Tunneling theory without the transfer-Hamiltonian formalism. I*

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Tunneling between two semi-infinite systems across an abrupt junction (of zero thickness) is discussed without invoking the transfer-Hamiltonian formalism. A lucid and novel interpretation of the significance of the transfer Hamiltonian is obtained. A rigorous and easily applied separation of the junction into its two component subsystems is introduced. The current is expressed in terms of characteristics of these two subsystems. Keldysh's perturbation theory for nonequilibrium processes is used to include the effects of the external potential V to all orders. In this, the analysis is similar to that of Caroli *et al.* The extreme-tight-binding approximation of these authors is avoided; this less-restricted formulation differs in important details from the preceding work. It is shown that tunneling current (density) within a differential energy interval can generally be expressed as proportional to the product of appropriately defined "left" and "right" local densities of states (in energy). This confirms the form of the extensions of the consequence of the transfer-Hamiltonian formalism, proposed by Appelbaum and Brinkman and by Caroli *et al.* The new formulation of tunneling manifestly applies in the zero-thickness extreme-strong-coupling limit, where the current formulation of the transfer Hamiltonian fails. The extension of the formalism to junctions of finite width has been worked out and is reported in a second paper, in which it is demonstrated that the results for the abrupt junction follow from those of the finite junction in the zero-width limit, and agree with them qualitatively. The formalism is specifically suited to include many-body interactions.

I. INTRODUCTION

A. Motivation for the study

The transfer-Hamiltonian formalism for the study of tunneling between two electrodes across an insulating barrier has enjoyed almost universal acceptance ever since it was suggested by Bardeen[1] and Cohen, Falicov, and Phillips[2] more than ten years ago. The fundamental premise of the transfer-Hamiltonian formalism is that tunneling between normal or superconducting electrodes can be described by time-dependent perturbation theory involving an appropriately defined transfer or coupling Hamiltonian. That is,

$$\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_T = \mathcal{H}_0 + \mathcal{H}_T , \tag{1.1}$$

where the transfer Hamiltonian $\mathcal{H}_T$ is normally taken in its second-quantized representation,

$$\mathcal{H}_T = \sum_{k,k'} V_{Rk;Lk'} a^{\dagger}_{Rk} a_{Lk'} + \text{H.c.} \tag{1.2}$$

The operators $a_{Lk}, a_{Rk'}$ are the destruction operators for the one-particle states which characterize the unperturbed left and right Hamiltonians (electrodes) $\mathcal{H}_L$ and $\mathcal{H}_R$.

A more involved though not necessarily more precise formulation of the tunneling problem asks for the linear response of the system described by $\mathcal{H}_0$ to the "external probe" represented by the transfer Hamiltonian $\mathcal{H}_T$.[3]

It is the purpose of this paper to determine in what sense the preceding can be justified from first principles, and the consequent limitations, if any, on its applicability to tunneling in general. In view of the considerable work that has been done on these questions, we shall find it convenient to summarize briefly the original motivation for the formalism and subsequent attempts to justify it, or at least interpret its significance. Following this survey it will be relatively simple to explain our approach and the novel results we were able to derive. This discussion occupies the remainder of Sec. I.

The actual derivation, which involves a reasonable amount of algebraic manipulation, is given in Secs. II and III.

B. Motivation for and main result of the transfer-Hamiltonian formalism

The initial motivation for the transfer-Hamiltonian formalism was the empirical observation by Giaever[4] that the current tunneling from a superconducting electrode across an insulating (oxide) barrier into a normal electrode could be described in terms of a properly normalized "tunneling density of states" $\mathfrak{N}_T(V)$, namely,

$$\left(\frac{dI_{NS}}{dV}\right)\left(\frac{dI_{NN}}{dV}\right)^{-1} = \frac{\mathfrak{N}_T(V)}{\mathfrak{N}_0(0)} . \tag{1.3}$$

In Eq. (1.3), $\mathfrak{N}_0(0)$ is the normal density of states at the Fermi level. V is the potential difference applied across the junction,

$$\mathfrak{N}_T(E) = \mathfrak{N}_0(0)\,\frac{d\epsilon}{dE}, \tag{1.4}$$

and ϵ, E are the single-particle energies in the normal (N) and superconducting (S) electrodes (measured relative to the Fermi level). It was noted that Eq. (1.3) could be derived from a perturbation theory subject to some further, presumably justifiable, assumptions. The crucial assumption is that *the transition rate for an electron in an initial (Bloch) state k' of the normal into a final quasiparticle state k of the superconducting electrode is given by the "Golden Rule":*

$$P_{fi} = (2\pi/\hbar)\,|M_{fi}|^2\,\delta(\epsilon_{k'} + V - E_k). \tag{1.5}$$

If the junction is planar and exhibits translational symmetry in that plane, then the transition rate out of the k' state can be written

$$P_{k'} = \frac{2\pi}{\hbar}\int n(k_z)\,\frac{dk_z}{d\epsilon_k}\,\frac{d\epsilon_k}{dE_k}\,|M_{fi}|^2\,\delta(\epsilon_{k'} + V - E_k)\,dk_z, \tag{1.6}$$

where k_z is the component of $\vec{k}$ normal to the junction. Equations (1.3) and (1.4) follow directly from Eq. (1.6) provided we make the following simplifying assumptions, which incidentally are not germane to the main argument: $|M_{fi}|$ is only weakly dependent on k and k', and hence may be removed from the integral and replaced by a constant. This constant is independent of the phase (normal or superconducting) of the electrode.[5,6]

The preceding discussion can be recast in a Green's-function formalism, which connects more clearly with the particular form of $\mathcal{H}_T$ chosen in Eq. (1.2), and which provides a calculational technique for evaluating $\mathfrak{N}_T$. Since the discussion applies equally to normal and superconducting electrodes, we shall henceforth restrict ourselves to the latter.

The assumption concerning the transition rate between electrodes immediately preceding Eq. (1.5) may be replaced by a more formal statement, viz.: The uncoupled electrodes are represented by $\mathcal{H}_0$ and a system of product (many-body) state vectors of $\mathcal{H}_0$. In particular the ground state of $\mathcal{H}_0$ is the product

$$|g\rangle = |g_L\rangle\,|g_R\rangle, \tag{1.7}$$

and a corresponding set of exact (product) excited states is

$$|n\rangle = |n'_L n_R\rangle. \tag{1.8}$$

The transfer Hamiltonian $\mathcal{H}_T$ couples the ground state to these excited states; i.e., the probability amplitude that a single bare electron be transferred from the right to the left is[7]

$$M_{fi} = \langle f|\mathcal{H}|i\rangle = \langle n'_L n_R|\mathcal{H}_T|g_L g_R\rangle = \sum_{k,k'} V_{Rk,Lk'}\langle n_R|a^\dagger_{Rk}|g_R\rangle\langle n'_L|a_{Lk'}|g_L\rangle. \tag{1.9}$$

According to the "Golden Rule" the total transition rate is

$$P = \frac{2\pi}{\hbar}\sum_{k,k_1;k_2k'} V_{Rk,Lk'}(V_{Rk_1,Lk_2})^* \sum_{n_R,n'_L}\delta(\epsilon_{n_R} - V - \epsilon_{n'_L})\langle g_R|a_{Rk_1}|n_R\rangle\langle n_R|a^\dagger_{Rk}|g_R\rangle\langle g_L|a^\dagger_{Lk_2}|n'_L\rangle\langle n'_L|a_{Lk'}|g_L\rangle, \tag{1.10}$$

where V is the potential difference across the junction. We now introduce the zero-temperature Green's functions $G^\pm$:

$$(2\pi i)^{-1}G^-(k,k';\omega) = \sum_n \delta(\omega - \epsilon_n)\langle g|a_k|n\rangle\langle n|a^\dagger_{k'}|g\rangle = \pi^{-1}[1 - f(\omega)][-\tfrac{1}{2}\rho(k,k';\omega)], \tag{1.11}$$

$$(2\pi i)^{-1}G^+(k,k';\omega) = \sum_n \delta(\omega - \epsilon_n)\langle g|a^\dagger_k|n\rangle\langle n|a_{k'}|g\rangle = -\pi^{-1}f(\omega)[-\tfrac{1}{2}\rho(k,k';\omega)] \tag{1.12}$$

Here $f(\omega)$ is the Fermi distribution and $\rho(k,k';\omega)$ is a spectral density function. When the states $|n\rangle$ are sharp in the index k, then $G^\pm$ are diagonal in k and can be expressed in terms of the retarded Green's function G^r, i.e.,[8]

$$\frac{1}{2\pi}\rho(k,k';\omega) = \rho(k;\omega)\delta_{kk'} = -\frac{1}{\pi}\,\mathrm{Im}G^r(k,\omega)\delta_{kk'}. \tag{1.13}$$

In the following we assume the validity of Eq. (1.13); hence we obtain for the net transition rate[9]

$$P = \frac{2\pi}{\hbar}\sum_{k,k'}|V_{kk'}|^2\int_{-\infty}^{\infty}[f_L(\omega - V) - f_R(\omega)]\times\rho_L(k';\omega - V)\rho_R(k;\omega)\,d\omega. \tag{1.14}$$

