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Theory of tunneling without transfer Hamiltonian: Relation between continuum and discrete formalisms, and equivalence with elementary theory for noninteracting systems

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The relation of the tunneling theory developed by Feuchtwang to the similar theory due to Caroli *et al.* is explained. Some previous assertions, concerning their discrete formulation of tunneling, reaffirmed in the companion comment, by Caroli *et al.* are disproved. A general proof for the equivalence of the elementary kinetic theory of tunneling and of the many-body formulation for a noninteracting system is given. The role of boundary conditions imposed at interfaces in junctions is discussed, and some of the results of an earlier analysis by Feuchtwang are shown to have a more general validity than suggested in the original work.

I. INTRODUCTION

Recently, we developed a tunneling theory for many-particle systems which does not involve the transfer Hamiltonian and elucidates its physical significance.[1,2] The theory like a similar formalism developed by Caroli *et al.*[3] is an adaptation of a novel transport theory due to Keldysh.[4] Both theories involve the determination of the full single-particle Green's function for a composite system in terms of Green's functions for appropriately defined uncoupled subsystems which are in thermal equilibrium. However, while Feuchtwang considers the problem in the continuous (coordinate) representation, Caroli *et al.* advocate a discrete representation suggested to them by an extreme tight-binding approximation. Formally, Feuchtwang computes the inverse operator (Green's function) for a differential equation, while Caroli *et al.* consider the inverse of a difference equation. There appears to be some question as to the precise relationship of these two formulations to each other and their relative advantages.[5] This paper is meant to (i) clarify these questions, and (ii) outline a general proof of the equivalence of the many-body theory and the elementary formulation of tunneling for noninteracting systems.

II. RELATION BETWEEN CONTINUOUS AND DISCRETE FORMULATIONS OF TUNNELING

The conversion of the Schrödinger equation for the tunneling of noninteracting particles into a second-order difference equation is an instance of a familiar procedure. This procedure has, however, limited utility except for the numerical integration of the Schrödinger (or any other differential) equation. In fact, a standard procedure for the analytic solution of difference equations is their conversion into differential equations. The procedure followed by Caroli *et al.* can, in fact, be applied to the integro-differential equation representing the effective single-particle Schrödinger equation for the interacting system when self-energy effects are allowed for in terms of an effective nonlocal potential. However, the procedure is manifestly cumbersome, and as we shall demonstrate below, confusing even to the experts.

Caroli *et al.* provide an interesting but erroneous argument for their preference for their formalism. In their first paper they admit that they did not know how to specify the conditions to be imposed on the wave and Green's functions of the uncoupled subsystems at the interfaces,[6] and that they thought the problem could be avoided by casting it into a Wannier-type representation. They indicate that the actual Wannier-type states will be sensitive to the site's location relative to the interface but do not pursue this point to the logical conclusion, that the difference equations will exhibit a variation of the coefficients with the site index. Such a variation is a standard procedure of incorporating boundary conditions into difference equations. Thus the choice to ignore the above variation constitutes an *arbitrary* though conceivably convenient boundary condition.

In their second paper (C-II), and in their comment on our recent work, Caroli *et al.* introduce a more strictly mathematical argument.[6,7] Namely, they assert that by the formal transcription of the Schrödinger equation into a second-order difference equation, they can avoid explicit discussion of the boundary conditions at the interface. Furthermore, the latter are presumed to be *uniquely* accounted for by the "discrete secular equations." This is in contrast to our proof of the inherent freedom in the choice of the homogenous boundary conditions to be imposed on the wave and Green's functions of the uncoupled subsystems at the interfaces. A little reflection isolates the fallacy in this circular argument: Caroli *et al.*'s difference equations are unique and correspond to the "fixed boundary condition," $\psi(x) = 0$ at the interface, because they implicitly chose to ignore all other admissible sets of difference equations corresponding to the more general class of boundary conditions we showed

to be admissible in the continuous representation.

