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Rigorous Formulation of High-Field Quantum Transport Applied to the Case of Electrons Scattered by Dilute Resonant Impurities

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A rigorous procedure is devised for generating quantum transport equations in an arbitrarily strong uniform electric field. An analytic implementation of the procedure is possible for the case of electrons scattering off a dilute random distribution of resonant-level impurities. In the limit of local scattering, the collision integral assumes a relaxation form, with a field-dependent relaxation time, thus reducing the calculation of the current to quadrature.

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It has been a long-standing theoretical problem to devise a scheme for calculating nonlinear transport phenomena.[1,2] Most reported results have been restricted to perturbation expansions in the external fields. The Keldysh[1] technique is a notable exception: the external fields are included in the free Hamiltonian thus permitting, at least in principle, a nonperturbative calculation. However, to our knowledge the Keldysh formalism has not been applied in practice to problems beyond quadratic response.[3]

The advent of the submicron semiconductor devices (where extremely high electric fields are commonplace) has increased the need for a formulation capable of going beyond the conventional semiclassical Boltzmann theory of transport. Levinson[4] and Barker and Ferry[5,6] have reported quantum transport equations where the collision integral differs from the Boltzmann case in two important aspects: (i) the driving fields are present in the collision integral leading to the so-called intracollisional field effect, and (ii) only in the limit of very large times is the irreversible Boltzmann-like structure recovered. In fact, recent calculations[7] of transient response indicate that the results obtained with these equations may differ significantly from those obtained with the conventional Boltzmann equation.

The construction of these quantum transport equations present serious analytical and computational problems. For example, Barker and Ferry[5,6] treated the electron-phonon scattering only to lowest order and included elastic impurity scattering phenomenologically by introducing a relaxation time. Even so only numerical solutions of the equations were possible.

In view of the above remarks it is clear that the field of nonlinear transport is in great need of rigorous results against which approximate formulations could be checked. We have studied a simple model problem where the exact analysis can be carried out much farther than is the case in the electron-phonon problem. The system investigated in this work is the resonant-level model (RLM)[8] in an arbitrarily strong uniform electric field. The RLM describes a localized level in a continuum: The conduction electrons make transitions between the localized level and the conduction band thus forming a scattering resonance. From our point of view the RLM is a model of an energy-dependent impurity scattering mechanism with particularly convenient mathematics related to it. The energy dependence of the RLM scattering mechanism allows one to study the intracollisional field effect in a very simple context.[9]

Our calculation is briefly summarized as follows. The field-dependent Green functions for free electrons in a uniform electric field are used to construct the single-site field-dependent T matrix for the RLM. By averaging over a dilute concentration of random resonant scatterers a self-energy functional is constructed and then used to evaluate the impurity-averaged field-dependent Green function. Finally, we use the generalized Baym-Kadanoff formalism[10] to write down the quantum transport equation for the RLM. In the limit of slow temporal and spatial variations a *nonlocal, field-dependent* collision integral is obtained. In the remainder of this Letter we expand on this summary.

Field-dependent free Green functions.—The equations of motion yield[11] the retarded Green function for a uniform electric field $[\vec{F}(t)$

$= -\partial\vec{A}(t)/\partial t$]:

$$G_r{}^{\varphi}(\vec{k},\vec{k}';t,t') = -i\,\theta(t-t')\,\delta\Big(\vec{k}-\vec{k}'-\int_{t'}^{t}dt_1\,\vec{F}(t_1)\Big)\exp\Big[-i\int_{t'}^{t}dt_1\,\epsilon\Big(\vec{k}-\int_{t'}^{t_1}dt_2\vec{F}(t_2)\Big)\Big] \tag{1a}$$

and

$$G_r{}^{A}(\vec{k},\vec{k}';t,t') = -i\theta(t-t')\,\delta(\vec{k}-\vec{k}')\exp\Big[-i\int_{t'}^{t}dt_1\,\epsilon(\vec{k}-\vec{A}(t_1))\Big], \tag{1b}$$

where the superscripts φ and A indicate that the electric field has been represented by a scalar or a vector potential, respectively. The advanced function G_a is obtained from (1) with the replacement $-i\theta(t-t')\to i\theta(t'-t)$. The results (1a) and (1b) are connected by the gauge transformation introduced by Levinson[4] and recently elaborated further by Calecki and Pottier.[12] The single-particle dispersion is denoted by $\epsilon(\vec{k})$.