It is normally assumed that $V_{kk'}$ can be removed from the sum so that[10]

$$P=\frac{2\pi}{\hbar}|V|^2\int_{-\infty}^{\infty}[f_L(\omega-V)-f_R(\omega)]\times\rho_L(\omega-V)\rho_R(\omega)\,d\omega\,, \tag{1.15}$$

where the density of states

$$\rho(\omega)=\sum_k\rho(k,\omega)=-\frac{1}{\pi}\sum_k \mathrm{Im}G^r(k,\omega)\,.$$

Recently a common phenomenological ansatz has been to consider V an energy-dependent pseudopotential matrix element, and to write

$$P=\frac{2\pi}{\hbar}\int_{-\infty}^{\infty}|V(\omega)|^2[f_L(\omega-V)-f_R(\omega)]\times\rho_L(\omega-V)\rho_R(\omega)\,d\omega\,; \tag{1.16}$$

such an expression has been derived by Appelbaum and Brinkman using an extension of Bardeen's work.[11]

To conclude, we have indicated the heuristic basis of the transfer Hamiltonian, and in Eqs. (1.13)–(1.15) the formal consequences of the theory. At this point two problems have to be considered: Can the operator satisfying Eqs. (1.1) and (1.2) be justified (derived) from first principles and applied to other scattering problems? How is the matrix element $V_{kk'}$, to be computed? These questions were considered by Bardeen,[1] Cohen *et al.*,[2] and Prange.[12] More recently Duke,[3] Appelbaum and Brinkman[11] and Caroli *et al.*[13] reconsidered the problem. In Sec. IC we shall review this work.

C. Previous analysis of the transfer Hamiltonian

Bardeen considered tunneling to be the transfer of a quasiparticle from a single (quasi) particle state of the left electrode to one of the right electrode. These states were localized within their respective electrodes by means of a barrier of finite height and infinite width.

The single-particle states of the actual Hamiltonian with a barrier of finite width ($x_a<x<x_b$) are expressed as linear combinations of the right states with a given left state[14]:

$$\psi_m=a_m(t)\phi_{L,m}e^{-iE_mt/\hbar}+\sum_n b_n(t)\phi_{R,n}e^{-iE_nt/\hbar}\,. \tag{1.17}$$

Subject to the standard initial conditions of time-dependent perturbation theory Bardeen obtains a Golden-Rule-like result,[15]

$$\frac{d}{dt}|b_n(t)|^2=\frac{2\pi}{\hbar}|\langle\phi_{R,n}|E_m-\mathcal{H}|\phi_{L,m}\rangle|^2\delta(E_m-E_n)\,. \tag{1.18}$$

The integrand in the matrix element on the right-hand side of Eq. (1.18) differs from zero only in the right electrode $x>x_b$; hence the matrix element can be rewritten

$$\int_{x>x_b}[\phi^*_{R,n}(\mathcal{H}-E_m)\phi_{L,m}-\phi_{L,m}(\mathcal{H}-E_n)\phi^*_{R,n}]\,dx\,. \tag{1.19}$$

Conservation of energy and an application of Green's theorem now reduce the above to

$$-\frac{\hbar^2}{2m}\int_{\mathcal{S}}(\phi^*_{R,n}\nabla\phi_{L,m}-\phi_{L,m}\nabla\phi^*_{R,n})\,ds$$

$$=-\tfrac{1}{2}i\hbar J_x(x_b)_{nm}\,. \tag{1.20}$$

If $\phi_{R,n}$ and $\phi_{L,m}$ are reasonably satisfactory approximate solutions of the Schrödinger equation in the barrier, $x_a<x<x_b$, then the precise location of the boundary surface $\mathcal{S}$ anywhere in the barrier is immaterial.

Bardeen argues that M_{fi} of Eq. (1.5) is to be identified with the expression given in Eq. (1.19). Bardeen does not concern himself with $\mathcal{H}_T$; rather he makes contact directly with Eq. (1.5).[16] Bardeen is not concerned in interpreting the particular form of M_{fi} nor does he present an estimate of the errors, if any, in his time-dependent perturbation theory.

The formal assertion that Giaever's experiment was to be interpreted in terms of a transfer Hamiltonian which satisfies Eqs. (1.1) and (1.2) was first made by Cohen *et al.*[2] They follow Bardeen's convention in their choice of one-particle basis states. They insist that the tunneling objects are normal electrons, but beyond that their analysis provides no further insight into the fundamental significance of $\mathcal{H}_T$.

Prange[12] attempted to find a single-particle basis set which would separate the general second-quantized Hamiltonian for a particularly simple case into three terms such as indicated by Eqs. (1.1) and (1.2). His failure to do so led Prange to suggest that $\mathcal{H}_T$ is an effective interaction which he expected to give strictly correct results only if it is used in first order calculations. While this conclusion has been challenged, Prange has undoubtedly successfully identified the major difficulty of the formalism, i.e., the precise specification of the one-particle basis and of the associated $\mathcal{H}_0=\mathcal{H}_L+\mathcal{H}_R$.

Duke pointed out the formal similarity between the transfer-Hamiltonian formulation of tunneling and Oppenheimer's discussion of field ionization of hydrogen.[17] Thus, writing

$$\mathcal{H}=-\frac{\hbar^2\nabla^2}{2m}-\frac{e^2}{r}-Fz=\mathcal{H}_a-Fz=-\frac{e^2}{r}+\mathcal{H}_b\,, \tag{1.21}$$

Oppenheimer writes

$$\psi_0 = a_0(t)\phi_{a,0}e^{-iE_0t/\hbar} + \sum_n b_n(t)\phi_{b,n}e^{-iE_nt/\hbar}, \tag{1.22}$$

where

$$(\mathcal{H}_a - E_0)\phi_{a,0} = 0, \quad (\mathcal{H}_b - E_n)\phi_{b,n} = 0. \tag{1.23}$$

An approximation equivalent to Eq. (1.18) is

$$\frac{d|b_n|^2}{dt} = \frac{2\pi}{\hbar}|\langle \phi_{b,n}|-Fz|\phi_{a,0}\rangle|^2\delta(E_n - E_0). \tag{1.24}$$

Bardeen's argument in proceeding from Eq. (1.18) is identified by Duke as based on the assumption that $\mathcal{H}$ is separable in the sense that

$$\mathcal{H} = \mathcal{H}' = \Theta(R_a)\mathcal{H}_a + \Theta(R_b)\mathcal{H}_b, \tag{1.25}$$

where $\Theta(R)$ is the characteristic function of the domain R (it is unity on R and vanishes everywhere else). If Eq. (1.25) applies, then the matrix element in Eq. (1.24) reduces to

$$\langle \phi_{b,n}|\mathcal{H} - E_0|\phi_{a,0}\rangle = -\frac{\hbar i}{e}\int_S J_{n0}\,ds, \tag{1.26}$$

where S is the boundary separating domains R_a and R_b. Duke now points out that Eqs. (1.23) and (1.24) are consistent only if the set $\{\phi_{a,n}; \phi_{b,m}\}$ forms a complete orthonormal product basis for $\mathcal{H}_0 = \mathcal{H}_a + \mathcal{H}_b$, that is, if

$$[\mathcal{H}_a, \mathcal{H}_b] = 0. \tag{1.27}$$

In this case, the transition rate from $\phi_{a,0}$ to $\phi_{b,n}$ is given by the Golden Rule,

$$P_{a,0;\,b,n} = \frac{2\pi}{\hbar}|\langle \phi_{b,n}|\mathcal{H}_T|\phi_{a,0}\rangle|^2\delta(E_n - E_0), \tag{1.28}$$

and

$$\mathcal{H}_T = \mathcal{H} - \mathcal{H}_0. \tag{1.29}$$

Neither Bardeen's nor Oppenheimer's models satisfy the preceding criteria. If they would, both would involve the same transfer Hamiltonian

$$\mathcal{H}_T = p^2/2m. \tag{1.30}$$

The preceding analysis leads Duke to suggest that the transfer-Hamiltonian method be viewed as a phenomenological formulation in which the trial function defined by Eqs. (1.22) and (1.23) is substituted in Eq. (1.21) and where $\mathcal{H}_T$ of Eq. (1.28) is defined by $\mathcal{H} - \mathcal{H}_a$.