Having examined the presumed advantages of the discrete formalism, we still have to check whether the latter is equivalent to the continuous one. It appears to us that the answer to this is a qualified yes. Namely, having derived the correct result in the continuous representation, one can always properly define the limiting processes implied in the discrete formalism to get agreement between the two formalisms. However, the discrete formalism is by itself ambiguous enough to have mislead even the authors themselves. This is evident upon comparing the expressions for the energy density of the tunneling current across a junction as stated by Caroli *et al.* in Eqs. (C-II. 40) and (C-IV. 16)[3]:

$$\langle J(\omega)\rangle = \frac{8e}{h}|\Lambda^r|^2 \operatorname{Im}\left(\frac{\partial^2}{\partial x \partial x'} g_L^r(x, x'; \omega)\Big|_{x=x'=x_0}\right) \times \operatorname{Im}\left(\frac{\partial^2}{\partial x \partial x'} g_R^r(x, x'; \omega)\Big|_{x=x'=x_0}\right)[f_L(\omega) - f_R(\omega)]\,. \tag{C-II. 40}$$

In their discussion of Eq. (C-II. 40), Caroli *et al.* categorically assert that "the properties of the electrodes do not appear in the current via the volume densities of state of the isolated (subsystems) M and M'." This statement, based on the form of (C-II. 40), is misleading. It depends, as does the derivation of this equation, on the particular boundary conditions imposed at the interface on the Green's functions for the uncoupled systems. However, Eq. (C-II. 40) is correct, and agrees with our result.[8] Turning to Eq. (C-IV. 16), we have

$$\langle J(\omega)\rangle = \frac{8e}{h}|T\Lambda^r|^2 \pi\rho_\alpha(\omega)\,\pi\rho_a(\omega) \times [f_L(\omega) - f_R(\omega)]\,. \tag{C-IV. 16}$$

Here Caroli *et al.* define the symbols $\rho_\alpha(\omega)$ as the local density of states at site α, the first site to the left of the interface, $\rho_\alpha = -(1/\pi)\mathrm{Im}g_L^r(x=\alpha, x'=\alpha;\ \omega)$; $\rho_\alpha(\omega)$ as the local density of states at site a, the first site to the right of the interface $\rho_a = -(1/\pi)\mathrm{Im}g_L^r(x=a, x'=a;\ \omega)$. On the face of it, the above equations are inconsistent. It is conceivable that T be interpreted as an operator such that

$$|T|[-\pi\rho_\alpha(\omega)] = \frac{\partial^2}{\partial x \partial x'} \mathrm{Im} g_L^r(x, x'; \omega)\Big|_{x=x_0=x'}\,. \tag{1.1}$$

However, this is surely a confusing notation, and moreover, is not the interpretation emerging from the discussion of Eq. (C-IV. 16) by Caroli *et al.*[9] The symbol T is evidently to be interpreted as an operator since it always has to appear in products such as Tg, or $Tc_i^\dagger c_j$.[10] However, the interpretation of Tg is not necessarily unique: The reduction of the Schrödinger equation to a difference equation[11] in fact suggests that T be interpreted as being proportional to the Laplacian, i.e., $T \sim -(\hbar^2/2m)(d^2/dx^2)$. This interpretation agrees with Duke's analysis of the transfer Hamiltonian[12] and with our interpretation of Bardeen's matrix elements of the transfer Hamiltonian.[13] However, this does not agree with Eq. (1.1). To compound this problem, Caroli *et al.*, spend considerable effort in discussing their limiting procedure in going from the discrete to the continuous representation. Nevertheless, they fail to give an explicit (operational) interpretation of the operator T which, in this limit, is formally singular.

In concluding this analysis of the relation between the discrete and continuous formalisms of tunneling, we wish to stress the following two points: (a) The two formalisms can be forced to agree. However, the continuous representation has the advantage of being more transparent. In case of (formal) disagreement, it should be used to interpret the result of the discrete analysis. (b) An important illustration of the above comment is the elucidation of the relation between the local density of states and the boundary conditions imposed at the surface of a subsystem, which emerges from our analysis.[14] This point is further emphasized below.

