# Theory of high-electric-field quantum transport for electron-resonant impurity systems

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A formalism is developed which allows a nonperturbative calculation of the effects of the electric field on electron-impurity scattering. The single-site T matrix is evaluated exactly and studied numerically for a model potential. For a dilute concentration of random impurities, the impurity-averaging procedure is carried out in a finite external field and a nonlinear integral equation is derived for the Green function. This equation is solved in an approximate, but consistent, manner. Finally, a quantum-transport equation is constructed with the generalized Baym-Kadanoff method of nonequilibrium quantum statistical mechanics. Special attention is paid to the field dependence of the collision integral. In particular, in the limit of slow spatial variations, a Boltzmann-type transport equation is derived with a nonlocal field-dependent collision integral.

# I. INTRODUCTION

It has been a long-standing theoretical problem to devise a scheme for calculating nonlinear transport phenomena. Most formalisms have been restricted to perturbation expansions in the external fields.<sup>1,2(a)</sup> The Keldysh<sup>3</sup> technique is a notable exception: The 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.<sup>2(b)</sup>

The development of 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. In semiconductor transport theory, the Boltzmann equation is usually written as

$$\frac{\partial f}{\partial t} + \vec{\nabla}_{\vec{k}} \epsilon(\vec{k}) \cdot \vec{\nabla}_{\vec{r}} f + [-\vec{\nabla}_{\vec{r}} U(\vec{r})] \cdot \vec{\nabla}_{\vec{k}} f$$
$$= \sum_{\vec{p}\, i} [K(\vec{p},\vec{p}\,')f(\vec{p}\,') - K(\vec{p}\,',\vec{p})f(\vec{p})] . \quad (1.1)$$

The research described in the present paper attempts to shed some light on the following questions.

(i) Under what conditions can the quantum-transport equations be cast in the form of Eq. (1.1)?

(ii) How does one include microscopically (and rigorously) the effect of the driving fields in the scattering rates  $K(\vec{p}, \vec{p}')$ ?

(iii) Does the structure of (1.1) prevail? One might expect to get additional time dependence or nonlocality on the right-hand side.

Rather than attempting to treat these questions exhaustively, and for a realistic submicron device, we have made several drastic simplifications to make the problem tractable. In doing so, we are able to carry out microscopic calculations which lead to explicit results under controlled approximations.

The system considered in this study consists of noninteracting electrons scattering off a dilute concentration of resonant scatterers under the influence of an arbitrarily strong, static, and uniform electric field. This system is simple enough to allow explicit calculations, but also sufficiently complex so as to reveal interesting physics when subjected to an analysis with the methods of quantumtransport theory. Our calculations must be viewed only as a first step towards a rigorous theory of transport in a small semiconductor device. In any calculation pertaining to a real device one should consider (i) electron-phonon scattering (which is not included in our explicit results; see, however, Appendix A), and (ii) some aspects of the spatial nonuniformity of the external field (important effects can be expected to take place in the transitional region between the low- and high-field areas of a realistic device). The greatest utility of our final results is that they can be used to study, and, in principle, exactly, how the electric field modifies the electron-resonant impurity collision integral. Many of the formal results and techniques developed in this work do have, however, a much wider range of validity and can be applied to any system where a nonperturbative treatment of the external field is desired.

The outline of this report is the following. In Sec. II we review the generalized Kadanoff-Baym (GKB) formalism for nonequilibrium quantum statistical mechanics.<sup>1,2</sup> In Sec. III we derive explicit expressions for field-dependent free Green functions which then are used as basic building blocks for the subsequent developments of the theory, Secs. IV and V. In Sec. IV we discuss the *dynamics* (single-particle properties) of the electron-impurity system, whereas Sec. V is devoted to the *kinetic* (distribution properties) of the system. In Appendix A we make a con-

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nection to the other existing formulations; in particular, the formalism developed in this study is used to derive, in a simple and self-contained fashion, results which formerly have emerged only after considerably more tedious calculations. Finally, Appendix B contains a technical note on the zero-field-limiting properties of the field-dependent Green functions.

# **II. FORMULATION OF THE THEORY**

In nonequilibrium problems one is concerned, say, with calculating currents arising due to the forces which drive the system out of equilibrium. A typical quantity one might want to evaluate is the current which is given by

$$\vec{j}(\vec{x},t) = \frac{1}{2i} (\vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}}) \langle \psi_H^{\dagger}(\vec{x}',t) \psi_H(\vec{x},t) \rangle .$$
(2.1)

The expectation value of the two Heisenberg-picture field operators closely resembles a Green function, and one might hope to be able to apply the conventional calculational schemes to extract the correlation function appearing in (2.1). In fact, in linear response this procedure becomes feasible due to the existence of the fluctuationdissipation theorem. In the nonlinear case, however, one has to resort to the full nonequilibrium theory.