In spite of this conclusion, Duke trusts the basic consequence of the formalism, namely Eq. (1.14). It therefore remains an open question whether the formalism, in spite of its conceptual weaknesses, does provide a reliable procedure for handling tunneling. One of the purposes of this paper is to adduce limits to the validity of this conjecture. In this work we shall follow an approach similar to that of Caroli *et al.*[13] Duke and co-workers have also recently discussed a new microscopic theory based on Green's functions, which, they argue, overcomes the conceptual difficulties of the transfer-Hamiltonian formalism.[18]

D. Outline of the present work

Recently Caroli *et al.* developed, in a series of four papers, a "direct" formulation of tunneling. They avoided the need to derive the transfer Hamiltonian, and in fact their work sheds light on possible fundamental shortcomings of that formalism.[19] This interesting work relies heavily on an extreme-tight-binding approximation which transforms the differential Schrödinger equation into a difference equation. The authors themselves were bothered by the possible lack of generality of their formulation and results. In the second of their papers they attempted to demonstrate the generality of their procedure. The rather indirect method used by Caroli *et al.* suggests to us the desirability of an independent analysis which would avoid any recourse to difference techniques. Our results partially corroborate those of Caroli *et al.* though they differ from them in some important details. We believe that the disagreement is due primarily to the incorrect definition of the Green's functions used by Caroli, which violate some of the analyticity requirements on such functions.

We shall show that subject to the separability criterion [Eq. (1.25)], the transfer Hamiltonian may be introduced quite naturally, as a pseudopotential, in agreement with the original conjecture of Prange. The operator has quite generally the form of a current operator, as suggested by Bardeen and Duke. However, this pseudopotential should and can be treated beyond first-order (time-dependent) perturbation theory; in fact, as already indicated by Caroli, it has to be treated to all orders.

In the present paper we restrict ourselves to an abrupt planar junction between two semi-infinite electrodes. Our approach consists of two distinct steps.

First, in Sec. II, the exact one-particle Green's function, in the absence of an external potential, is computed in terms of "zero order" or uncoupled Green's functions for the two half-spaces. The Green's functions for the half-spaces are not unique. The consequences of the resultant flexibility in the description of the full Green's func-

tion are discussed. This work enables us to resolve the controversy concerning the proper definition of $\mathcal{H}_0$ and of the "right" and "left" propagators. We also obtain a clear interpretation of Bardeen's matrix element (of the transfer Hamiltonian) as a device to assure the proper continuity of the Green's (and wave) function at the abrupt junction.

Then, in Sec. III we follow Caroli *et al.* in applying a generalization of real-time Green's-function techniques, due to Keldysh,[20] to calculate the tunneling current at an abrupt junction in the presence of an applied potential. It should be emphasized that by extending the perturbation theoretic techniques for many-body systems in thermal equilibrium to nonequilibrium processes, Keldysh's formalism enables us to go beyond the first-order time-dependent perturbation theory which characterized all work on tunneling prior to Caroli *et al.* In the present paper we restrict ourselves to the case of noninteracting electrons. Extensions to include electron-electron and electron-phonon interactions as well as the consideration of barriers of finite width have been developed and will be dealt with in future publications. Here it should be stressed that the abrupt junction obviously represents the limiting case of an infinitely thin junction; thus, we are here dealing with the so-called strong-coupling case, which is the opposite extreme of the thick-barrier (weak-coupling) limit. It was only in the latter limit that Duke was able to demonstrate the agreement of the transfer-Hamiltonian analysis of the tunneling of free electrons across a (square) barrier with the exact (single-particle) elementary solution.[21] While it is not clear how, if at all, the transfer-Hamiltonian formalism, as currently formulated, can be applied to our case, we show in the second paper of this series that the abrupt junction results derived in the present paper are indeed obtained from those for the finite junction in the limit of vanishing width.[22] Conversely our conclusions are independent of the width of the junction.

In Sec. IV we discuss our conclusions and results, of which the three most important ones are (i) a clear statement of the significance of the transfer Hamiltonian; (ii) the precise limits of the validity of the current formulations of tunneling in terms of this Hamiltonian; (iii) the development of a formalism for tunneling which is no more cumbersome to apply than the current transfer-Hamiltonian formalism, and is free of the many inherent difficulties of the latter. It is well known that the transfer-Hamiltonian formulation fails to explain several experimental observations. This point has been made quite emphatically by Duke in a recent publication.[18]

II. EQUILIBRIUM GREEN'S FUNCTION

A. Definitions

We wish to compute the Green's function for an abrupt junction in the absence of an applied potential in terms of the Green's functions of the uncoupled electrodes.

The abrupt junction is defined below,[23]

$$\mathcal{H} = \Theta(-x)\mathcal{H}_L + \Theta(x)\mathcal{H}_R . \tag{2.1}$$

The Hamiltonians $\mathcal{H}_L, \mathcal{H}_R$ characterize the uncoupled, generally distinct, left and right electrodes. It is convenient to include in the definition of the Green's functions g for the uncoupled electrodes the fact that these are semi-infinite rather than infinite systems. This is done by imposing on these functions boundary conditions at the interface. The Green's functions for these uncoupled electrodes are distinguished from the ordinary Green's functions (for the corresponding infinite electrode) because they satisfy *homogeneous boundary conditions at the interface*, i.e.,

$$(\hbar\omega - \mathcal{H}_L)\, g_L(x, x'; \omega) = \delta(x - x'), \tag{2.2}$$

and at the interface,

$$\alpha g_L(0, x' < 0; \omega) + \beta \frac{\partial}{\partial x} g_L(0, x' < 0; \omega) = 0$$

$$= \alpha g_L(x < 0, 0; \omega) + \beta \frac{\partial}{\partial x'} g_L(x < 0, 0; \omega), \tag{2.3}$$

while at infinity,

$$\lim_{x \to -\infty} a_- g_L(x, x'; \omega) + b_- \frac{\partial}{\partial x} g_L(x, x'; \omega) = 0 . \tag{2.4}$$

Here the coefficients α, β are completely at our disposal, and are to be chosen so as to simplify the calculation of the full Green's function. One might expect that setting one of these coefficient equal to zero could simplify the analysis. It is, however, not clear which of two possible choices is preferable. We shall see that choosing $\alpha = 0$ leads to a tunneling theory which is physically more transparent.[24]

The coefficients a_-, b_- do not have to be specified at all, but are understood to represent "outgoing waves" boundary conditions.

Note that g_L exists everywhere. The "localization" to the left half-space is not forced by making g_L vanish identically on the right space, nor by making it decay exponentially. The function has no immediate significance on the right half-space.

This is the standard procedure for boundary-value problems, and we emphasize it only because of the incorrect choice of Caroli *et al.* to force g_L to vanish on the entire right half-space.

The Green's function for the right half-space is defined analogously,

$$(\hbar\omega - \mathcal{H}_R)\, g_R(x, x'; \omega) = \delta(x - x'), \tag{2.5}$$

where at the interface,

$$\alpha g_R(0, x' > 0; \omega) + \beta \frac{\partial}{\partial x} g_R(0, x' > 0; \omega) = 0$$

$$= \alpha g_R(x > 0, 0; \omega) + \beta \frac{\partial}{\partial x'} g_R(x > 0, 0; \omega), \tag{2.6}$$

and at infinity

$$\lim_{x \to +\infty} a_+ g_R(x, x'; \omega) + b_+ \frac{\partial}{\partial x} g_R(x, x'; \omega) = 0. \tag{2.7}$$

The Green's function for the entire junction satisfies homogeneous boundary conditions only at $\pm\infty$:

$$(\hbar\omega - \mathcal{H}) G(x, x'; \omega) = \delta(x - x'), \tag{2.8}$$

$$\lim_{x \to \mp\infty} a_\mp G(x, x'; \omega) + b_\mp \frac{\partial}{\partial x} G(x, x'; \omega) = 0. \tag{2.9}$$

B. Determination of G

The Green's function G can be represented in terms of the functions $g_{R,L}$ by two alternative procedures: The direct procedure is to apply Green's theorem over the two half-intervals, and to express G in terms of its "boundary values" at the interface, $x = 0$. Alternatively the "inhomogeneous boundary values" satisfied by G at $x = 0$ may be treated as an inhomogeneous (source) term in the differential equation. That is, one may introduce a pseudo-Hamiltonian $\mathcal{H}'$ and represent G in terms of an integral equation. The Hamiltonian $\mathcal{H}'$ is in fact just the transfer Hamiltonian whose matrix elements were given by Bardeen.

