)=P\int_{-\infty}^{\infty}\frac{\rho(\vec{r},\vec{r}';\omega')}{\omega-\omega'}\frac{d\omega'}{2\pi}-\frac{i}{2}\rho(\vec{r},\vec{r}';\omega)=[g^{a}(\vec{r},\vec{r}';\omega)]^{\dagger}=[g^{a}(\vec{r}',\vec{r};\omega)]^{*}\,. \tag{3.8}$$

In Eqs. (3.6)–(3.8), f is the Fermi function

$$f(\omega)=[1-\exp[(\hbar\omega-\mu)/k_BT]\,, \tag{3.9}$$

μ is the chemical-potential, P denotes the Cauchy principal part of the integral, and $\rho(\mathrm{r},\mathrm{r}';\omega)$ is the spectral density function.[27] To conclude this review of pertinent relations we note that Eqs. (3.5) imply

$$G^{a}-G^{r}=G^{+}-G^{-}\,. \tag{3.10}$$

Upon substituting Eq. (3.4) into Eq. (3.3) and using Eq. (3.10), we can derive the three-dimensional analogs to Eqs. (I3.20) and (I3.21), i.e., when the general homogenous boundary conditions Eq. (2.3) are specialized by setting $\alpha\equiv 0$, $\beta\equiv 1$, we have

$$\frac{2m}{e\hbar}B\langle\bar{J}(\omega)\rangle=-\iint_B ds\,ds_1[g_1^{+}(\vec{r},\vec{r}_1;\omega)\Gamma^{-}(\vec{r}_1,\vec{r};\omega)-g_1^{-}(\vec{r},\vec{r}_1;\omega)\Gamma^{+}(\vec{r}_1,\vec{r};\omega)] \tag{3.11}$$

$$\frac{2m}{e\hbar}B\langle\bar{J}(\omega)\rangle=\iint_B ds\,ds_1[g_2^{+}(\vec{r},\vec{r}_1;\omega)\Gamma^{-}(\vec{r}_1,\vec{r};\omega)-g_2^{-}(\vec{r},\vec{r}_1;\omega)\Gamma^{+}(\vec{r}_1,\vec{r};\omega)]\,. \tag{3.12}$$

Here, we defined the tensor

$$\underline{\Gamma}^{\nu}(\vec{r},\vec{r}';\omega)=-\frac{\hbar^2}{2m}\nabla_r\nabla_{r_1}G^{\nu}(\vec{r},\vec{r}_1;\omega)\,,\quad \nu=\pm,r,a\,, \tag{3.13}$$

and its (n,n_1) component

$$\Gamma^{\nu}(\vec{r},\vec{r}_1;\omega)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial n\,\partial n_1}G^{\nu}(\vec{r},\vec{r}_1;\omega)\,,\quad \nu=\pm,r,a\,, \tag{3.14}$$

where $\partial/\partial n$ is the derivative along the positive normal to the surface B.

Next, using the continuity of $\partial G^{+}(\vec{r}:\vec{r}';\omega)/\partial n'$ when $\vec{r},\vec{r}'$ are on B, we find that when $\vec{r}_1,\vec{r}'\in B$,

$$0=\int_B\{[g_1^{r}(\vec{r}_1,\vec{r}_2;\omega)+g_2^{r}(\vec{r}_1,\vec{r}_2;\omega)]\Gamma^{\pm}(\vec{r}_2,\vec{r}';\omega)+[g_1^{\pm}(\vec{r}_1,\vec{r}_2;\omega)+g_2^{\pm}(\vec{r}_1,\vec{r}_2;\omega)]\Gamma^{a}(\vec{r}_2,\vec{r}';\omega)\}ds_2\,. \tag{3.15}$$

Multiplying Eq. (3.15) by $\Gamma^{r}(\vec{r},\vec{r}_1;\omega)$ and integrating (with respect to the $\vec{r}_1\in B$) over B, we find upon substituting Eq. (2.19) that when $\vec{r}$ and $\vec{r}'\in B$,

$$\frac{2m}{\hbar^2}\Gamma^{\pm}(\vec{r},\vec{r}';\omega)=-\iint_B ds_1\,ds_2\Gamma^{r}(\vec{r},\vec{r}_1;\omega)[g_1^{\pm}(\vec{r}_1,\vec{r}_2;\omega)+g_2^{\pm}(\vec{r}_1,\vec{r}_2;\omega)]\Gamma^{a}(\vec{r}_2,\vec{r}';\omega)\,. \tag{3.16}$$

Hence, substituting Eq. (3.16) into Eq. (3.12),

$$\frac{\hbar}{e}B\langle\bar{J}(\omega)\rangle=\left(\frac{\hbar^2}{2m}\right)^2\iiiint_B ds\,ds_1\,ds_2\,ds_3[g_1^{+}(\vec{r},\vec{r}_1;\omega)\Gamma^{r}(\vec{r}_1,\vec{r}_2;\omega)g_2^{-}(\vec{r}_2,\vec{r}_3;\omega)\Gamma^{a}(\vec{r}_3,\vec{r};\omega)-g_1^{-}(\vec{r},\vec{r}_1;\omega)\Gamma^{r}(\vec{r}_1,\vec{r}_2;\omega)g_2^{+}(\vec{r}_2,\vec{r}_3;\omega)\Gamma^{a}(\vec{r}_3,\vec{r};\omega)]\,. \tag{3.17}$$