The expression (2.1) for the current suggests defining the following real-time correlation functions:

$$G^{\langle (1,1') = -i \langle \psi_H(1)\psi_H^{\dagger}(1') \rangle},$$
  

$$G^{\langle (1,1') = i \langle \psi_H^{\dagger}(1')\psi_H(1) \rangle}.$$
(2.2)

The current is then readily expressed in terms of  $G^{<}$ ,

$$\vec{j}(\vec{R},T) = -i \sum_{\vec{p},p_0} \vec{p} G^{<}(\vec{p},p_0;\vec{R},T)$$
 (2.3)

In (2.3) we have introduced the so-called Wigner coordinates,

$$\vec{\mathbf{r}} = \vec{\mathbf{x}} - \vec{\mathbf{x}}', \ \tau = t - t', \ \vec{\mathbf{R}} = \frac{1}{2}(\vec{\mathbf{x}} + \vec{\mathbf{x}}'), \ T = \frac{1}{2}(t + t')$$
 (2.4)

This is a convenient way of separating the fast and slow spatial and temporal scales; in what follows, a Fourier transformation is performed with respect to  $\vec{r}$  and  $\tau$ , and quantities are often expanded in terms of the gradients of the slow variables  $\vec{R}$  and T (see below).

Another quantity of great importance, which is directly expressible in terms of  $G^{<}$ , is the Wigner distribution function  $f(\vec{p}, \vec{R}, T)$ ,

$$f(\vec{\mathbf{p}},\vec{\mathbf{R}},T) = \int d^3 r \, e^{-i\,\vec{\mathbf{p}}\cdot\vec{\mathbf{r}}} \langle \psi_H^{\dagger}(\vec{\mathbf{R}}-\frac{1}{2}\,\vec{\mathbf{r}},T)\psi(\vec{\mathbf{R}}+\frac{1}{2}\,\vec{\mathbf{r}},T) \rangle$$
$$= -i \sum_{p_0} G^{<}(\vec{\mathbf{p}},p_0;\vec{\mathbf{R}},T) \,. \tag{2.5}$$

Thus the main task of the nonequilibrium theory is to set up a calculational scheme for the functions (2.2). The main difficulty lies in the fact that the Feynman-Dyson perturbation expansion does not exist for functions such as (2.2). However, one can obtain equations for the correlation functions (2.2) by analytic continuation from the Dyson equations satisfied by the imaginary-time Green functions. There are many equivalent ways of performing this step; our method is closest to the GKB scheme,<sup>1,2</sup> even though some essential ingredients can be found in Keldysh's<sup>3</sup> work as well.

Conceptually, the nonequilibrium calculation splits into two steps. First, the dynamics, or single-particle properties, are described by quantities which possess well-defined Dyson equations, and hence, at least in principle, are tractable. Examples of these quantities are the retarded and advanced Green functions. Second, the description of the distribution of the particles requires the aforementioned correlation functions which satisfy a "kinetic" equation derived by analytic continuation.

In the GKB formalism,<sup>2</sup> the basic equations are

$$G_{r,a} = G_{r,a}^{0} + G_{r,a}^{0} U G_{r,a} + G_{r,a}^{0} \Sigma_{r,a} G_{r,a} , \qquad (2.6a)$$
$$[(G^{0})^{-1} - U - \Sigma, G^{\gtrless}] - [\Sigma^{\gtrless}, G]$$
$$= -\frac{1}{2} \{\Sigma^{<}, G^{>}\} + \frac{1}{2} \{\Sigma^{>}, G^{<}\} . \qquad (2.6b)$$

In (2.6) all external forces are denoted by the operator  $U_{i}$ whereas all scattering processes (impurities, phonons, and electron-electron interactions) are collected in the selfenergy  $\Sigma_{r,a}$ . We have also defined the real part of the Green function and the self-energy by  $G = \frac{1}{2}(G_a + G_r)$  and  $\Sigma = \frac{1}{2}(\Sigma_a + \Sigma_r)$ , respectively. To have a closed set of equations one needs to know the self-energy as a functional of the Green function. The two-step structure discussed above is evident: One needs the solutions of the Dyson equation (2.6a) as an input for the "quantum kinetic" equation (2.6b). Equations (2.6) should be interpreted as matrix equations: Integrals over intermediate position and time variables are implied throughout. For the derivation of (2.6) the reader is referred to Appendix A of Ref. 2(a); it should be noted that in the present study we use slightly different definitions for the correlation functions than what was used in Ref. 2.<sup>4</sup> Consequently, our basic equation (2.6b) differs slightly from the corresponding equation (A19) of Ref. 2(a).

A very similar two-step structure is obtained in the Keldysh formalism:<sup>3</sup> Our equations (2.6a) and (2.6b) correspond to the diagonal and off-diagonal components of the Keldysh matrix equation, respectively.