Applying Green's theorem to

$$\int_0^\infty \{ G(x_1, x'; \omega)[\hbar\omega - \mathcal{H}_R(x_1)]\, g_R(x, x_1; \omega)$$

$$- g_R(x, x_1; \omega)[\hbar\omega - \mathcal{H}(x_1)]\, G(x_1, x'; \omega)]\, d\omega, \tag{2.10}$$

we obtain, with help of Eqs. (2.5)–(2.9),

$$G(x, x'; \omega) = g_R(x, x'; \omega)\Theta(x')$$

$$+ \frac{\hbar^2}{2m} \{ g_R(x, x_1; \omega)$$

$$\times \frac{\partial}{\partial x_1} G(x_1, x'; \omega) - \frac{\partial}{\partial x_1}[g_R(x, x_1; \omega)]$$

$$\times G(x_1, x'; \omega)\} \big|_{x_1 = 0^+}, \quad x \geq 0. \tag{2.11}$$

Evidently we can rewrite Eq. (2.11) as

$$\Theta(x) G(x, x'; \omega) = g_R(x, x'; \omega)\Theta(x')\Theta(x)$$

$$+ \int_{-\infty}^{\infty} g_R(x, x_1; \omega)\Theta(x)\Theta(x_1)\mathcal{H}_R'(x_1)$$

$$\times G(x_1, x'; \omega)\, dx_1, \tag{2.12}$$

where

$$\mathcal{H}_R'(x) = \lim_{\epsilon \to 0^+} \frac{\hbar^2}{2m} \left(\delta(x - \epsilon), \frac{\partial}{\partial x} \right)_+. \tag{2.13}$$

This, however, amounts to the statement that

$$[\hbar\omega - (\mathcal{H}_R + \mathcal{H}_R')]\, G(x, x'; \omega) = \delta(x - x') \quad \text{if } x > 0. \tag{2.14}$$

The same argument can be applied to the left half-space, i.e.,

$$G(x, x'; \omega) = g_L(x, x'; \omega)\Theta(-x') - \frac{\hbar^2}{2m} \Big(g_L(x, x_1; \omega)$$

$$\times \frac{\partial}{\partial x_1} G(x_1, x'; \omega) - \frac{\partial}{\partial x_1}[g_L(x, x_1; \omega)]$$

$$\times G(x_1, x'; \omega) \Big) \big|_{x_1 = 0^-}, \quad x \leq 0. \tag{2.15}$$

In the preceding we have followed the convention that

$$\Theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$

and

$$\Theta(-x) = \begin{cases} 1, & x \leq 0 \\ 0, & x > 0. \end{cases}$$

While not the common definition of the unit step function, this is the most convenient convention for our purposes and will be followed throughout the remainder of this paper.

An alternative version of Eqs. (2.11) and (2.15) is

$$G(x, x'; \omega) = g_R(x, x'; \omega)\Theta(x) - \frac{\hbar^2}{2m} \Big(G(x, x_1; \omega)$$

$$\times \frac{\partial}{\partial x_1} g_R(x_1, x'; \omega) - \frac{\partial}{\partial x_1}[G(x, x_1; \omega)]$$

$$\times g_R(x_1, x'; \omega) \Big) \big|_{x_1 = 0^+}, \quad x' \geq 0 \tag{2.11'}$$

and

$$G(x, x'; \omega) = g_L(x, x'; \omega)\Theta(-x) + \frac{\hbar^2}{2m} \Big(G(x, x_1; \omega)$$

$$\times \frac{\partial}{\partial x_1} g_L(x_1, x'; \omega) - \frac{\partial}{\partial x_1}[G(x, x_1; \omega)]$$

$$\times g_L(x_1, x'; \omega) \Big) \big|_{x_1 = 0^-}, \quad x' \leq 0. \tag{2.15'}$$

Thus we conclude that the "boundary values" $G(0, x'; \omega)$ and $\partial G(x, x'; \omega)/\partial x|_{x=0}$, which enter Eqs. (2.11) and (2.15), can be expressed in terms of the constants

$$G(0,0;\omega),\quad \frac{\partial G}{\partial x}(x,x_1;\omega)\big|_{x=x_1^+=0},$$
$$\frac{\partial G}{\partial x_1}(x,x_1;\omega)\big|_{x=x_1^+=0},\qquad (2.16)$$
$$\frac{\partial^2 G}{\partial x\,\partial x_1}(x,x_1;\omega)\big|_{x=x_1=0}.$$

Here we note that $G(x,x_1;\omega)$ is continuous at $x=x_1$, but has a characteristic discontinuity in its first derivative,

$$\frac{\partial G}{\partial x}(x,x_1;\omega)\Big|_{x=x_1^-}^{x=x_1^+}=\frac{2m}{\hbar^2}=\frac{\partial G}{\partial x_1}(x,x_1;\omega)\Big|_{x_1=x^-}^{x_1=x^+}. \qquad (2.17)$$

Finally, the mixed second derivative $\partial^2 G(x,x_1;\omega)/\partial x\,\partial x_1$ is continuous at $x=x_1$. The same comments apply to $g_{R,L}(x,x_1;\omega)$.

Combining Eqs. (2.11) and (2.15) and Eqs. (2.17), one can determine the constants listed in Eq. (2.16); in particular one obtains

$$G(0,0;\omega)=\frac{g_R(0,0;\omega)g_L(0,0;\omega)}{g_R(0,0;\omega)+g_L(0,0;\omega)} \qquad (2.18)$$

as well as an alternative equivalent expression,

$$G(0,0;\omega)=\frac{\partial}{\partial x}g_L(x,x_1=x^-;\omega)\,\frac{\partial}{\partial x}g_R(x,x_1=x^+;\omega)\big|_{x=0}\times\left(\frac{\partial^2}{\partial x\,\partial x_1}[g_L(x,x_1;\omega)+g_R(x,x_1;\omega)]\,\big|_{x=x_1=0}\right)^{-1}. \qquad (2.18')$$

Equation (2.18) is formally identical to the "surface Green's function" derived by Garcia-Moliner and Rubio.[25] When the general homogeneous boundary conditions imposed on $g_{R,L}$ at the interface are specialized by setting $\beta=0$ in Eqs. (2.3) and (2.6), then Eq. (2.18) becomes indeterminate and Eq. (2.18′) reduces to[26]

$$G(0,0;\omega)=-\left(\frac{2m}{\hbar^2}\right)^2\left(\frac{\partial^2}{\partial x\,\partial x_1}[g_L(x,x_1;\omega)+g_R(x,x_1;\omega)]\right)^{-1}. \qquad (2.18'')$$

For future reference, we note that Eq. (2.18″) was derived by Caroli *et al.*, using a totally different approach.[27] Thus we conclude that implicit in Caroli's analysis is the convention that $g_{R,L}$ vanish at the interface.

We can combine Eqs. (2.11) and (2.15) into a single equation,

$$G(x,x';\omega)=g(x,x';\omega)+\int_{-\infty}^{\infty}g(x,x_1;\omega)\times\mathcal{K}'(x_1)G(x_1,x';\omega)\,dx_1, \qquad (2.19)$$

where

$$g(x,x';\omega)=[\Theta(-x)\Theta(-x')g_L(x,x';\omega)+\Theta(x)\Theta(x')g_R(x,x';\omega)]\times[1-\tfrac{1}{2}\Theta(x)\Theta(x')\Theta(-x)\Theta(-x')], \qquad (2.20)$$

and

$$\mathcal{K}'(x)=\lim_{\epsilon\to 0^+}\frac{\hbar^2}{2m}\left([\delta(x-\epsilon)-\delta(x+\epsilon)],\frac{\partial}{\partial x}\right)_+ =-[\mathcal{K}(x)]^\dagger. \qquad (2.21)$$

Equations (2.19)–(2.21) enable us to identify Bardeen's "transition current" with the corresponding matrix element of $\mathcal{K}'$. Evidently the role of $\mathcal{K}'$ is to assure the continuity of G (and hence also of the wave function ψ) across the discontinuity of the potential at the interface.

Before concluding this section we shall indicate the complete representation of $G(x,x';\omega)$ in terms of $g_{L,R}$ for the two simple homogeneous boundary conditions at the interface: When the Green's functions $g_{R,L}$ vanish at the interface, we need in Eqs. (2.11) and (2.15) the boundary values $G(0,x';\omega)$, which according to Eqs. (2.11′) and (2.15′) are

$$G(0,x';\omega)=\mp\frac{\hbar^2}{2m}G(0,0;\omega)\,\frac{\partial}{\partial x_1}g_{R,L}(x_1,x';\omega)\big|_{x_1=0^\pm},\quad x'\gtrless 0 \qquad (2.22)$$

where $G(0,0;\omega)$ is given by Eq. (2.18″).

When the normal derivative of Green's functions $g_{R,L}$ vanishes at the interface, then we need in Eqs. (2.11) and (2.15) the boundary values $\partial G(x=0,x';\omega)/\partial x$, which are again determined from Eqs. (2.11′) and (2.15′):

$$\frac{\partial G}{\partial x}(x,x';\omega)\big|_{x=0}=\pm\left(\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x\,\partial x_1}G(x,x_1;\omega)\big|_{x=0=x_1}\times g_{R,L}(0,x';\omega),\quad x'\gtrless 0 \qquad (2.23)$$

where, by virtue of the characteristic singularity of G at $x=x'$,

$$\frac{\partial^2}{\partial x\,\partial x_1}G(x,x_1;\omega)\big|_{x=0=x_1}=-\left(\frac{2m}{\hbar^2}\right)^2[g_R(0,0;\omega)+g_L(0,0;\omega)]^{-1}. \qquad (2.24)$$

III. TUNNELING CURRENT

A. Generalities

We shall express the current across the interface in terms of the Green's function G^+, to be defined below, and then use the formalism of Keldysh to express G^+ in terms of related left and right functions.