III. RELATION OF THE MANY-BODY TO THE KINETIC FORMULATION OF TUNNELING

In this section we present a general proof of the equivalence of our many-body formalism and the elementary kinetic (single-particle) formulation of tunneling for a noninteracting system. The derivation also demonstrates that our expression for the energy density of the tunneling current $\langle J(\omega)\rangle$ does not depend on the boundary conditions imposed on the wave and Green's functions for the uncoupled subsystems at the interfaces. To keep the algebra to a minimum, we consider only an abrupt junction with Hamiltonian

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

where, $\Theta(x)$ is the unit step function. The analysis extends without difficulty to the finite junction.

Let $\{\psi_L^{(1)}(x;\omega),\ \psi_L^{(1)*}(x;\omega)\}$ and $\{\psi_R^{(2)}(x;\omega),\ \psi_R^{(2)*}(x;\omega)\}$ be two pairs of linearly independent solutions of the Schrödinger equation for the uncoupled subsystems,

$$(\hbar\omega - \mathcal{H}_\gamma)\,\psi_\gamma(x;\omega) = 0; \quad \gamma = L, R\,. \tag{2.2}$$

Let $\psi_L^{(1)}(x;\omega)$, $\psi_R^{(2)}(x;\omega)$, respectively, satisfy "outgoing wave" boundary conditions at $x = \pm\infty$.

A solution for the composite full system can be written

$$\psi(x;\omega)=\begin{cases}\psi_L^{(1)*}(x;\omega)+R_L\psi_L^{(1)}(x;\omega), & x<0\\ S_R\psi_R^{(2)}(x;\omega), & x>0.\end{cases} \tag{2.3}$$

Hence the ratio of the flux transmitted to the right to that incident from the left is

$$\left.\frac{\psi_R^{(2)*}(x;\omega)\frac{d}{dx}[\psi_R^{(2)}(x;\omega)]-\frac{d}{dx}[\psi_R^{(2)*}(x;\omega)]\psi_R^{(2)}(x;\omega)}{\psi_L^{(1)}(x;\omega)\frac{d}{dx}[\psi_L^{(1)*}(x;\omega)]-\frac{d}{dx}[\psi_L^{(1)}(x;\omega)]\psi_L^{(1)*}(x;\omega)}\right|_{x=0} |S_R|^2=|T|^2, \tag{2.4}$$

where, the continuity of the logarithmic derivative of ψ across the junction determines,

$$S_R=\left.\frac{\psi_L^{(1)*}(x;\omega)\frac{d}{dx}[\psi_L^{(1)}(x;\omega)]-\frac{d}{dx}[\psi_L^{(1)*}(x;\omega)]\psi_L^{(1)}(x;\omega)}{\psi_R^{(2)}(x;\omega)\frac{d}{dx}[\psi_L^{(1)}(x;\omega)]-\frac{d}{dx}[\psi_R^{(2)}(x;\omega)]\psi_L^{(1)}(x;\omega)}\right|_{x=0}. \tag{2.5}$$

It is now a simple matter to verify that

$$|T|^2=4\,\mathrm{Im}\left(\frac{\psi_L^{(1)}(x;\omega)}{\frac{d}{dx}\psi_L^{(1)}(x;\omega)}\right)\mathrm{Im}\left(-\frac{\psi_R^{(2)}(x;\omega)}{\frac{d}{dx}\psi_R^{(2)}(x;\omega)}\right)\left|\frac{\psi_L^{(1)}(x;\omega)}{\frac{d}{dx}\psi_L^{(1)}(x;\omega)}-\frac{\psi_R^{(2)}(x;\omega)}{\frac{d}{dx}\psi_R^{(2)}(x;\omega)}\right|_{x=0}^{-2} \tag{2.6}$$

$$=4\,\mathrm{Im}\left(-\frac{\frac{d}{dx}\psi_L^{(1)}(x;\omega)}{\psi_L^{(1)}(x;\omega)}\right)\mathrm{Im}\left(\frac{\frac{d}{dx}\psi_R^{(2)}(x;\omega)}{\psi_R^{(2)}(x;\omega)}\right)\left|-\frac{\frac{d}{dx}\psi_L^{(1)}(x;\omega)}{\psi_L^{(1)}(x;\omega)}+\frac{\frac{d}{dx}\psi_R^{(2)}(x;\omega)}{\psi_R^{(2)}(x;\omega)}\right|_{x=0}^{-2}. \tag{2.7}$$

In the elementary treatment of one dimensional junctions, the current is written

$$\langle J\rangle=\frac{2e}{h}\int|T(\omega)|^2\{f_L(\omega)[1-f_R(\omega)]+f_R(\omega)[1-f_L(\omega)]\}\frac{d\omega}{2\pi}, \tag{2.8}$$

where, $f_\gamma(\omega)$ is the Fermi function for the γth subsystem.