A completely analogous derivation obtains when $\alpha\equiv 1$, $\beta\equiv 0$; in this case, Eq. (2.20) rather than Eq. (2.19) applies, and

$$\frac{\hbar}{e}B\langle\bar{J}(\omega)\rangle=\left(\frac{\hbar^2}{2m}\right)^4\iiiint_B\Big(\frac{\partial^2}{\partial n\,\partial n_1}[g_1^+(\vec{r},\vec{r}_1;\omega)]G^r(r_1,r_2;\omega)\frac{\partial^2}{\partial n_2\,\partial n_3}[g_2^-(\vec{r}_2,\vec{r}_3;\omega)]G^a(\vec{r}_3,\vec{r};\omega)$$
$$-\frac{\partial^2}{\partial n\,\partial n_1}[g_1^-(\vec{r},\vec{r}_1;\omega)]G^r(\vec{r}_1,\vec{r}_2;\omega)\frac{\partial^2}{\partial n_2\,\partial n_3}[g_2^+(\vec{r}_2,\vec{r}_3;\omega)]G^a(\vec{r}_3,r;\omega)\Big)\,ds\,ds_1\,ds_2\,ds_3\ . \quad (3.18)$$

We can now eliminate the uncoupled Green's functions $g_\delta^\pm$ in favor of the corresponding spectral densities introduced in Eqs. (3.6)–(3.9). Thus Eq. (3.17) reduces to

$$\frac{\hbar}{e}B\langle\bar{J}(\omega)\rangle=[f_1(\omega)-f_2(\omega)]\iiiint_B ds\,ds_1\,ds_2\,ds_3\,\rho_1(\vec{r},\vec{r}_1;\omega)\rho_2(\vec{r}_2,\vec{r}_3;\omega)\left[\left(\frac{\hbar^2}{2m}\right)\Gamma^r(\vec{r}_1,\vec{r}_2;\omega)\right]\left[\left(\frac{\hbar^2}{2m}\right)\Gamma^r(\vec{r},\vec{r}_3;\omega)\right]^*, \quad (3.19)$$

while Eq. (3.18) leads to the formally different, though numerically identical, result

$$\frac{\hbar}{e}B\langle\bar{J}(\omega)\rangle=[f_1(\omega)-f_2(\omega)]\iiiint_B ds\,ds_1\,ds_2\,ds_3\frac{\partial^2}{\partial n\,\partial n_1}[\rho_1(\vec{r},\vec{r}_1;\omega)]\frac{\partial^2}{\partial n_2\,\partial n_3}[\rho_2(\vec{r}_2,\vec{r}_3;\omega)]$$
$$\times\left[\left(\frac{\hbar^2}{2m}\right)^2G^r(\vec{r}_1,\vec{r}_2;\omega)\right]\left[\left(\frac{\hbar^2}{2m}\right)^2G^r(\vec{r},\vec{r}_3;\omega)\right]^*\ . \quad (3.20)$$

Equations (3.19) and (3.20) represent the general extension into three dimensions of the one-dimensional results stated in Eqs. (I3.24) and (I3.21). Before we proceed to discuss our results, we shall briefly drive more explicit expressions for the ordered planar junction.

It should be emphasized that the relatively simple structure of Eqs. (3.19) and (3.20) arises from the correspondingly simple structure of Eqs. (3.11) and (3.12). In either case the integration over all two dimensional (surface) variables, i.e., of the normal component of $\langle\vec{J}(\vec{r};\omega)\rangle$ over the surface B, indicated in Eq. (3.2), is essential. The expression for $\langle\vec{J}(\vec{r};\omega)\rangle$, corresponding to Eq. (3.11) is indicated as

$$\frac{\hbar}{e}\langle J(\vec{r};\omega)\rangle\Big|_{\vec{r}\in D_2}=\frac{\hbar^2}{2m}\iint_B ds_1\,ds_2[\nabla_r g_2^r(\vec{r},\vec{r}_1;\omega)\Gamma^r(\vec{r}_1,\vec{r}_2;\omega)g_2^+(\vec{r}_2,\vec{r};\omega)-g_2^+(\vec{r},\vec{r}_1;\omega)\Gamma^a(\vec{r}_1,\vec{r}_2;\omega)\nabla_r g_2^a(\vec{r}_2,\vec{r};\omega)$$
$$+\nabla_r g_2^+(\vec{r},\vec{r}_1;\omega)\Gamma^a(\vec{r}_1,\vec{r}_2;\omega)g_2^a(\vec{r}_2,\vec{r};\omega)+\nabla_r g_2^r(\vec{r},\vec{r}_1;\omega)\Gamma^+(\vec{r}_1,\vec{r}_2;\omega)g_2^a(r_2,\vec{r};\omega)$$
$$-g_2^r(\vec{r},\vec{r}_1;\omega)\Gamma^r(\vec{r}_1,\vec{r}_2;\omega)\nabla_r g_2^+(\vec{r}_2,\vec{r};\omega)-g_2^r(\vec{r},\vec{r}_1;\omega)\Gamma^+(\vec{r}_1,\vec{r}_2;\omega)\nabla_r g_2^a(\vec{r}_2,\vec{r};\omega)]\ . \quad (3.21)$$

The boundary conditions imposed on g_δ^ν, the characteristic singularity of $g_\delta^{r,a}$, and the continuity of $g_\delta^\pm$ assure the consistency of Eq. (3.21) with Eqs. (3.4), (3.11), and (3.16).[28] In fact,

$$\frac{\hbar}{e}\langle J_n(r;\omega)\rangle\Big|_{r\to B_\delta(\mathrm{in})}=(-1)^\delta\frac{\hbar^2}{2m}\int_B ds_1[\,\Gamma^r(\vec{r},\vec{r}_1;\omega)g_\delta^+(\vec{r}_1,\vec{r};\omega)-g_\delta^+(\vec{r},\vec{r}_1;\omega)\Gamma^a(\vec{r}_1,\vec{r};\omega)$$
$$+\Gamma^+(\vec{r},\vec{r}_1;\omega)g_\delta^a(\vec{r}_1,\vec{r};\omega)-g_\delta^r(\vec{r},\vec{r}_1;\omega)\Gamma^+(\vec{r}_1,\vec{r};\omega)]\ . \quad (3.22)$$

Integrating Eq. (3.22) with respect to $\vec{r}$ over the interface B and using Eq. (3.10) one obtains Eqs. (3.11) and (3.12).