It is a simple matter to verify that the average

of J,

$$\langle J(x)\rangle = -\frac{e\hbar}{2m}\lim_{x',\, t'\to x,\, t}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)G^{+}(x,t;x't') = \langle J(0)\rangle\ . \tag{3.1}$$

The last equation in Eq. (3.1) follows from the one-dimensional equation of continuity. The Green's function G^{+} is defined below:

$$G^{+}(x,t;x',t') = i\langle\psi^{\dagger}(x',t')\psi(x,t)\rangle\ . \tag{3.2}$$

Taking the Fourier transform of Eq. (3.1) with respect to t, we obtain[28]

$$\langle J(0)\rangle = \frac{e\hbar}{2m}\int\lim_{x'\to x}\frac{\partial}{\partial x}[G^{+}(x',x;\omega) - G^{+}(x,x';\omega)]\,|_{x=0}\frac{d\omega}{2\pi}\ . \tag{3.3}$$

B. Summary of Keldysh's formalism

Keldysh[20] has demonstrated that for nonequilibrium processes, G^{+} can be determined in terms of three related Green's functions which satisfy the (matrix) Dyson equation indicated symbolically below:

$$\begin{pmatrix}0 & G^{a}\\ G^{r} & F\end{pmatrix} = \begin{pmatrix}0 & g^{a}\\ g^{r} & f\end{pmatrix}\left[\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}+\begin{pmatrix}\Omega & \Sigma^{r}\\ \Sigma^{a} & 0\end{pmatrix}\begin{pmatrix}0 & G^{a}\\ G^{r} & F\end{pmatrix}\right], \tag{3.4}$$

In Eq. (3.4) multiplication of matrix elements is to be interpreted as an integration with respect to both space and time variables. Using a more compact matrix notation, we may rewrite Eq. (3.4) as

$$\underline{G} = \underline{g} + \underline{g}\,\underline{\Sigma}\,\underline{G}\ . \tag{3.5}$$

The Hermitian adjoint equation also applies; i.e.,

$$\underline{G} = \underline{g} + \underline{G}\,\underline{\Sigma}^{\dagger}\underline{g}\ . \tag{3.6}$$

In the present discussion, the "unperturbed" Green's functions in Eqs. (3.4)–(3.6) are to be defined in terms of left and right functions by an equation such as Eq. (2.20). For an instantaneous interaction, such as the pseudo-Hamiltonian $\mathcal{H}'$ defined in Eq. (2.21), the self-energy matrix reduces to a symmetric matrix with vanishing diagonal elements.[29] Since $\mathcal{H}'$ is a single-particle operator, we obtain, furthermore,

$$\underline{\Sigma} = \begin{pmatrix}0 & \mathcal{H}'\\ \mathcal{H}' & 0\end{pmatrix}\ . \tag{3.7}$$

To illustrate the preceding remarks, we have, for instance,

$$G^{a}(x,x';\omega) = \left[\left(g_{L}^{a}(x,x';\omega)\Theta(-x') + \int_{-\infty}^{0} g_{L}^{a}(x,x_1;\omega)\mathcal{H}'(x_1)G^{a}(x_1,x';\omega)\,dx_1\right)\Theta(-x) + \left(g_{R}^{a}(x,x';\omega)\Theta(x') + \int_{0}^{\infty} g_{R}^{a}(x,x_1;\omega)\mathcal{H}'(x_1)G^{a}(x_1,x';\omega)\,dx_1\right)\Theta(x)\right]\left[1-\tfrac{1}{2}\Theta(x)\Theta(x')\Theta(-x)\Theta(-x')\right]. \tag{3.8}$$

It remains now to define the several Green's functions introduced above. In terms of the field operators ψ and $\psi^{\dagger}$,[30]

$$\begin{aligned} g^{+}(x,t;x',t') &= i\langle\psi^{\dagger}(x',t')\psi(x,t)\rangle_{0},\\ g^{-}(x,t;x',t') &= -i\langle\psi(x,t)\psi^{\dagger}(x',t')\rangle_{0},\\ g^{r,a}(x,t;x',t') &= \mp i\langle[\psi(x,t),\psi^{\dagger}(x',t')]_{+}\rangle_{0}\Theta(\pm t\mp t'),\\ g(x,t;x',t') &= -i\langle T[\psi(x,t)\psi^{\dagger}(x',t')]\rangle_{0},\\ f(x,t;x',t') &= -i\langle[\psi(x,t),\psi^{\dagger}(x',t')]_{-}\rangle_{0}. \end{aligned} \tag{3.9}$$

From Eqs. (3.9) it follows immediately that

$$g^{\pm} = \tfrac{1}{2}(f \pm g^{a} \mp g^{r})\ . \tag{3.10}$$

The subscript 0 denotes that the average indicated by the angular brackets is with respect to the unperturbed density matrix. The full Green's functions G are defined by the same formal expressions [Eqs. (3.9)] except that the averages are taken with respect to the full density matrix.

Below we shall find use for the following relations between the time Fourier transforms of the several g's[31]:

$$g^{+}(x,x';\omega) = -2if(\omega)[-\tfrac{1}{2}\rho(x,x';\omega)], \tag{3.11}$$

$$g^{-}(x,x';\omega) = 2i[1-f(\omega)][-\tfrac{1}{2}\rho(x,x';\omega)], \tag{3.12}$$

$$g^{r}(x,x';\omega) = P\int\frac{\rho(x,x';\omega')}{\omega-\omega'}\frac{d\omega'}{2\pi} - \frac{i}{2}\rho(x,x';\omega) = [g^{a}(x,x';\omega)]^{\dagger} = [g^{a}(x',x;\omega)]^{*}\ . \tag{3.13}$$

In these equations,

$$f(\omega) = \{1+\exp[(\hbar\omega-\mu)(k_B T)^{-1}]\}^{-1}; \tag{3.14}$$

P denotes the principal part of the integral; and $\rho(x, x'; \omega)$ is the so-called spectral-density function, which is discussed in Sec. IV. Here we only wish to note that the function is in general complex, but when $x = x'$ it is real and positive for real values of ω. Equations (3.11)–(3.14) apply only if the unperturbed system is in thermal equilibrium.[32]

C. Calculation of the current

Using the formalism of Keldysh as summarized in Sec. III B, we can determine G^+ in terms of the unperturbed functions g, and thus express $\langle J(0) \rangle$ in terms of these quantities. In the following we shall drop, whenever this causes no confusion, the argument ω.

Upon substitution of Eq. (3.7) and (3.10) into Eq. (3.4), we obtain

$$G^+(x, x') = g^+(x, x') + \int_{-\infty}^{\infty} dx_1 [g^+(x, x_1)\mathcal{H}'(x_1) \times G^a(x_1, x') + g^r(x, x_1)\mathcal{H}'(x_1)G^+(x_1, x')] . \tag{3.15}$$

We note that if the uncoupled subsystems are defined to be in thermal equilibrium when $\mathcal{H}' = 0$, then Eq. (3.11) implies that[33]

$$\lim_{\substack{x' \to x \\ x = 0^-}} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) g^+(x, x'; \omega) = 0 . \tag{3.16}$$

Thus, the integrand on the right side of Eq. (3.3) can be written with the help of Eq. (3.15) and its adjoint,

$$\frac{2m}{\hbar e} \langle J(0; \omega) \rangle$$

$$= \lim_{\substack{x' \to x \\ x = 0^-}} \left(\frac{\partial}{\partial x} \int_{-\infty}^{0} [G^+(x, x_1; \omega)\mathcal{H}'(x_1) g_L^a(x_1, x'; \omega) + G^r(x, x_1; \omega)\mathcal{H}'(x_1) g_L^+(x_1, x'; \omega)] \, dx_1 + \frac{\partial}{\partial x'} \int_{-\infty}^{0} [g_L^+(x, x_1; \omega)\mathcal{H}'(x_1) G^a(x_1, x'; \omega) + g_L^r(x, x_1; \omega)\mathcal{H}'(x_1) G^+(x_1, x'; \omega)] \, dx_1 \right) . \tag{3.17}$$

At this point we shall drop the general homogeneous boundary conditions at the interface in favor of the simpler requirement that the normal derivative of $g_{R,L}$ vanish at the interface. In the Appendix, we outline the analysis in terms of Green's functions $\bar{g}_{R,L}$ subject to the second "simple" boundary condition at the interface, namely those that vanish there.

Using Eqs. (2.21) and (2.24), the relation

$$G^a - G^r = G^+ - G^- , \tag{3.18}$$

and the boundary conditions

$$\frac{\partial}{\partial x} g_{R,L}(x, x' \gtrless 0; \omega)|_{x=0} = 0 = \frac{\partial}{\partial x'} g_{R,L}(x \gtrless 0, x'; \omega)|_{x'=0} , \tag{3.19}$$

we obtain from Eq. (3.17)

$$\frac{2m}{\hbar e} \langle J(0; \omega) \rangle = \frac{\hbar^2}{2m} \left(g_L^+(0, 0; \omega) \frac{\partial^2}{\partial x \partial x'} G^-(x, x'; \omega) - g_L^-(0, 0; \omega) \frac{\partial^2}{\partial x \partial x'} G^+(x, x'; \omega) \right) \Big|_{x = 0^- = x'} . \tag{3.20}$$

However, the left side of Eq. (3.17) could have been evaluated in the limit $x \to 0^+$, in which case we obtain

$$\frac{2m}{\hbar e} \langle J(0; \omega) \rangle = \frac{\hbar^2}{2m} \left(g_R^+(0, 0; \omega) \frac{\partial^2}{\partial x \partial x'} G^-(x, x'; \omega) - g_R^-(0, 0; \omega) \frac{\partial^2}{\partial x \partial x'} G^+(x, x'; \omega) \right) \Big|_{x = 0^+ = x'} . \tag{3.21}$$

The continuity of the mixed second derivative of Green's functions allows us to drop in Eqs. (3.20) and (3.21) the distinction between left- and right-hand limits, $x = 0^-, 0^+$.