The spectral density is constructed according to $A \equiv i(G_r - G_a)$:

$$A(\vec{k},\vec{R};\tau,T) = \exp\Big[-i\int_{T-\tau/2}^{T+\tau/2}dt_1\,\epsilon(\vec{k}-\vec{A}(t_1))\Big]. \tag{2}$$

In (2) we have used the Wigner frame $[(\vec{x},\vec{x}')\to((\vec{x}-\vec{x}'),(\vec{x},\vec{x}')/2)\equiv(\vec{r},\vec{R})$; $\vec{k}$ is the Fourier transform of $\vec{r}$] which is convenient in the description of transport phenomena. In the limit of slow time variations the Fourier transform of (2) with respect to the difference variable τ reduces to the expression used earlier by Barker[6]:

$$A(\vec{k},\vec{R};\omega,T) = 2\pi\,\delta[\omega-\epsilon(\vec{k}-\vec{A}(T))]. \tag{3}$$

Single-site field-dependent RLM.—Here we summarize the results of our earlier work.[11] The RLM zero-field Green function is written as $G = G_0 + G_0 T G_0$; when a static uniform electric field is turned on, the T matrix generalizes to

$$T^{\varphi} = V(\vec{k})V(\vec{k}')/[\omega - E - i\Gamma^{\varphi}(\omega)], \tag{4}$$

where E defines the position of the localized level with respect to the conduction band and $V(\vec{k})$ is the hybridization matix element between the conduction band and the localized level. The level width $\Gamma^{\varphi}(\omega)$ for a Gaussian model $V(k) = V_0 \times\exp(-\lambda^2k^2/2)$ (λ is a parameter describing the range of the interaction) is

$$\begin{aligned}\Gamma^{\varphi}(\omega) &= \operatorname{Im}\sum_{\vec{q}_1,\vec{q}_2} V(\vec{q}_1)G_r{}^{\varphi}(\vec{q}_1,\vec{q}_2;\omega)V(\vec{q}_2)\\ &= \Gamma(\omega)\exp(\tfrac{2}{3}\lambda^6F^2)\int_{-\infty}^{\alpha(F)}dx\,\mathrm{Ai}(-x),\end{aligned} \tag{5}$$

where $\Gamma(\omega)$ is the zero-field level width. Here $\alpha(F) = 2\omega/F^{2/3} - \lambda^4F^{4/3}$, and $\mathrm{Ai}(x)$ is the Airy function.[13] From (4) and (5) we infer the following important conclusions. The coupling between the conduction electrons and the resonant level [which is characterized by the level width $\Gamma^{\varphi}(\omega)$] *vanishes* for very high fields and it approaches its *zero-field* value as the energy is increased. Reference 11 offers a more complete discussion on these points.

It should be noted that the exact single-site T matrix available for the resonant-level model enables one to obtain an explicit form for the transport equations (see below). Much of the analysis however can be carried out formally with a T matrix which is known only implicitly.[11b]

Dilute concentration of resonant scatterers.—We follow the standard procedure[14]: The Dyson equation for a fixed configuration of impurities is iterated and averaged term by term and finally an infinite resummation is carried out to construct a self-energy functional. Working to linear order in the concentration of impurities c, one obtains the following self-consistent equations:

$$\begin{aligned}&\overline{G}^{\varphi} = G^{\varphi} + G^{\varphi}\Sigma[\overline{G}^{\varphi}]\overline{G}^{\varphi},\\ &\Sigma[\overline{G}^{\varphi}] = c\int\frac{d^3R}{\Omega}\,\frac{\exp[-i(\vec{q}_1-\vec{q}_2)\cdot\vec{R}]\,V(\vec{q}_1)V(\vec{q}_2)}{\omega - E - F[\overline{G}^{\varphi}]},\end{aligned} \tag{6}$$

where

$$F[\overline{G}^{\varphi}] = \sum_{\vec{p},\vec{q}}\exp[i(\vec{p}-\vec{q})\cdot\vec{R}]\,V(\vec{p})\overline{G}^{\varphi}(\vec{p},\vec{q};\omega)V(\vec{q}).$$

In the zero-field case the self-consistent equations (6) can be solved to yield $\Sigma[\overline{G}] = c\,V(\vec{q})^2/[\omega - E - i\Gamma(\omega)]$. Thus the imaginary part of the self-energy (which is related to the relaxation time) displays the expected resonant structure.