We shall now demonstrate that [upon substitution into Eq. (2.8)] Eqs. (2.6) and (2.7) correspond to Eqs. (II3.24)(II3.26). The procedure to be followed utilizes the Wronskian technique for the calculation of one dimensional Green's functions,[15] that is,

$$g(x,x';\omega)=\frac{2m}{\hbar^2}[W(\psi^{(1)},\psi^{(2)})]^{-1}\times\psi^{(1)}(x;\omega)\psi^{(2)}(x;\omega);\quad x<x', \tag{2.9a}$$

$$g(x,x';\omega)=\frac{2m}{\hbar^2}[W(\psi^{(1)},\psi^{(2)})]^{-1}\times\psi^{(2)}(x;\omega)\psi^{(1)}(x';\omega);\quad x>x', \tag{2.9b}$$

is the solution of the inhomogeneous differential equation

$$(\hbar\omega-\mathcal{H}_\gamma)g(x,x';\omega)=\delta(x-x');\quad \gamma=L,R, \tag{2.10}$$

provided $\{\psi^{(i)}(x;\omega)\}$ is a pair of linearly independent solutions of the homogeneous equation, Eq. (2.2), satisfying appropriate boundary conditions. $W(\psi^{(1)},\psi^{(2)})$ is the Wronskian of these solutions and is (for the Schrödinger equation) a constant. Thus, in particular, we have

$$g_L(x,x';\omega)=\frac{2m}{\hbar^2}W_L^{-1}\psi_L^{(1)}(x;\omega)\psi_L^{(2)}(x';\omega),\quad x<x' \tag{2.11a}$$

$$g_L(x,x';\omega)=\frac{2m}{\hbar^2}W_L^{-1}\psi_L^{(2)}(x;\omega)\psi_L^{(1)}(x';\omega),\quad x>x' \tag{2.11b}$$

where

$$W_L=-\left(\frac{\alpha}{\beta}\psi_L^{(1)}(x;\omega)+\frac{d}{dx}\psi_L^{(1)}(x;\omega)\right)\psi_L^{(2)}(x;\omega)\Big|_{x=0}. \tag{2.12}$$

Here, $\psi_L^{(1)}(x;\omega)$ satisfies "outgoing wave" boundary conditions at $x=-\infty$, and

$$\alpha\psi_L^{(2)}(x;\omega)+\beta\frac{d}{dx}\psi_L^{(2)}(x;\omega)\Big|_{x=0}=0, \tag{2.13}$$

α, β are real constants.[16] Similarly,

$$g_R(x,x';\omega)=\frac{2m}{\hbar^2}W_R^{-1}\psi_R^{(1)}(x;\omega)\psi_R^{(2)}(x';\omega);\quad x<x', \tag{2.14a}$$

$$g_R(x,x';\omega)=\frac{2m}{\hbar^2}W_R^{-1}\psi_R^{(2)}(x;\omega)\psi_R^{(1)}(x';\omega);\quad x>x', \tag{2.14b}$$

where now

$$W_R=\frac{\alpha}{\beta}\left(\psi_R^{(2)}(x;\omega)+\frac{d}{dx}\psi_R^{(2)}(x;\omega)\right)\psi_R^{(1)}(x;\omega)\Big|_{x=0}, \tag{2.15}$$

whereas $\psi_R^{(2)}(x;\omega)$ satisfies "outgoing wave" boundary conditions at $x=\infty$, and

$$\alpha\psi_R^{(1)}(x;\omega)+\beta\frac{d}{dx}\psi_R^{(1)}(x;\omega)\Big|_{x=0}=0. \tag{2.16}$$