Combining Eqs. (3.18) with the Dyson equation satisfied by $G^{r,a}$, one obtains the following relation between the mixed second derivatives of G^+ and G^- at the interface:

$$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x \partial x'} [G^+(x, x'; \omega) - G^-(x, x'; \omega)]|_{x = 0 = x'} = \frac{2m}{\hbar^2} [g_R^+(0, 0; \omega) + g_L^+(0, 0; \omega) - g_R^-(0, 0; \omega) - g_L^-(0, 0; \omega)] \times \{[g_R^a(0, 0; \omega) + g_L^a(0, 0; \omega)][g_R^r(0, 0; \omega) + g_L^r(0, 0; \omega)]\}^{-1} . \tag{3.22}$$

We can now eliminate $G^{\pm}$ between Eqs. (3.20)–(3.22), and obtain

$$\langle J(0;\omega)\rangle = \frac{e}{\hbar}\,|\,g_R^r(0,0;\omega)+g_L^r(0,0;\omega)\,|^{-2} \times[g_L^+(0,0;\omega)\,g_R^-(0,0;\omega) - g_L^-(0,0;\omega)\,g_R^+(0,0;\omega)]\,. \tag{3.23}$$

Using Eqs. (3.11) and (3.12) to eliminate $g^{\pm}$ in favor of g^r, we obtain

$$\langle J(0;\omega)\rangle = \frac{4e}{\hbar}\,|\Lambda^r(\omega)|^2\,\mathrm{Im}g_L^r(0,0;\omega) \times \mathrm{Im}g_R^r(0,0;\omega)[f_L(\omega)-f_R(\omega)]; \tag{3.24}$$

here, the right and left Fermi distributions $f_{R,L}$ are defined in terms of the right and left chemical potentials $\mu_{R,L}$, which are displaced by a potential V. The "matrix element" $\Lambda^r(\omega)$ is given by

$$\Lambda^r(\omega)=[g_R^r(0,0;\omega)+g_L^r(0,0;\omega)]^{-1}\,. \tag{3.25}$$

In the Appendix we show that the energy density of the tunneling current, $\langle J(0;\omega)\rangle$, can be expressed in terms of the Green's functions $\bar{g}_{R,L}$, which vanish at the interface. In this case,

$$\langle J(0;\omega)\rangle = \frac{4e}{\hbar}\,|\bar{\Lambda}^r(\omega)|^2\,\frac{\partial^2}{\partial x\,\partial x'}\,[\mathrm{Im}\bar{g}_L^r(x,x';\omega)] \times \frac{\partial^2}{\partial x\,\partial x'}\,[\mathrm{Im}\bar{g}_R^r(x,x';\omega)]\,|_{x=0=x'}\,[f_L(\omega)-f_R(\omega)]\,, \tag{3.26}$$

where

$$\bar{\Lambda}^r(\omega)=\left(\frac{\partial^2}{\partial x\,\partial x'}\,[\bar{g}_R^r(x,x';\omega) +\bar{g}_L^r(x,x';\omega)]\,|_{x=0=x'}\right)^{-1}\,. \tag{3.27}$$

The two alternative expressions for $J(0;\omega)$ are compared and discussed in Sec. IV.

IV. DISCUSSION OF RESULTS

It is well known that the retarded single-particle Green's function is related to the energy density of states $\rho(\omega)$ as follows[34]:

$$-\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{Im}g^r(x,x;\omega)\,dx=\frac{1}{2\pi}\int_{-\infty}^{\infty}\rho(x,x;\omega)\,dx=\rho(\omega)\,, \tag{4.1}$$

where the complex spectral density, $\rho(x,x';\omega)$, is defined by the relation,

$$g^r(x,x';\omega)=\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{\rho(x,x';\omega')}{\omega-\omega'+i\epsilon}\,\frac{d\omega'}{2\pi} =P\int_{-\infty}^{\infty}\frac{\rho(x,x';\omega')}{\omega-\omega'}\,\frac{d\omega'}{2\pi}-\frac{i}{2}\rho(x,x',\omega)\,, \tag{4.2}$$

and

$$\mathrm{Im}\rho(x,x;\omega)=0\,.$$

Equations (4.1) and (4.2) suggest that for inhomogeneous systems, it may be convenient to introduce the notion of a "local" energy density of states,

$$\rho(x,\omega)=-\frac{1}{\pi}\,\mathrm{Im}g^r(x,x;\omega)>0\,, \tag{4.3}$$

which satisfies the two sum rules,

$$\int_{-\infty}^{\infty}\rho(x,\omega)\,dx=\rho(\omega)$$

and

$$\int_{-\infty}^{\infty}\rho(\omega)\,d\omega=1\,.$$

Evidently Eq. (3.24) can be written in the form

$$\langle J\rangle=\frac{2e}{\hbar}\int_{-\infty}^{\infty}(2\pi)^2\,|\,\Lambda^r(\omega)\,|^2[f_L(\omega)-f_R(\omega)] \times\rho_L(0;\omega)\rho_R(0;\omega)\,\frac{d\omega}{2\pi}\,, \tag{4.4}$$

where we have now summed over spin orientations. Equation (4.4) represents our version of Appelbaum's extension of the transfer-Hamiltonian formalism, except that the "matrix element" $\Lambda^r(\omega)$ is inherently defined within our formalism in terms of the Green's functions $g_{R,L}$, and is strictly speaking no matrix element at all.

Turning to Eq. (3.26), we note that here the right-hand side does not depend on $\mathrm{Im}g^r(x,x;\omega)$ but rather on

$$\frac{\partial^2}{\partial x\,\partial x'}\,\mathrm{Im}g^r(x,x';\omega)\,|_{x=x'}\,.$$

This manifestly reasonable result follows from the fact that $\bar{g}^r(0,0;\omega)$ vanishes; thus an expression such as Eq. (3.24) would be indeterminate if we were to replace g by $\bar{g}$. In fact, one might interpret Eq. (3.26) as resulting from Eq. (3.24) following a repeated application of l'Hôpital's rule. It thus is obvious that besides Eq. (4.4), an equally correct expression for the tunneling current is

$$\left(\frac{h}{2e}\right)\langle J\rangle=\int d\omega\,|\,\bar{\Lambda}^r(\omega)\,|^2[f_L(\omega)-f_R(\omega)] \times\frac{\partial^2}{\partial x\,\partial x'}\left(-\frac{1}{\pi}\,\mathrm{Im}\bar{g}_L^r(x,x';\omega)\right) \times\frac{\partial^2}{\partial x\,\partial x'}\left(-\frac{1}{\pi}\,\mathrm{Im}\bar{g}_R^r(x,x';\omega)\right)\Big|_{x=0=x'}(2\pi)^2\,. \tag{4.5}$$

However, Eq. (4.5) has the drawback that it no longer displays an explicit dependence on the local

densities of states. Instead, it involves a reasonably complicated functional of these quantities. It should be emphasized, however, that the local densities of states clearly depend on the arbitrary choice of the particular homogeneous boundary conditions imposed at the interface. More precisely, the local densities of states entering Eq. (4.4) characterize the semi-infinite electrodes provided we impose on their wave functions the condition that they have a vanishing normal derivative at surface $x=0$.