For finite external fields the solution (6) is considerably harder because the self-energy is nondiagonal in its momentum labels. Rather than analyzing (6) numerically we give here the following approximate solution. Observe that in the zero-field case the correct result can be obtained by using the *free* Green function in the self-energy. Via this *Ansatz* the *field-dependent* free Green function in (6) yields

$$\Sigma = c\int\frac{d^3R}{\Omega}\,\frac{\exp[-i(\vec{q}_1-\vec{q}_2)\cdot\vec{R}]\,V(\vec{q}_1)V(\vec{q}_2)}{\omega - E - i\Gamma^{\varphi}(\omega + FR_{\parallel})}. \tag{7}$$

Note that the level width appears with an energy argument which is increased by $FR_{\parallel}$, where $R_{\parallel}$ is the distance traveled parallel to the uniform electric field. Now recall the result obtained in the single-site calculation: The level width approaches its zero-field value as the energy is increased. Hence for field strengths occurring in submicron devices, after a few angstroms in the sample the charge carrier has been accelerated to such a high energy that we can approximate $\Gamma^{\varphi}(\omega+FR_{\parallel}) \simeq \Gamma(\omega)$. The now trivial R integral yields a self-energy diagonal in the momentum labels $\vec{q}$, and an exact solution of Eqs. (6) is possible. A lengthy but straightforward calculation gives

$$\overline{G}_{r,a}{}^{\varphi}(\vec{k},\vec{k}';\omega) = G_{r,a}{}^{\varphi}(\vec{k},\vec{k};\omega)\exp\left(-\frac{i}{F}\int_{k_{\parallel}'}^{k_{\parallel}} dq_{\parallel}\,\frac{cV(q_{\parallel},\vec{k}_{\perp})^2}{\omega - E \mp i\Gamma(\omega)}\right), \tag{8}$$

where $G^{\varphi}(\vec{k},\vec{k};\omega)$ is the time Fourier transform of the field-dependent free Green function (1a). It can be shown[11b] that (8) is indeed a self-consistent solution to (6) if V is an insensitive function of $\vec{k}$. It should also be noted that (8) reduces to the correct zero-field result when $F \to 0$.[15]

Equation (8) is one of our main results: To our knowledge no previous explicit solutions to the field-dependent Dyson equation exist. The retarded and advanced Green functions as given by (8) are needed in the construction of spectral densities which form an input to the generalized Baym-Kadanoff equations.

Transport equations for the RLM.—Using the results (6) and (8) we can follow the prescription for constructing a quantum transport equation with the generalized Baym-Kadanoff formalism.[10] Rather than giving the cumbersome equation in full we pass to the limit where external perturbations are slowly varying and examine the approximate equations for which the physics is more transparent. We use the following procedure. (1) All relevant quantities are assumed to be slowly varying functions of the "center-of-mass" variables $(\vec{R}, T)$. (2) A gradient expansion is performed in these variables and only the lowest-order terms are retained. Then, using the Gaussian model interaction, we find

$$\{\nabla_p \epsilon_{\vec{p}}\cdot\nabla_{\vec{R}} + \vec{F}\cdot\nabla_p\} f(\vec{p},\vec{R}) = \frac{c}{(\epsilon_{\vec{p}} - \vec{F}\cdot\vec{R} - E)^2 + \Gamma^2}\sum_{\vec{p}'}\int d^3R'\,\frac{\exp[-(\vec{R}-\vec{R}')^2/2\lambda^2]}{(2\pi\lambda^2)^{3/2}}$$

$$\times V^2(\vec{p})V^2(\vec{p}')\delta(\epsilon_{\vec{p}} - \epsilon_{\vec{p}'} - \vec{F}\cdot(\vec{R}-\vec{R}'))[f(\vec{p},\vec{R}) - f(\vec{p}',\vec{R}')]. \tag{9}$$

It is worth noting that in order to obtain in the collision term the resonant prefactor characteristic of the RLM one has to go beyond the Born approximation and use the T matrix form (7) for the self-energy [see also Eq. (4)].

The transport equation (9) resembles the Boltzmann equation but the collision integral has two important differences: it is nonlocal in space and field dependent. The nonlocality results from the finite range of the model interaction. The field-dependent energy shifts in (9) are easily understood if one recalls that the zero of the potential energy of the system is position dependent as a result of the applied electric field. One should note that (9) cannot be reduced to a relaxation-time form as in the case with the ordinary impurity Boltzmann equation.