C. Current across ordered planar junction

We have already remarked several times that Eqs. (3.19) and (3.20) are formal expressions of the tunneling current. By this we meant that they involved explicitly the full Green's function of the junction, i.e., the functions $\partial^2G^r(\vec{r},\vec{r}_1;\omega)/\partial n\,\partial n_1$ [or $G^r(\vec{r},\vec{r}_1;\omega)$] evaluated at the interface B. However, no explicit expression for these functions was given for the general junction. In the following we shall indicate how the notation developed in Sec. II C 1, and the result stated by Eq. (2.35), lead to a more complete, explicit solution for the tunneling current across a planar ordered junction.

The position independent tunneling current can be expanded in a (space) Fourier series

$$\langle\bar{J}(\omega)\rangle=\sum_m\int_{BZ}\frac{d^2k_\rho}{a_c^*}\langle J(\vec{k}_\rho;\vec{m},\vec{m};\omega)\rangle$$
$$=\mathrm{Tr}\int_{BZ}\frac{d^2k_\rho}{a_c^*}\langle\underline{J}(\vec{k}_\rho;\omega)\rangle\ . \quad (3.23)$$

Here, $a_c^*=(2\pi)^2/a_c$ is the area of the (first) Brillouin zone, Tr denotes the trace of the matrix to the right. We have seen that in k space the integrations over the interface B reduce to matrix products. Thus, in particular, we obtain from Eqs. (3.11) and (3.12)

$$(-1)^\delta\frac{2m}{\hbar^2}B\frac{\hbar}{e}\langle\underline{J}(\vec{k}_\rho;\omega)\rangle$$
$$=g_\delta^+(0,0;\vec{k}_\rho;\omega)\underline{\Gamma}^-(0,0;\vec{k}_\rho;\omega)$$
$$-g_\lambda^-(0,0;\vec{k}_\rho;\omega)\underline{\Gamma}^+(0,0;\vec{k}_\rho;\omega)\ . \quad (3.24)$$

Here we defined, in analogy to Eq. (3.14), the matrices

$$\underline{\Gamma}^{\nu}(z,z_1;\vec{k}_\rho;\omega) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z\,\partial z_1}\underline{G}^{\nu}(z,z_1;\vec{k}_\rho;\omega)\,, \qquad \nu = \pm, r, a\,. \tag{3.25}$$

The matrices $\underline{g}^{\nu}$ and $\underline{\Gamma}^{\nu}$ are continuous at $z = z_1$. We can now deduce, either directly from Eq. (3.4) and its transpose, or by a Fourier transformation of Eqs. (3.16), that

$$(2m/\hbar^2)\underline{\Gamma}^{\pm} = -\underline{\Gamma}^{a}(\underline{g}_1^{\pm}+\underline{g}_2^{\pm})\underline{\Gamma}^{r}(\underline{g}_1^{\pm}+\underline{g}_2^{\pm})\underline{\Gamma}^{a}\,, \tag{3.26}$$

where, from Eq. (2.35) and the Dyson equations Eq. (3.4′),

$$\underline{\Gamma}^{r,a} = (2m/\hbar^2)(\underline{g}^{r,a}+\underline{g}^{r,a})^{-1}\,. \tag{3.27}$$

Thus, combining Eqs. (3.24), (3.26), and (3.6)–(3.9), or by direct transformation of Eq. (3.19), we find

$$B\frac{\hbar}{e}\langle\bar{J}(\omega)\rangle = \left(\frac{\hbar^2}{2m}\right)^2[f_1(\omega)-f_2(\omega)] \times \mathrm{Tr}\int_{BZ}\frac{d^2k_\rho}{a_c^*}\underline{\rho}_1(0,0;\vec{k}_\rho;\omega)\underline{\Gamma}^{r}(0,0;\vec{k}_\rho;\omega)\underline{\rho}_2 \times(0,0;\vec{k}_\rho;\omega)\underline{\Gamma}^{a}(0,0;\vec{k}_\rho;\omega)\,. \tag{3.28}$$

In Eq. (3.28) we reinserted the variables that were suppressed in Eqs. (3.26) and (3.27). It should be emphasized that the matrix equation Eq. (3.27) allows an explicit representation of the tunneling current strictly in terms of the uncoupled Green's functions, i.e., parameters of the semi-infinite electrodes.

IV. DISCUSSION AND SUMMARY OF RESULTS

In the fourth publication of this series on tunneling we have extended the one-dimensional theory developed in I to a full three-dimensional treatment of the abrupt (tunneling) junction for a noninteracting system. The versatility and soundness of a tunneling theory based on Keldysh's (perturbation) theory for nonequilibrium processes was demonstrated by the relative ease with which the one-dimensional results could be extended, while new, significant insight into tunneling was achieved.

In Eq. (2.11) we obtained a three-dimensional expression for the pseudo Hamiltonian $\mathcal{H}'(\vec{r})$ (i.e., the perturbing pseudopotential) whose matrix elements correspond to Bardeen's transition current.

Two alternative, exact and general expressions of the space average (over the interface of the abrupt junction) of the (normal component) of the tunneling current density in terms of the spectral densities of the two electrodes were derived. The expression indicated in Eq. (3.19) is the closest to that commonly derived by means of the transfer Hamiltonian formalism.[2–10] Equations (3.19) and (3.20) were derived subject to the restriction that the uncoupled Green's functions g_δ satisfy respectively Neumann and Dirichlet boundary conditions at the interface. However it can be shown that these expressions hold under the slightly more general conditions that, respectively, $\beta \neq 0$ and $\alpha \neq 0$. The proof is a simple extension of the one dimensional argument presented in III, and establishes also the equivalence of the many-body formalism for the noninteracting system with the more elementary kinetic treatment.