We now turn to compare our results with those of Caroli *et al.* As noted in the discussion of Eq. (2.18″), Caroli *et al.* work in terms of the functions which we designated $\bar{g}_{R,L}$, which vanish at the interface. In fact, our Eq. (3.26) agrees (within a factor of 2, representing the sum over spin orientations and minor errors) with Eq. (II.40) of Caroli.[35] However, our analysis demonstrates that the results derived by Caroli *et al.* for their discrete model have a considerably more restricted validity than claimed by them. This conclusion follows from a comparison of our Eq. (3.26) and Eq. (IV.13) of Caroli *et al.*, which we rewrite as

$$\langle J(0;\omega)\rangle = \frac{4e}{\hbar}|\bar{\Lambda}_c^r(\omega)T|^2\,\mathrm{Im}\bar{g}_L^r(0,0;\omega) \times \mathrm{Im}\bar{g}_R^r(0,0;\omega)[f_L(\omega)-f_R(\omega)], \quad (4.6)$$

where

$$|\bar{\Lambda}_c^r(\omega)T|^2 = |[1-T^2\bar{g}_L^r(0,0;\omega)\bar{g}_R^r(0,0;\omega)]^{-1}T|^2. \quad (4.7)$$

T is asserted to be an appropriate matrix element of the interaction which couples the two semi-infinite electrodes between which the tunneling occurs. In Eqs. (4.6) and (4.7) we transcribed the discrete indices used by Caroli as the first two arguments of our Green's functions. The comparison of Eq. (3.26) and the physical significance of T indicate that in the continuous limit, one should interpret

$$T\,\mathrm{Im}\bar{g}^r(0,0;\omega) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x_1}\mathrm{Im}\bar{g}^r(x,x_1;\omega)|_{x=0=x_1}, \quad (4.8)$$

and in order to secure agreement between the "matrix element" $|\bar{\Lambda}_c^r(\omega)|$ and the corresponding factor in Eq. (3.26), specified by Eq. (3.27), we have to interpret

$$\begin{aligned}|1-T^2\bar{g}_L^r(0,0;\omega)\bar{g}_R^r(0,0;\omega)| &= |1-T\bar{g}_L^r(0,0;\omega)T\bar{g}_R^r(0,0;\omega)| \\ &= \frac{\hbar^2}{2m}\left|\frac{\partial^2}{\partial x\,\partial x_1}\bar{g}_L^r(x,x_1;\omega)\right|_{x=0=x_1} \\ &\quad + \frac{\partial^2}{\partial x\,\partial x_1}\bar{g}_R^r(x,x_1;\omega)|_{x=0=x_1}|. \end{aligned} \quad (4.9)$$

Caroli *et al.* indeed claim to have proved these relations, though while not committing themselves, they seem to identify T with $p^2/2m$. Without belaboring this ambiguity in the proper limit of the discrete model of Caroli *et al.*, we do have to stress that contrary to their assertion, Eq. (4.6) [which corresponds to Eq. (3.26)] does not depend explicitly on the local energy densities of states.[36] Such a dependence is displayed only by the right side of Eq. (3.24). Thus if we wish to interpret the tunneling current in a "transfer-Hamiltonian-like" fashion, or more precisely, if we wish to use tunneling experiments to study the local density of states, we have to study the uncoupled subsystems in terms of the functions $g_{R,L}$ which have a vanishing normal derivative at the boundary.

To conclude, we have obtained a simple interpretation of Bardeen's matrix element of the transfer Hamiltonian as a pseudopotential representing the boundary conditions at the interface. We have obtained a simple definition of the uncoupled subsystems and we have derived from first principles an expression for the tunneling current which formally agrees with an obvious generalization of the one obtained by means of the transfer-Hamiltonian formalism. We have indicated the connection between the rather arbitrary definition of the uncoupled subsystems and the dependence of the tunneling current on the local density of states. Our formalism is inherently free of the justified objections raised with regard to transfer Hamiltonian, and it has the added advantage of containing an explicit procedure for calculating the "matrix element" which enters the transfer Hamiltonian in an *ad hoc* fashion. Our formalism avoids the ambiguities involved in the extreme tight-binding approximation of Caroli *et al.* and enabled us to detect a basic inconsistency in their results.

We have checked our formalism by applying it to the trivial case, where the two electrodes are identical free-electron (Bohr-Sommerfeld) metals. In this case we obtain, upon summing over spin orientations,

$$\begin{aligned}\langle J\rangle &= \frac{8e}{h}\int_{-\infty}^{\infty}\frac{kK}{(k+K)^2}[f(\omega)-f(\omega+V)]\,d\omega \\ &= \frac{2e}{h}\int_{-\infty}^{\infty}|T(\omega)|^2[f(\omega)-f(\omega+V)]\,d\omega, \end{aligned} \quad (4.10)$$

where

$$(hk)^2/2m = h\omega = (hK)^2/2m + V. \quad (4.11)$$

This result is obtained by substituting $g_{R,L}$ into Eq. (4.4) or $\bar{g}_{R,L}$ into Eq. (4.5); it is identical to that obtained in the elementary analysis of the current across a potential step whose transmission coefficient is $|T|^2$. Incidentally, this elementary problem cannot be handled in terms of the conven-

tional transfer-Hamiltonian formalism.

While this check of our formalism does not constitute an independent proof of its correctness, it increases our confidence in it.

We have extended our analysis to a junction of finite width, i.e., to a system consisting of three distinct regions, rather than the two-region case considered above. This work, reported in the second paper of this series, confirms the conclusions we have drawn from the simpler model. We are presently extending our formalism to a full three-dimensional analysis.

APPENDIX: CALCULATION OF THE TUNNELING CURRENT IN TERMS OF $\bar{g}_{R,L}$

If we wish to use the Green's functions $\bar{g}_{R,L}$, which vanish at the interface, then it is more convenient to use the adjoint of the right side of Eq.(3.17),

$$\frac{2m}{\hbar e}\langle J(0;\omega)\rangle = \lim_{\substack{x'\to x\\ x\to 0^-}} -\left(\frac{\partial}{\partial x}\int_{-\infty}^{0}[g_L^+(x,x_1;\omega)\mathcal{K}'(x_1)G^a(x_1,x';\omega)+g_L^r(x,x_1;\omega)\mathcal{K}'(x_1)G^+(x_1,x';\omega)]dx_1\right.$$
$$\left.+\frac{\partial}{\partial x'}\int_{-\infty}^{0}[G^+(x,x_1;\omega)\mathcal{K}'(x_1)g_L^a(x_1,x';\omega)+G^r(x,x_1;\omega)\mathcal{K}'(x_1)g_L^+(x_1,x';\omega)]dx_1\right). \tag{A1}$$

Using Eq. (3.18) and the boundary conditions,

$$\bar{g}_{R,L}(0,x'\gtrless 0;\omega)=0=\bar{g}_{R,L}(x\gtrless 0,0;\omega). \tag{A2}$$

We now obtain

$$\frac{2m}{\hbar e}\langle J(0;\omega)\rangle=\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x\,\partial x_1}\bar{g}_L^+(x,x_1;\omega)G^-(0,0;\omega)-\frac{\partial^2}{\partial x\,\partial x_1}\bar{g}_L^-(x,x_1;\omega)G^+(0,0;\omega)\right)\Big|_{x=0^-=x_1}, \tag{A3}$$

and similarly, letting $x\to 0^+$,

$$\frac{2m}{\hbar e}\langle J(0;\omega)\rangle=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x\,\partial x_1}\bar{g}_R^+(x,x_1;\omega)G^-(0,0;\omega)\right.$$
$$\left.-\frac{\partial}{\partial x\,\partial x_1}\bar{g}_R^-(x,x_1;\omega)G^+(0,0;\omega)\right)\Big|_{x=0^+=x_1} \tag{A4}$$

The continuity of the mixed second derivatives of $\bar{g}_{R,L}$ and of the functions G at $x=x'$ allows us to drop in Eqs. (A3) and (A4) the distinction between the limits $x=0^-, 0^+$.

From the matrix Dyson equation, Eq. (3.4), we obtain

$$G^{r,a}(x,x';\omega)=g^{r,a}(x,x';\omega)+\int_{-\infty}^{\infty}g^{r,a}(x,x_1;\omega)\mathcal{K}'(x_1)G^{r,a}(x_1,x';\omega)\,dx_1. \tag{A5}$$

Thus, Eq. (2.18″) defines $G^{r,a}(0,0;\omega)$ in terms of $\bar{g}_{L,R}^{r,a}$. Using Eq. (3.18) we obtain now

$$G^+(0,0;\omega)-G^-(0,0;\omega)$$
$$=-\left(\frac{2m}{\hbar^2}\right)[(\bar{\gamma}_L^+ +\bar{\gamma}_R^+)-(\bar{\gamma}_L^- +\bar{\gamma}_R^-)][(\bar{\gamma}_L^a +\bar{\gamma}_R^a)(\bar{\gamma}_L^r +\bar{\gamma}_R^r)], \tag{A6}$$

where

$$\bar{\gamma}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x_1}\bar{g}(x,x_1;\omega)\big|_{x=0=x_1}. \tag{A7}$$

We can now eliminate $G^{\pm}$ between Eqs. (A3)–(A7), and obtain

$$\langle J(0;\omega)\rangle=\frac{e}{\hbar}|\bar{\gamma}_L^r+\bar{\gamma}_R^r|^{-2}(\bar{\gamma}_L^+\bar{\gamma}_R^- -\bar{\gamma}_L^-\bar{\gamma}_R^+). \tag{A8}$$

Using Eqs. (3.11) and (3.12) to eliminate $\bar{\gamma}^{\pm}$ in favor of $\bar{\gamma}^r$ we obtain Eq. (3.26) from Eq. (A8).

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[1]J. Bardeen, Phys. Rev. Lett. 6, 57 (1961).

[2]M. H. Cohen, L. M. Falicov, and J. C. Phillips, Phys. Rev. Lett. 8, 316 (1962).

[3]C. B. Duke, *Tunneling in Solids, Solid State Physics Suppl.* (Academic, New York, 1969), Vol. 10, p. 207.

[4]I. Giaever, Phys. Rev. Lett. 5, 147 (1960); 5, 464 (1960).