Evidently, as long as $\beta \neq 0$,

$$|g_L(0,0;\omega)+g_R(0,0;\omega)|^{-2} = \left|\frac{\alpha}{\beta}\frac{\psi_L^{(1)}}{\psi_L^{(1)\prime}}+1\right|^2\left|\frac{\alpha}{\beta}\frac{\psi_R^{(2)}}{\psi_R^{(2)\prime}}+1\right|^2\left|\frac{\psi_L^{(1)}}{\psi_L^{(1)\prime}}-\frac{\psi_R^{(2)}}{\psi_R^{(2)\prime}}\right|^{-2}, \tag{2.17}$$

and

$$\mathrm{Im}g_L(0,0;\omega) = \mathrm{Im}\left(\frac{\psi_L^{(1)}}{\psi_L^{(1)\prime}}\right)\left|\frac{\alpha}{\beta}\frac{\psi_L^{(1)}}{\psi_L^{(1)\prime}}+1\right|^{-2}, \tag{2.18}$$

$$\mathrm{Im}g_R(0,0;\omega) = \mathrm{Im}\left(\frac{\psi_R^{(2)}}{\psi_R^{(2)\prime}}\right)\left|\frac{\alpha}{\beta}\frac{\psi_R^{(2)}}{\psi_R^{(2)\prime}}+1\right|^{-2}, \tag{2.19}$$

where we denoted

$$\frac{d}{dx}\psi_\gamma^{(i)}(x;\omega)\big|_{x=0} = \psi_\gamma^{(i)\prime} \tag{2.20}$$

and

$$\psi_\gamma^{(i)}(x;\omega)\big|_{x=0} = \psi_\gamma^{(i)}. \tag{2.21}$$

Substituting Eqs. (2.17)–(2.19) into Eq. (2.6), we obtain

$$|T|^2 = 4\frac{\mathrm{Im}g_L(0,0;\omega)\,\mathrm{Im}g_R(0,0;\omega)}{|g_L(0,0;\omega)+g_R(0,0;\omega)|^2}. \tag{2.22}$$

The preceding calculation is invalid when, in Eq. (2.16), $\beta = 0$. That is, when,

$$\psi_L^{(2)}(0;\omega) = 0 = \psi_R^{(1)}(0;\omega). \tag{2.23}$$

In this case, and in fact whenever $\alpha \neq 0$, we can show by a completely analogous calculation, omitted here, that Eq. (2.7) reduces to,

$$|T|^2 = 4\left|\frac{\frac{\partial^2}{\partial x\partial x'}[\mathrm{Im}g_L(x,x';\omega)]\frac{\partial^2}{\partial x\partial x'}[\mathrm{Im}g_R(x,x';\omega)]}{\left|\frac{\partial^2}{\partial x\partial x'}\mathrm{Im}g_L(x,x';\omega)+\frac{\partial^2}{\partial x\partial x'}\mathrm{Im}g_R(x,x';\omega)\right|^2}\right|_{x=0=x'}. \tag{2.24}$$

Evidently, substituting Eqs. (2.22) or (2.24) into Eq. (2.8), we obtain, respectively, Eqs. (I3.24) and (I3.26), reproduced below,

$$\frac{\hbar}{4e}\langle J(0;\omega)\rangle = |\Lambda^r(\omega)|^2\,\mathrm{Im}g^r_L(0,0;\omega)\,\mathrm{Im}g^r_R(0,0;\omega)\times[f_L(\omega)-f_R(\omega)] \tag{2.25}$$

and

$$\frac{\hbar}{4e}\langle J(0;\omega)\rangle = |\bar{\Lambda}^r(\omega)|^2\frac{\partial^2}{\partial x\partial x'}\mathrm{Im}g^r_L(x,x';\omega)\times\mathrm{Im}g^r_R(x,x';\omega)[f_L(\omega)-f_R(\omega)], \tag{2.26}$$

where

$$|\Lambda(\omega)|^2 = |g_L(0,0;\omega)+g_R(0,0;\omega)|^{-2}, \tag{2.27}$$

and

$$|\bar{\Lambda}(\omega)|^2 = \left|\frac{\partial^2}{\partial x\partial x'}[g_L(x,x';\omega)+g_R(x,x';\omega)\big|_{x=0=x'}\right|^{-2}. \tag{2.28}$$