In spite of the apparent similarity between Eq. (3.19) and the commonly used expression for the tunneling current, the two differ in significant respects. In the common expression for the current

$$B\frac{\hbar}{2e}\langle J\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(2\pi)^2[f_1(\omega)-f_2(\omega)]\,|\,\Lambda^{r}(\omega)\,|^2\rho_1(\omega)\rho_2(\omega), \tag{4.1}$$

the quantity $\rho_\delta(\omega)$ is the *position-independent bulk energy density* of states characteristic of the δth electrode; $|\Lambda^{r}(\omega)|^2$ is the square of the "matrix element" of the transfer (pseudo) Hamiltonian. In contrast, in the simplest model, i.e., for the case of a planar junction which is invariant under translation parallel to the plane of the junction, Eq. (3.19) reduces to

$$B\frac{\hbar}{2e}\langle\bar{J}\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(2\pi)^2[f_1(\omega)-f_2(\omega)]\iiiint_B ds\,ds_1\,ds_2\,ds_3\,[\Lambda^{r}(0,0;(\vec{\rho}_1-\vec{\rho}_2);\omega)\Lambda^{r*}(0,0;(\vec{\rho}-\vec{\rho}_3);\omega)] \times\rho_1(0,0,(\vec{\rho}-\vec{\rho}_1);\omega)\rho_2(0,0,(\vec{\rho}_2-\vec{\rho}_3);\omega)\,, \tag{4.2}$$

where

$$\Lambda^{r}(0,0;\vec{\rho};\omega) = \frac{\hbar^2}{2m}\Gamma^{r}(0,0;\vec{\rho};\omega) = -\left(\frac{\hbar^2}{2m}\right)^2\frac{\partial^2}{\partial z\,\partial z_1}G^{r}(z,z_1;\vec{\rho};\omega)\,|_{z=0=z_1} = \int\frac{d^2k_\rho}{(2\pi)^2}e^{i\vec{k}_\rho\cdot\vec{\rho}}[\,g_1^{r}(0,0;\vec{k}_\rho;\omega)+g_2^{r}(0,0;\vec{k}_\rho;\omega)]^{-1}\,. \tag{4.3}$$

In Eqs. (4.1) and (4.2), a factor of 2 was included to account for the sum over spins. The right-hand side of Eq. (4.2) can be simplified considerably by means of a Fourier transform with respect to the variables $\vec{\rho}_i$:

$$B\frac{\hbar}{2e}\langle\bar{J}\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(2\pi)^2[f_1(\omega)-f_2(\omega)]\int\int_{-\infty}^{\infty}\frac{d^2k_\rho}{(2\pi)^2}\,|\,\Lambda^{r}(0,0;\vec{k}_\rho;\omega)\,|^2\rho_1(0,0;\vec{k}_\rho;\omega)\rho_2(0,0;\vec{k}_\rho;\omega)\,, \tag{4.4}$$

where

$$\rho(0,0;(\vec{\rho}_1-\vec{\rho}_2);\omega)=\iint_{-\infty}^{\infty} e^{i\vec{k}_\rho\cdot(\vec{\rho}_1-\vec{\rho}_2)}\rho(0,0;\vec{k}_\rho;\omega)\frac{d^2k_\rho}{(2\pi)^2}\,, \tag{4.5}$$

and the diagonal term of the spectral density $\rho(z,z;0;\omega)$ is proportional to the *local* density of states, i.e., the usual density of states is given by

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\rho(z,z;0;\omega)\,dz=\rho(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dz\iint_{-\infty}^{\infty}\frac{d^2k_\rho}{(2\pi)^2}\rho(z,z;\vec{k}_\rho;\omega)\,. \tag{4.6}$$

Similarly,

$$\Lambda^r(0,0;(\vec{\rho}_1-\vec{\rho}_2);\omega)=\iint\frac{d^2k_\rho}{(2\pi)^2}e^{i\vec{k}_\rho\cdot(\vec{\rho}_1-\vec{\rho}_2)}\Lambda^r(0,0;\vec{k}_\rho;\omega)\,. \tag{4.7}$$

We see that tunneling current energy density is not simply proportional to the product of the energy densities of states of the two electrodes; instead it involves an integral over the two-dimensional k space of the product of the two-dimensional Fourier transforms of the spectral densities evaluated at the interface and weighted by an appropriate k- (and energy) dependent matrix element. Here we emphasize that the matrix element is in fact a definite, simple function of the uncoupled Green's functions given by Eq. (4.3).

The physical interpretation of Eq. (4.4) is quite obvious: If the junction is invariant under translations in the plane of the junction, the problem is separable. The k integral is simply a sum over the separation constant of the effective "one-dimensional" tunneling current densities given by Eq. (I4.4). The equivalence of Eqs. (4.3) and (4.4) with the result obtained by an elementary treatment of the noninteracting system has been demonstrated in III.[29] The relatively simple dependence of the tunneling current energy density on spectral densities indicated in Eqs. (4.3)–(4.6) applies only for strictly separable problems. Thus, any attempt to account for the periodic potential in an ordered planar junction involves the replacement of Eqs. (4.3) and (4.4) by Eqs. (3.27) and (3.28). These equations involve the spectral densities in a much more complicated way than Eqs. (4.3)–(4.6). In fact, except for the calculational advantage presented by Eq. (3.27) as compared to Eq. (2.19), one might just as well consider the generally valid coordinate representation, given by Eqs. (2.19) and (3.19). Thus, for the general junction as well as for the ordered planar junction, the tunneling current energy density involves an average of the spectral densities over the interface with respect to "generalized matrix elements" which in fact couple the two densities. This suggests that the determination of (local) densities of states, or rather spectral densities averaged over the interface, from experimental data on tunneling junction may require considerably more effort than has been hitherto assumed. This point is implicit in a calculation of the field emitted current from a planar electrode by Caroli *et al.* In this paper the authors outline an extension of their one-dimensional tunneling formalism to three dimensions and they quote, without derivation, an expression which is essentially equivalent to Eq. (3.20).[30]