[5]J. R. Schrieffer [in *Tunneling Phenomena in Solids*, edited by E. Burstein and S. Lundquist (Plenum, New York, 1969), p. 287,] gives an excellent survey of the current view on single-particle tunneling in superconductors.

[6]Compare the preceding discussion with that on pp. 292–294 of Ref. 5 above, in particular our Eq. (1.6) with Eqs. (12) and (13).

[7]See Eq. (6) of Ref. 5.

[8]In Eqs. (1.11) and (1.12) we follow the notation of Caroli

et al. (see Ref. 13) in denoting by $G^{\pm}(k,\omega)$ the functions introduced by Kadanoff and Baym as $G^{\gtrless}(k,\omega)$ [L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Menlo Park, Calif., 1962), Chap. 2]. The second equality in Eqs. (1.11) and (1.12) represents the zero-temperature version of a well-known result. See, for instance, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971), pp. 292–295. The only difference between the formulas in the above reference and Eqs. (1.11) and (1.12) is due to our convention

$$G^{r}(k,\omega)=\lim_{\epsilon\to 0^{+}}\int_{-\infty}^{\infty}d\omega'\,(\omega-\omega'+i\epsilon)^{-1}\rho(k\omega')\,d\omega'\,; \qquad \text{(a)}$$

hence, instead of Eq. (31.20) of Fetter *et al.* we have

$$\mathrm{Im}\,G^{r}(k,\omega)=-\pi\rho(k,\omega). \qquad \text{(b)}$$

[9]By net we mean the difference in the rate out of $|g\rangle$ and that into $|g\rangle$. We also made use of Eq. (b) in Ref. 8 above.

[10]See Ref. 3, Eqs. (18.29), (15.2), and (19.33).

[11]See J. A. Appelbaum and W. F. Brinkman, Phys. Rev. 186, 464 (1969), Eq. (2.23).

[12]R. E. Prange, in *Lectures on the Many Body Problem*, edited by E. R. Caianello (Academic, New York, 1964), Vol. 2, p. 137.

[13]C. Caroli, R. Combescot, P. Noziere, and D. Saint James, J. Phys. C 4, 916 (1971); 4, 2599 (1971); 4, 2611 (1971); 5, 21 (1972). These papers will be referred to as Caroli I, etc. Equations in these papers will be referred to by indicating the paper with a roman numeral preceding the number of the equation, e.g. (I.3).

[14]$\phi_{L,m}$ and $\phi_{R,n}$ are assumed to be valid approximate solution of $\mathcal{H}$ inside the barrier and in the left and right electrodes, respectively.

[15]This is not the golden rule proper; in deriving Eq. (1.18) Bardeen assumed that

$$\left|\sum_{n'}\frac{i}{\hbar}b_{n'}(t)\langle\phi_{R,n}|E_{n'}-\mathcal{H}|\phi_{R,n'}\rangle\right.$$
$$\times\exp[-i(E_{n'}-E_{n})t\hbar^{-1}]-\frac{\partial a_{m}}{\partial t}\langle\phi_{R,n}|\phi_{L,m}\rangle$$
$$\left.\times\exp[-i(E_{m}-E_{n})t\hbar^{-1}]\right|\ll\left|\frac{i}{\hbar}a_{m}\langle\phi_{R,n}|E_{m}-\mathcal{H}|\phi_{L,m}\rangle\right.$$
$$\left.\times\exp[-i(E_{m}-E_{n})t\hbar^{-1}]\right|.$$

The first term on the left-hand side has a different structure from that of the corresponding term in ordinary time-dependent theory, and the second term is absent in that theory.

[16]Note that in effect the assertion is equivalent to the claim that $V_{kk'}=-(ih/e)J_{x,nm}$.

[17]See Ref. 3, p. 208.

[18]C. B. Duke, C. G. Kleinman, and T. E. Stakelon, Phys. Rev. B 6, 2389 (1972).

[19]See comments preceding Eq. (I.13) of Ref. 13.

[20]L. V. Keldysh, Zh. Eksp. Teor. Fiz. 47, 1515 (1964) [Sov. Phys.-JETP 20, 1018 (1965)]. See also R. A. Craig, J. Math. Phys. 9, 605 (1969).

[21]See Ref. 3, p. 218.

[22]T. E. Feuchtwang, following paper, Phys. Rev. B 10, 4135 (1974), Sec. IV.

[23]Note that in principle, Eq. (2.1) does not represent an essential restriction, since one may always include in $\mathcal{H}_{L}$ an additional term representing the perturbation of the left system by the presence of the right system. This effect has then to be treated by perturbation theory and represents an additional scattering mechanism for the left (right) incident current.

[24]One might also choose the boundary conditions specified by α, β so that they are satisfied by the exact Green's function for the isolated (semi-infinite) electrodes, $G_{L,R}$. These Green's functions $G_{L,R}$ satisfy homogenous boundary conditions at $x=\pm\infty$. The choice of α, β such that, e.g.,

$$\alpha G_{L}(0,x'<0;\omega)+\beta\frac{\partial}{\partial x}G_{L}(x,x'<0;\omega)\Big|_{x=0}=0$$
$$=\alpha G_{L}(x<0,0;\omega)+\beta\frac{\partial}{\partial x'}G_{L}(x<0,x';\omega)\Big|_{x=0} \qquad \text{(c)}$$

can thus be made only after $G_{L}(x,x';\omega)$ is known. In general neither α nor β will vanish in this case, and these parameters will generally also depend on the electrodes. Unless the interface is chosen so that $\mathcal{H}_{L,R}$ are identical to the Hamiltonians of the actual semi-infinite electrodes when $x\gtrless 0$, $g_{L,R}\neq G_{L,R}$ even though these functions satisfy the same boundary conditions. In practice one may neither wish nor be able to satisfy this condition, and hence the relationship between the functions $G_{L,R}$ and $g_{L,R}$ may be quite untransparent. Furthermore, even if $g_{L,R}=G_{L,R}$ the tunneling current acquires a much more complicated dependence on the local densities of states than that resulting from the convention $\alpha=0$. Thus it is doubtful whether the increased complexity of the formal analysis following from the convention Eq. (c) is warranted. However, such a convention was indeed adopted by Garcia-Moliner and Rubio (Ref. 25).

[25]F. Garcia-Moliner and J. Rubio, J. Phys. C 2, 1789 (1969). These authors defined their $g_{R,L}$ differently. We have not checked whether the two sets of Green's functions are equivalent.

[26]In deriving Eq. (2.18''), we used the fact that when $g_{R,L}$ vanish at the interface, their characteristic singularity implies that

$$\frac{\partial}{\partial x}g_{L}(x,x_{1}=x^{-})\Big|_{x=0}=\frac{2m}{\hbar^{2}}=-\frac{\partial}{\partial x}g_{R}(x,x_{1}=x^{+})\Big|_{x=0}.$$

[27]See Eqs. (II.22) and (II.30) in Ref. 13.

[28]Because the definition of G^{+} (in terms of the left and right Green's functions) changes across $x=0$, the limit $x\to 0$ has to be one sided. The choice 0^{-} as opposed to 0^{+} is arbitrary and of no consequence.

[29]See Ref. 13, Appendix A of Caroli I.

[30]Our definition of $g^{r,a}$ follows the standard convention, rather than Keldysh's. In addition, the step function $\Theta(t)$ involved in the definition of $g^{r,a}$ is the conventional one rather than the one we have been using, i.e.,

$$\Theta(t)=\begin{cases}1, & t>0\\ 1, & t>0\end{cases}.$$

[31]These equations can be easily obtained from Eq. (31.24) of Fetter and Walecka, Ref. 8 above.

[32]Equations (3.11)–(3.14) are the configuration space version of Eqs. (31.20), (31.25), and (31.26) of Ref. 8.

[33]This formal assertion is strictly obvious since in thermal equilibrium there is no net current.

[34]See A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinsky, *Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1968), p. 64. Also Ref. 8, p. 294; note that most textbooks consider only homogenous systems so that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\rho(x, x; \omega)\,dx = \int_{-\infty}^{\infty}\rho(k, \omega)\,dk\,.$$

[35]Equation (II.40) has the wrong sign, and as can be checked by direct substitution of Eqs. (III.38) into (II.37), the denominator should be

$$|\gamma(x_0)+\tilde{\gamma}(x_0)^*|^2 = (\hbar^2/2m)^2\left|\frac{\partial^2}{\partial x\,\partial x_1}[g^r(x, x_1; \omega) + \tilde{g}^r(x, x_1; \omega)]\right|_{x=x_0=x_1}\Bigg|^2 .$$

[36]In Ref. 13, Eq. (IV. 16), Caroli *et al.* rewrite Eq. (4.6) of the present paper [i.e., (IV.13)] as

$$\left(\frac{2e}{h}\right)^{-1}\langle J\rangle = \int\left|\frac{\hbar^2}{2m}\Lambda^r(\omega)\right|^2[f_L(\omega)-f_R(\omega)] \times\rho_L(0;\omega)\rho_R(0;\omega)\,d\omega\,.$$

where $\Lambda^r(\omega)$ is defined by Eq. (4.7).