The point to note is that these results have now been shown to have an additional generality: Equations (2.22) and (2.25) or (2.24) and (2.26) apply when we impose at the interface self-adjoint homogeneous boundary conditions;

$$\left.\begin{aligned}&\alpha g_L(x,x'<0;\omega)+\beta\frac{\partial}{\partial x}g_L(x,x'<0;\omega)=0,\\ &\text{and}\\ &\alpha g_R(x,x'>0;\omega)+\beta\frac{\partial}{\partial x}g_R(x,x'>0;\omega)=0.\end{aligned}\right\}\ \alpha,\beta=\text{real} \tag{2.29}$$

provided that, respectively, $\beta \neq 0$ or $\alpha \neq 0$. That is, whenever both Eqs. (2.25) and (2.29) are meaningful, they are equivalent. When Dirichlet boundary conditions are imposed at the interface, only Eqs. (2.22) and (2.25) apply; when Neuman boundary conditions are imposed at the interface, only Eqs. (2.24) and (2.26) apply. The preceding supplements the more restricted previous demonstration of the equivalence of the many-body and elementary formulations of tunneling for noninteracting systems. It also sheds further light on the precise significance of the local densities of states which figure prominently in a current modification of the transfer-Hamiltonian formalism, [17,18] as well as in our own tunneling theory.

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[1] T. E. Feuchtwang, Phys. Rev. B 10, 4121 (1970). Equations in this paper will be referred to by I followed by the number of the equation.

[2] T. W. Feuchtwang, Phys. Rev. B 11, 4135 (1974).

[3] C. Caroli, R. Combescot, R. Nozière, 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 CI, etc. Equations in these papers will be referred to by indicating the paper with C-I, etc. preceding the number of the equation.

[4] L. V. Keldysh, Zh. Eksp. Theo. Fiz. 47, 1515 (1964) [Sov. Phys.-JETP 20, 1018 (1965)].

[5] C. Caroli *et al.*, preceding paper, Phys. Rev. B 12, 3977 (1975).

[6] C. Caroli *et al.*, J. Phys. C 4, 916 (1971), Sec. (2.1) and, in particular, the two last sentences in this sec-

tion.

[7]C-II, Sec. 1.

[8]Recall that Caroli *et al.* require their uncoupled Green's functions to vanish at the interface. Hence Eqs. (I-3.26), (I-3.27) apply.

[9]See C-IV, the discussion following (C-IV.16). There $T\Lambda^r$ is identified as an effective matrix element analogous to that introduced by Applebaum and Brinkman, Phys. Rev. 186, 464 (1969). The authors thus clearly imply that T does not operate on the local density of states. This point is further emphasized in the paper by R. Combescot and G. Schreder, J. Phys. C 6, 1363 (1973) who apply the formalism of Caroli *et al.* to a metal-semiconductor contact and conclude explicitly that: "The change in the tunneling current ··· arises only from the modification of the density of states of the isolated semiconductor at the interface."

[10]This is particularly obvious from the continuous representation, $T = \lim_{\epsilon \to 0^+} \hbar^2/2m\epsilon^2$.

[11]See C-11, Sec. 2. In particular, Eqs. (C-II. 8), (C-II.11), and Eqs. (3), (4) in Ref. 5.

[12]C. B. Duke, *Tunneling in Solid State Physics Suppl.* 10 (Academic, New York, 1969), p. 212.

[13]See Eqs. (I2.19) and (I2.21).

[14]See Sec. IV in I.

[15]P. H. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), p. 529; see also E. A. Kraut, *Fundamentals of Mathematical Physics* (McGraw-Hill, New York, 1967), p. 295.

[16]Note that in order to assure that the uncoupled systems are in thermal equilibrium, the homogeneous boundary conditions have to be self-adjoint, i.e., α, β have to be real. This point has not been stated in Ref. 1.

[17]D. Penn, R. Gomer, and M. H. Cohen, Phys. Rev. B 5, 768 (1972); Phys. Rev. Lett. 27, 26 (1971).

[18]D. Penn, Phys. Rev. B 9, 844 (1974).