In conclusion, we wish to note that Eq. (4.4) bears a considerable formal similarity to Appelbaum and Brinkman's expression for the tunneling current within their version of the transfer Hamiltonian formalism which we rewrite[31]

$$B\frac{\hbar}{2e}\langle\bar{J}\rangle=\int_{-\infty}^{\infty}\left(\frac{d\omega}{2\pi}(2\pi)^2[f_1(\omega)-f_2(\omega)]\iint\frac{d^2k_\rho}{(2\pi)^2}\sum_{k_z,l_z}|T(k_z,l_z;\vec{k}_\rho;\omega)|^2\rho_1(k_z,\vec{k}_\rho;\omega)\rho_2(l_z,\vec{k}_\rho;\omega)\right)\,. \tag{4.8}$$

Evidently Appelbaum and Brinkman *assume each electrode to be invariant under translation in the direction normal to the interface*, i.e., their spectral density functions depend only on the coordinate difference $z-z_1$. If furthermore the matrix elements of the (pseudo) tunneling Hamiltonian T are independent of k_z and l_z, or else replaced by their average over k_z and l_z, i.e., if we can write

$$T(k_z,l_z;\vec{k}_\rho;\omega)=\overline{T}(\vec{k}_\rho;\omega)\,, \tag{4.9}$$

then the sums over k_z, l_z reduce to the single term

$$\overline{T}(\vec{k}_\rho;\omega)\rho_1(z-z_1;\vec{k}_\rho;\omega)\big|_{z=z_1}\rho_2(z-z_1;\vec{k}_\rho;\omega)\big|_{z=z_1}\,. \tag{4.10}$$

Equations (4.8)–(4.10) are clearly identical to Eq. (4.4) in the case where the electrodes are invariant under translation along the direction normal to the interface. Admittedly the assumption of translational invariance along the z direction is inconsistent with existence of an interface and the semi-infinite nature of the electrodes. Furthermore, it is difficult to rationalize the imposition of Eq. (4.9)

on the transfer Hamiltonian defined by Appelbaum and Brinkman. However, our analysis which identified the effective tunneling matrix element with the right-hand side of Eq. (4.3) clearly demonstrates Λ^r to be a transfer matrix which for the abrupt junction is to be evaluated at the interface. That is, formally we could indeed replace Λ^r by its average Fourier transform with respect to z and z_1. Whereas the preceding discussion sheds some light on the relation between our results and those based on one of the current versions of the transfer Hamiltonian formalism, a considerably more satisfying understanding of the relation between our theory and the transfer Hamiltonian formalism is obtained by comparing an alternative version of Appelbaum and Brinkman's theory to ours. Rewriting Appelbaum and Brinkman's expression in our notation we have[11a]

$$B\langle \bar{J}\rangle \frac{\hbar}{2e} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}[f_1(\omega) - f_2(\omega)] \iint_B ds\, ds_1 \Big(\rho_1(\vec{r}, \vec{r}_1; \omega) \frac{\partial^2}{\partial z_1 \partial z} \rho_2(\vec{r}_1, \vec{r}; \omega) + \frac{\partial^2}{\partial z \partial z_1}[\rho_1(\vec{r}, \vec{r}_1; \omega)]\rho_2(\vec{r}_1, \vec{r}; \omega)$$
$$- \frac{\partial}{\partial z}[\rho_1(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z_1}[\rho_2(\vec{r}_1, \vec{r}; \omega)] - \frac{\partial}{\partial z_1}[\rho_1(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z}[\rho_2(\vec{r}_1, \vec{r}; \omega)] \Big) . \qquad (4.11)$$

This expression agrees with our theory when it is linearized in the pseudo Hamiltonian $\mathcal{H}'$. That is, substituting into Eq. (3.2) the linearized approximation of Eq. (3.4) and of its transpose, we obtain for the planar junction

$$B\langle \bar{J}\rangle \frac{\hbar}{2e} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_B \Big(\lim_{\substack{z\to 0^+;\rho\to\rho' \\ z'\to 0^-}} \frac{\partial}{\partial z} G^+(\vec{r}, \vec{r}'; \omega) - \lim_{\substack{z\to 0^-;\rho\to\rho' \\ z'\to 0^+}} \frac{\partial}{\partial z'} G^+(\vec{r}, \vec{r}'; \omega) \Big) ds$$
$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Big(\frac{\hbar^2}{2m}\Big) \iint_B \Big(- \frac{\partial}{\partial z}[g_2^r(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z_1}[g_1^+(\vec{r}_1, \vec{r}; \omega)] + \frac{\partial^2}{\partial z \partial z_1}[g_2^r(\vec{r}, \vec{r}_1; \omega)] g_1^+(\vec{r}_1, \vec{r}; \omega)$$
$$- \frac{\partial}{\partial z}[g_2^+(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z_1}[g_1^a(\vec{r}_1, \vec{r}; \omega)] + \frac{\partial^2}{\partial z \partial z_1}[g_2^+(\vec{r}, \vec{r}_1; \omega)] g_1^a(\vec{r}_1, \vec{r}; \omega) - g_1^+(\vec{r}, \vec{r}_1; \omega) \frac{\partial^2}{\partial z \partial z_1} g_2^a(r_1, r; \omega)$$
$$+ \frac{\partial}{\partial z_1}[g_1^+(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z}[g_2^a(r_1, r; \omega)] - g_1^r(r, r_1; \omega) \frac{\partial^2}{\partial z \partial z_1} g_2^+(\vec{r}_1, \vec{r}; \omega)$$
$$+ \frac{\partial}{\partial z_1}[g_1^r(\vec{r}, \vec{r}_1; \omega)] \frac{\partial}{\partial z}[g_1^+(\vec{r}_1, \vec{r}; \omega)] \Big) ds\, ds_1 . \qquad (4.12)$$