The main emphasis of our work will be on the study of transport phenomena which are nonlinear in the external fields. In particular, we aim at a nonperturbative treatment of the external fields. In practice this amounts to treating the system consisting of noninteracting particles and the external fields exactly. In other words, the particles are "dressed" with the external fields, and the Green functions describing these dressed particles are then used as the basic building blocks in the subsequent developments of the theory.

The field-dependent Green functions are defined by

$$G_{r,a}^{U} = G_{r,a}^{(0)} + G_{r,a}^{(0)} U G_{r,a}^{U} , \qquad (2.7)$$

in terms of which the GKB equations are

$$G_{r,a} = G_{r,a}^{U} + G_{r,a}^{U} \Sigma_{r,a} G_{r,a}$$

$$[(G^{U})^{-1} - \Sigma, G^{\gtrless}] - [\Sigma^{\gtrless}, G]$$

$$= -\frac{1}{2} \{\Sigma^{<}, G^{>}\} + \frac{1}{2} \{\Sigma^{>}, G^{<}\} . \qquad (2.8)$$

The idea of including the external fields exactly in the Green functions occurs already in Keldysh's work (but only on a formal level); to our knowledge, however, our work is the first practical realization of such a procedure.

In many physical situations the external fields vary slowly on microscopic time or length scales. This suggests a division between "macroscopic" and "microscopic" quantities; the microscopic quantities are treated exactly, whereas one performs a gradient expansion in the slowly varying macroscopic quantities. More explicitly, one transforms into center-of-mass and difference variables [i.e., to the Wigner coordinates defined in (2.4)], Fouriertransforms with respect to the difference variables, and gradient-expands in the center-of-mass variables. What one needs then is a prescription for evaluating commutators and anticommutators. The rules are

$$\frac{1}{i} \int d^{4}\bar{x} [A(x,\bar{x})B(\bar{x},x') - B(x,\bar{x})A(\bar{x},x')] \rightarrow \frac{\partial}{\partial p_{0}} A(\vec{p},p_{0};\vec{R},T) \frac{\partial}{\partial T} B(\vec{p},p_{0};\vec{R},T) - \frac{\partial}{\partial T} A(\vec{p},p_{0};\vec{R},T) \frac{\partial}{\partial p_{0}} B(\vec{p},p_{0};\vec{R},T) - \vec{\nabla}_{\vec{p}} A(\vec{p},p_{0};\vec{R},T) \cdot \vec{\nabla}_{\vec{R}} B(\vec{p},p_{0};\vec{R},T) + \vec{\nabla}_{\vec{R}} A(\vec{p},p_{0};\vec{R},T) \cdot \vec{\nabla}_{\vec{p}} B(\vec{p},p_{0};\vec{R},T) + \cdots$$
(2.9a)

and

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$$\frac{1}{2} \int d^{4}\overline{x} [A(x,\overline{x})B(\overline{x},x') + B(x,\overline{x})A(\overline{x},x')] \rightarrow A(\overrightarrow{p},p_{0};\overrightarrow{R},T)B(\overrightarrow{p},p_{0};\overrightarrow{R},T) + \cdots$$
(2.9b)

The somewhat tedious derivation for (2.9) can be found in Ref. 2(a). As an application of (2.9) let us consider the first term in the kinetic equation (2.6a),

$$[G_0^{-1}, G^{\gtrless}] \rightarrow \frac{\partial}{\partial p_0} (p_0 - \epsilon_{\vec{p}}) \frac{\partial}{\partial T} G^{\gtrless} - \vec{\nabla}_{\vec{p}} (p_0 - \epsilon_{\vec{p}}) \cdot \vec{\nabla}_{\vec{R}} G^{\gtrless} .$$
(2.10)

We identify the contribution arising from (2.10) as pieces of the driving terms of the Boltzmann equation. This is an important feature of the gradient expansion: It can be used as a device to derive Boltzmann equations from more fundamental equations (such as the GKB equations).

This concludes our discussion of the theoretical preliminaries; in subsequent sections we construct transport equations for the resonant-level model (RLM; see below) starting from the modified basic equations (2.8) which allow a nonperturbative treatment of the external fields.