There is, however, a relaxation-time form for a localized interaction ($\lambda \to 0$), and an exact prescription of the current is possible. In this limit (9) reduces to

$$\{\nabla_p \epsilon_{\vec{p}}\cdot\nabla_{\vec{R}} + \vec{F}\cdot\nabla_p\} f(\vec{p},\vec{R}) = [\tau(\epsilon_p - \vec{F}\cdot\vec{R})]^{-1}[f(\vec{p},\vec{R}) - f_0(\epsilon_{\vec{p}})]. \tag{10}$$

Here $1/\tau(\epsilon) = cV_0{}^4/[(\epsilon - E)^2 + \Gamma^2]$ and $f_0(\epsilon_{\vec{p}})$ is the equilibrium distribution function. Using the solution of (10) in the expression for the current, $\vec{j} = \sum_{\vec{p}} \vec{p} f(\vec{p})$, one finally obtains[16]

$$\vec{j}(\vec{R}) = \sum_{\vec{p}} \vec{p}\int_0^{\infty} ds\, e^{-s} f_0(\vec{p} - s\vec{F}\tau(\epsilon_{\vec{p}} - \vec{F}\cdot\vec{R})). \tag{11}$$

In linear theory (11) gives the ordinary Boltzmann-equation result for the conductivity.

In summary, we have outlined a rigorous method to calculate nonlinear transport properties. An application to a simple model system reveals new and interesting structure in a Boltzmann-type collision integral. Only in the limit of a localized interaction *and* in linear theory does the transport equation (9) reduce to the ordinary Boltzmann equation used earlier[17] to discuss the transport properties of the RLM.

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[1] L. V. Keldysh, Zh. Eksp. Teor. Fiz. 47, 1945 (1964) [Sov. Phys. JETP 20, 1018 (1965)].

[2] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).

[3] C. Caroli, D. Lederer-Rozenblatt, B. Roulet, and S. Saint-James, Phys. Rev. B 8, 4552 (1973).

[4] I. B. Levinson, Zh. Eksp. Teor. Phys. 57, 660 (1967) [Sov. Phys. JETP 30, 362 (1970)].

[5] J. R. Barker, J. Phys. C 6, 2663 (1973); J. R. Barker and D. K. Ferry, Phys. Rev. Lett. 42, 1776 (1979).

[6] J. R. Barker, J. Phys. (Paris) Colloq. 42, C7-245 (1981).

[7] D. K. Ferry and J. R. Barker, Solid-State Electron. 23, 545 (1980).

[8] See, for example, P. W. Anderson, Phys. Rev. 124, 41 (1961); J. Friedel, Can. J. Phys. 34, 1190 (1956), and Nuovo Cimento Suppl. 7, 287 (1958).

[9] We point out that in the case of elastic impurity scattering discussed within the Born approximation the field dependence of the collision integral vanishes. Thus the RLM has two attractive features: One is able to go beyond the Born approximation and a nontrivial field dependence occurs even in Bolzmann-like equations.

[10] D. C. Langreth and J. W. Wilkins, Phys. Rev. B 6, 3189 (1972); D. C. Langreth, in *Linear and Nonlinear Electron Transport in Solids*, edited by J. T. Devreese and E. van Boren (Plenum, New York, 1976).

[11a] A. P. Jauho, J. W. Wilkins, and F. P. Esposito, J. Phys. Colloq. 42, C7-301 (1981).

[11b] A. P. Jauho, Ph.D. thesis, Cornell University, 1982 (unpublished).

[12] D. Calecki and N. Pottier, J. Phys. Colloq. 42, C7-271 (1981); N. Pottier and D. Calecki, Physica (Utrecht) 110A, 471 (1982).

[13] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards, Washington, D. C., 1964), pp. 446–452.

[14] See, for example, A. A. Arbrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975), Sec. 39.2.

[15] The apparent nonanalytic dependence on the external field can be circumvented if one interprets (8) as a generalized function. For details, see Ref. 11b.

[16] It is easy to verify that the distribution function used in (11) is a solution of (10) by making use of the identity $\{\nabla_p \epsilon_{\vec{p}} \cdot \nabla_R + \vec{F} \cdot \nabla_p\}(\epsilon_{\vec{p}} - \vec{F} \cdot \vec{R}) \equiv 0$. The integration constant in the expression for the distribution function is fixed so that the equilibrium function is recovered when the field is turned off.

[17] H. Smith and J. W. Wilkins, Phys. Rev. Lett. 24, 221 (1970).

ERRATUM

SITE PERCOLATION IN A SQUARE LATTICE WITH SECOND- AND DILUTE FIRST-NEIGHBOR BONDS. P. Murilo Oliveira [Phys. Rev. Lett. 47, 1423 (1981)].

In Table I, the value 1.601 should be replaced by 1.275, and accordingly, the value 2.618 should be replaced by 2.084.