Using Eqs. (3.6)–(3.10) the right-hand side of Eq. (4.12) reduces to Eq. (4.11). It should be noted that the difference between Eqs. (3.2) and the first equation of Eq. (4.12) is only apparent: If the correct correlation function G^+ is used, then the limits are in any case simply $\vec{r} \to \vec{r}'$, however, the particular limit chosen simplifies the algebra of reducing Eq. (4.12) to Eq. (4.11). The other point to note is that in Eqs. (4.11) and (4.12) no use was made of any particular boundary conditions imposed on the uncoupled Green's functions at the interface. Appelbaum and Brinkman chose their functions to satisfy a pair of left and right problems, which are each defined over *all space*. Hence they imposed on their Green's functions "outgoing wave" boundary conditions at infinity.[32] Evidently these functions cannot satisfy any homogenous boundary conditions at the interface. In fact, Eq. (4.11) is not valid when the "uncoupled" Green's functions are subject to homogenous boundary conditions at the interface, for then the right side vanishes identically. In order to understand this conclusion one has to recall that the boundary conditions imposed on the uncoupled Green's functions enter our theory explicitly only when Eq. (3.2) is transformed into Eq. (3.11), or an equivalent expression when Dirichlet conditions are imposed at the interface. That is, Eqs. (3.2)–(3.10) are valid regardless of the detailed choice of the uncoupled Green's functions.[33] This choice is however crucial in determining the final expression of the tunneling current in terms of the spectral densities. It is clear, upon further examination of the equations, that unless homogenous boundary conditions are imposed on the uncoupled Green's functions at the interface, the algebra becomes completely unmanageable.

Our somewhat lengthy discussion clearly confirms the original conjecture that the transfer Hamiltonian formalism is only valid to first order in the matrix elements of the transfer (pseudo) Hamiltonian.[34] Equation (4.11) is evidently a satisfactory approximation if and only if the correction represented by the surface integral on the right-hand side of Eq. (2.8) is small. This in turn will be the case when both $g_6(\vec{r}, \vec{r}_1; \omega)$ and

$\nabla_{r_1} g_\delta(\vec{r}, \vec{r}_1; \omega)$ are negligible for $\vec{r}_1 \in B$. One case where this occurs is when the "interface" is located inside a thick barrier such that each "electrode" includes a thick region in which the single-particle eigenfunctions of the uncoupled Hamiltonian $\mathcal{H}_\delta$ exhibit a roughly exponential decay in the coordinate normal to the interface. It is in this sense that the transfer Hamiltonian formalism represents (like the classical WKB approximation) a "thick-barrier approximation." This observation has already been made by Duke in his explicit comparison of the formalism with the kinetic theory for a thick barrier.[35] The same conclusion was also reached by Griffin and Demers from their calculation of quasiparticle tunneling in a normal metal-insulator-superconducting junction.[36] Since the barrier width is inherently dependent on the applied external bias potential V we may conclude that the transfer Hamiltonian formalism is also a "small (bias) potential approximation." The thick barrier is certainly a sufficient, while a small potential is a necessary condition for the applicability of the transfer Hamiltonian. However, the precise conditions under which Eq. (4.11) is a satisfactory approximation are difficult to assess, primarily since $\mathcal{H}'$ does not involve a small parameter; on the contrary, it is a singular operator.

A final point that should be made concerns Eq. (2.34). This equation represents the plane-wave expansion of the surface Green's function introduced by Garcia-Moliner and Rubio.[12] Isolated values of ω for which

$$\det[\underline{g}_1(0,0;\vec{k}_\rho;\omega)+\underline{g}_2(0,0;\vec{k}_\rho;\omega)]=0\ , \qquad (4.13)$$

and which do not fall into one of the several branch-cuts (in the ω-plane) for either of the uncoupled Green's functions, $\underline{g}_\delta(0,0;\vec{k}_\rho;\omega)$, identify the "interfacial" states. That is, eigenstates of the junction which are localized at the interface, since they do not fall into one of the allowed bands of the electrodes. Thus we may conclude from Eqs. (3.27) and (3.28) that, at least for the ordered junction, our theory explicitly accounts for the contribution of interfacial states to the tunneling current. This conclusion is in agreement with the one-dimensional result, and thus, while gratifying, is not really surprising.

However, an important consequence of the above is that, in general, one may not assume the transfer matrix $\Gamma^r(0,0;\vec{k}_\rho;\omega)$ to have any particular, simple $\vec{k}_\rho$ dependence. In particular, one cannot assert it to be sharply peaked at $\vec{k}_\rho=0$, as is commonly suggested for the matrix element or transmission coefficient of the transfer Hamiltonian formalism on the basis of the WKB approximation applied to effective, one-dimensional models of tunneling junctions.[37,38]

APPENDIX: DISCONTINUITY OF UNCOUPLED GREEN'S FUNCTIONS g_δ AT BOUNDARY (INTERFACE) B

In this appendix we shall examine the characteristic singularity of the Green's function for the (single-particle) Schrödinger equation and the consequent discontinuity imposed on this function across a boundary surface on which it has to satisfy homogenous boundary conditions. These are obvious generalizations of the corresponding one-dimensional results quoted in I. The defining equation for the Green's function can be written

$$\left(\nabla_r^2+\frac{2m}{\hbar^2}[\omega-V(\mathbf{r})]\right)g(\vec{r},\vec{r}';\omega)=\frac{2m}{\hbar^2}\delta(\vec{r}-\vec{r}')\ . \qquad (A1)$$

Applying the divergence theorem over a volume D bounded by a surface S we find that

$$\int_S \nabla_r g(\vec{r},\vec{r}';\omega)\cdot d\vec{s}+\frac{2m}{\hbar^2}\int_D[\omega-V(\vec{r})] \times g(\vec{r},\vec{r}';\omega)\,d^3\boldsymbol{\gamma}=\frac{2m}{\hbar^2}\Theta_D(\vec{r}')\ . \qquad (A2)$$

Consider now $D=D_\epsilon$ to contain the point $\vec{r}'$, on the surface S, and bounded by two (finite) surfaces S^+, S^- separated by an infinitesimal distance ϵ along their normal. If, as we shall show, the volume integral on the left-hand side of Eq. (A2) is $0(\epsilon)$, then

$$\lim_{\substack{S^+\to S\\ S^-\to S}}\oint_{S^+-S^-}\nabla_r g(\vec{r},\vec{r}'\omega)\cdot d\vec{s} =\lim_{\epsilon\to 0}\oint_S \nabla_r g(\vec{r},\vec{r}'\omega)\Big|_{z=z'-\epsilon}^{z=z'+\epsilon}\cdot d\vec{s}=\frac{2m}{\hbar^2}\ , \qquad (A3)$$

where z is the coordinate along the positive normal to S.

We can therefore conclude that the normal derivative of g is discontinuous across S by the amount

$$\Delta_S\frac{\partial}{\partial n}g(\vec{r},\vec{r}';\omega)=\frac{2m}{\hbar^2}\delta^{(2)}(\mathbf{r}_S-\mathbf{r}'_S)\ . \qquad (A4)$$

Thus we have established the validity of Eq. (2.4). To finish our proof we note that for bounded potentials

$$\left|\frac{2m}{\hbar^2}\int_{D_\epsilon}[\omega-V(x)]g(\vec{r},\vec{r}';\omega)\right|d^3\boldsymbol{\gamma} \le\frac{2m}{\hbar^2}(\omega+V_{\max})\int_{D_\epsilon}|g(\vec{r},\vec{r}';\omega)|\,d^3\boldsymbol{\gamma}\ . \qquad (A5)$$

The only possibly significant contribution to the integral on the right-hand side arises from the neighborhood of $\vec{r}'$ where we can bound g by $|\vec{r}-\vec{r}'|^{-1}$, and the integral is thus $O(\epsilon)$.

Turning to the discontinuity of g_δ at the boundary, we recall Green's theorem: for $\vec{r}\in D$

$$\frac{\hbar^2}{2m}\int_{B_\delta}[\nabla_{r_1}g_\delta(\vec{r},\vec{r}_1;\omega)f(\vec{r}_1;\omega)-g_\delta(\vec{r},\vec{r}_1;\omega)\times\nabla_{r_1}f(\vec{r}_1;\omega)]\cdot d\vec{s}_1=h(\vec{r};\omega) \tag{A6}$$

is a solution of

$$[\omega-\mathcal{H}(r)_\delta]h(\vec{r};\omega)=0\ , \tag{A7}$$

which satisfies on B_δ the boundary conditions

$$h(\vec{r};\omega)=f(\vec{r};\omega)\ ,\quad\left(\frac{\partial}{\partial n}\right)f(\vec{r};\omega)=\left(\frac{\partial}{\partial n}\right)f(\vec{r};\omega)\ , \tag{A8}$$

provided that f satisfies Eq. (A7). If, in particular, g_δ and f satisfy the same boundary conditions except at the interface B on which g_δ is supposed to satisfy the homogenous boundary conditions

$$\left(\alpha(r_1)+\beta(r_1)\frac{\partial}{\partial n_1}\right)g_\delta(\vec{r},\vec{r}_1;\omega)=0\ ,\quad r\in D_\delta\ , \tag{A9}$$

then we can eliminate $\nabla_{r_1}g$ from the integral in Eq. (A6) and obtain

$$\left(\frac{\alpha(r)}{\beta(r)}+\frac{\partial}{\partial n}\right)f(\vec{r};\omega)=-\frac{\hbar^2}{2m}(-1)^\delta\int_B\left(\frac{\alpha(r)}{\beta(r)}+\frac{\partial}{\partial n}\right)\times g_\delta(\vec{r},\vec{r}_1;\omega)\left(\frac{\alpha(r)}{\beta(r)}+\frac{\partial}{\partial n_1}\right)f(\vec{r}_1;\omega)\,ds_1\ . \tag{A10}$$

Thus we conclude that if $\beta(r)\neq 0$ on B_δ, then

$$\lim_{\vec{r}\to B_\delta(\mathrm{in})}\left(\frac{\alpha(r)}{\beta(r)}+\frac{\partial}{\partial n}\right)g_\delta(\vec{r},\vec{r}_1;\omega)\Big|_{\vec{r}_1\in B}=-(-1)^\delta\frac{2m}{\hbar^2}\delta^{(2)}(\vec{r}_B-\vec{r}_B')\ . \tag{A11}$$

This proves Eq. (2.5). The proof of the remaining discontinuity conditions, Eqs. (2.5′), (2.6), and (2.6′), is similar, and will be omitted. We note that Eq. (A11) could be deduced directly from Eqs. (A4) and (A9), for

$$\lim_{\vec{r}\to B_\delta(\mathrm{in})}g_\delta(\vec{r},\vec{r}';\omega)-\lim_{r\to B_\delta(\mathrm{out})}g_\delta(\vec{r},\vec{r}';\omega)\Big|_{\vec{r}'\in B}=0\ . \tag{A12}$$

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[11a]See Eq. (2.2) of the second paper in Ref. 3.

[12]F. Garcia-Moliner and J. Rubio, Proc. R. Soc. Lond. A 324, 257 (1971).

[13]There is no real advantage in using general homogeneous boundary conditions. In practice we shall consider only the two simple boundary conditions: Neumann conditions $\alpha\equiv 0$, $\beta\equiv 1$; and Dirichlet conditions $\alpha\equiv 1$, $\beta\equiv 0$. However, it is convenient to develop the theory as far as possible for the general conditions. We recall that the "transfer-Hamiltonian-like" results were obtained in I only for the Neumann conditions. However, in III we demonstrated that these same results hold whenever $\beta\neq 0$.

[14]The notation, though apparently cumbersome, allows simultaneous treatment of (a) planar geometry: semi-infinite electrodes filling the half-spaces $z\lessgtr 0$ and a plane interface $B=\{x,y,z;z=0\}$, and (b) Spherical geometry, a finite spherical electrode bounded by the spherical interface $B=\{\vec{r};r=R\}$.

[15]Thus for the planar system, we could impose on the dependence on x,y periodic boundary conditios at some planes $x=\pm X$; $y=\pm Y$. And "outgoing-wave" boundary conditions at $z\to\pm\infty$.

[16]The analysis in I clearly demonstrates this point which also follows from the subsequent work below.

[17]Equation (2.4) is a particular case of the classical discontinuity (boundary condition) imposed on the normal component of the electric field across surface charge density.

[18]Thus, for planar geometry, $B_{1,2}(\mathrm{in})=\{\vec{r},\ z=0^{\mp}\}$.

[19]These equations are derived in Appendix A.

[20]Throughout we assume the convention that when $\vec{r}$ is integrated over B, $\vec{r}=\vec{r}_B$.

[21]This applies in particular to vacuum-crystal interface since free space can be assigned any periodic structure desired.

[22]We shall see below that for (planar) systems which are translationally invariant, or at least periodic, in the plane of the junction such a solution can be constructed by means of the convolution theorem for Fourier transforms.

[23]Obviously a completely translationally invariant junction is a rather trivial special case of the above. In fact, for translationally invariant cases (i.e., separable potentials), the integrations over the two-dimensional wave vector $\vec{k}_\rho$ extend over all space, and the summations with respect to $\vec{m}$, $\vec{m}'$ drop out. The matrix equations thus reduce to scalar equations.

[24]This expansion is the two-dimensional analog of the ordinary plane wave expansion of the Green's function for a three-dimensional lattice. Note that the Green's function is not translationally invariant (i.e., it is not just a function of the difference $(\vec{\rho}-\vec{\rho}')$; it is invariant under the simultaneous translation of $\vec{\rho}$ and $\vec{\rho}'$ by (the same) net translation vector.

[25]The general expression for $[\partial^2 G(z, z_1; \vec{k}_\rho; \omega)/\partial z\, \partial z_1]_{z=0=z_1}$ is considerably more involved due to the noncommutative algebra of the matrices considered.

[26]Note that as suggested in the references above, Eqs. (2.35) and (2.36) could have been deduced directly from Eqs. (2.19) and (2.20).

[27]This function is briefly discussed in Sec. III B of I and in Refs. 19–22 cited therein. For a noninteracting system, $\rho(\vec{r}, \vec{r}\,'; \omega) = \sum_i \psi_i(\vec{r})\psi_i^*(\vec{r}\,')\,\delta(\epsilon_i - \omega)$, where $\{\psi_i\}$ is a complete set of orthonormal eigenfunctions of $\mathcal{H}$, with energies $\omega = \epsilon_i$.

[28]Note that we imposed on g^ν the boundary conditions

$$\frac{\partial}{\partial n} g_\delta^\nu(\vec{r}, \vec{r}_1; \omega)\Big|_{\substack{\vec{r}\in B \\ \vec{r}\,'\in D_\delta}} = 0 = \frac{\partial}{\partial n'} g_\delta^\nu(\vec{r}, \vec{r}\,'; \omega)\Big|_{\substack{\vec{r}\,'\in B \\ \vec{r}\in D_\delta}} .$$

Hence, the characteristic singularity of the Green's functions implies that

$$\frac{\partial}{\partial n} g_\delta^{r,a}(\vec{r}, \vec{r}_1; \omega)\Big|_{\substack{\vec{r}\in B \\ \vec{r}_1 \to B_\delta(\text{out})}} = (-1)^\delta \frac{2m}{\hbar^2}\, \delta^{(2)}(r_B - r_{1B})$$

$$= \frac{\partial}{\partial n'} g_\delta^{r,a}(\vec{r}, \vec{r}_1; \omega)\Big|_{\substack{\vec{r}_1\in B \\ \vec{r}\to B_\delta(\text{out})}} .$$

[29]The one-dimensional analysis in III extends immediately to the separable three-dimensional problem. One simply has to replace the functions $\psi(x; \omega)$ by $\psi(z; \vec{k}_\rho; \omega)$.

[30]See Eq. (17) of Ref. 11. This equation is obtained upon taking in Eq. (3.20) the limits $f_1(\omega) = \Theta(\mu_1 - \omega)$, i.e., $T \to 0$ and $f_2(\omega) = 0$, i.e., $\mu_2 \to -\infty$. Note however, that Caroli's equation has a mistake: $[G_\omega^a(x_0, \vec{\rho}_2 \mid x_0 \vec{\rho}_3)]^*$ should have the arguments $\vec{\rho}_2$ and $\vec{\rho}_3$ interchanged. Note also that $\lim g^\nu(x_0 \pm \epsilon, \vec{\rho} \mid x_0 \pm \epsilon, \vec{\rho}_1)$ as $\epsilon \to 0$ is to be interpreted as $[\partial^2 g^\nu(x, \vec{\rho} \mid x_1, \vec{\rho}_1)/\partial x\, \partial x_1]_{x=0=x_1}$.

[31]See Eq. (2.23) of the first paper in Ref. 3.

[32]This is obvious upon examination of Eqs. (2.7)–(2.11) of the second paper in Ref. 3.

[33]Note also that in particular Eq. (2.8) applies no matter what boundary conditions are imposed on g_δ at the interface. Consequently the same holds for Eqs. (2.9)–(2.11).

[34]In fact, Appelbaum and Brinkman make explicit use of this fact in deriving their version of the theory.

[35]See Ref. 8, p. 218.

[36]A. Griffin and J. Demers, Phys. Rev. B 4, 2202 (1971).

[37]D. R. Penn and E. W. Plummer, Phys. Rev. B 9, 1216 (1974).

[38]The effective-mass approximation is often used to reduce tunneling to an effectively one-dimensional problem. However, the effective-mass approximation leads to a separable (effectively one-dimensional) problem only if the normal to the interface B is parallel to one of the principal axes of the effective-mass tensor.