# **III. FIELD-DEPENDENT FREE GREEN FUNCTIONS**

#### A. Introduction

In this section we derive expressions for the fielddependent free Green functions (2.6) discussed in the preceding section. Exact expressions are given for timedependent but spatially uniform electric fields. The generalization to nonuniform fields seems to be difficult (see below). However, within the gradient expansion the problem simplifies considerably. As an example, we derive the Boltzmann equation driving terms for position- and timedependent (but slowly varying) electric and magnetic fields. We will also compare our results with those obtained elsewhere.<sup>3,5-7</sup> Some of the results of this section have been briefly discussed before.<sup>8,9</sup>

#### **B.** Exact expressions

The exact expressions are constructed by solving the equations of motion. In a general electromagnetic field, these equations read

$$\begin{vmatrix} i\frac{\partial}{\partial t} - \epsilon(-i\vec{\nabla} - \vec{A}(\vec{x},t)) - \phi(\vec{x},t) \end{vmatrix} G(\vec{x},\vec{x}\,';t,t') = \delta(\vec{x} - \vec{x}\,')\delta(t-t'), (3.1) 
$$\left[ -i\frac{\partial}{\partial t'} - \epsilon(i\vec{\nabla}\,' - \vec{A}(\vec{x}\,',t')) - \phi(\vec{x}\,',t') \right] G(\vec{x},\vec{x}\,';t,t') = \delta(\vec{x} - \vec{x}\,')\delta(t-t').$$$$

To determine these functions completely, a boundary condition is needed. This condition can be, for example, that the solution of (3.1) is of the retarded or of the advanced type. In (3.1) we denote the single-particle dispersion by  $\epsilon(\vec{k})$ , and we have chosen a system of units where  $m_e = \hbar = e = 1$ .

Equations (3.1), in their present form, cannot be solved explicitly. Consider now the case where there is no magnetic field, and the system is subject to a time-dependent electric field  $\vec{F}(t)$ . Then we can choose

$$\vec{\mathbf{A}}(t) = -\int_0^t d\vec{t} \ \vec{\mathbf{F}}(\vec{t}), \ \phi(\vec{\mathbf{x}},t) \equiv 0.$$
(3.2)

With this assumption one can Fourier-transform with respect to the spatial coordinates to obtain

$$\left[i\frac{\partial}{\partial t} - \epsilon(\vec{k} - \vec{A}(t))\right] G^{\vec{A}}(\vec{k}, \vec{k}'; t, t') = \delta(t - t')\delta(\vec{k} - \vec{k}') ,$$
(3.3)

which can be integrated to yield

$$G_{r}^{\vec{A}}(\vec{k},\vec{k}';t,t') = -i\Theta(t-t')\delta(\vec{k}-\vec{k}')$$

$$\times \exp\left[-i\int_{t'}^{t} d\vec{t}\,\epsilon(\vec{k}-\vec{A}(\vec{t}))\right]. \quad (3.4)$$

In (3.4) the boundary condition has been chosen to correspond to the retarded function. The advanced function  $G_a^A$  is obtained from (3.4) with the replacement  $-i\Theta(t-t')\rightarrow i\Theta(t'-t)$ . Finally, the superscript  $\vec{A}$  indicates that the external field is represented by a vector potential.

Consider now the case where the electric field is represented by a scalar potential,

$$\vec{\mathbf{A}}(\vec{\mathbf{x}},t) = \vec{\mathbf{0}}, \quad \phi(\vec{\mathbf{x}},t) = -\vec{\mathbf{x}} \cdot \vec{\mathbf{F}}(t) \ . \tag{3.5}$$

The equation of motion now reads

$$\left[ i \frac{\partial}{\partial t} - \epsilon(\vec{k}) + i \vec{F}(t) \cdot \vec{\nabla}_{\vec{k}} \right] G^{\phi}(\vec{k}, \vec{k}'; t, t')$$
  
=  $\delta(t - t') \delta(\vec{k} - \vec{k}')$ , (3.6)

from which the retarded function is as follows:

$$G_{r}^{\phi}(\vec{\mathbf{k}},\vec{\mathbf{k}}';t,t') = -i\Theta(t-t')\delta\left[\vec{\mathbf{k}}-\vec{\mathbf{k}}'-\int_{t'}^{t}d\vec{t}\ \vec{\mathbf{F}}(\vec{t})\right] \times \exp\left[-i\int_{t'}^{t}d\vec{t}\ \epsilon\left[\vec{\mathbf{k}}-\int_{\vec{t}}^{t}dt_{1}\vec{\mathbf{F}}(t_{1})\right]\right]. \quad (3.7)$$

In the case of a dc electric field (3.7) reduces to

$$G_{r}^{\phi}(\vec{\mathbf{k}},\vec{\mathbf{k}}';t-t') = -i\Theta(t-t')\delta(\vec{\mathbf{k}}-\vec{\mathbf{k}}'-\vec{\mathbf{F}}(t-t'))$$

$$\times \exp\left[-i\int_{0}^{t-t'}dt_{1}\,\epsilon(\vec{\mathbf{k}}-t_{1}\vec{\mathbf{F}})\right],$$
(3.8)

and has a simple interpretation when compared to the zero-field Green function

$$G_{r}^{0}(\vec{\mathbf{k}};\vec{\mathbf{k}}';t-t') = -i\Theta(t-t')\delta(\vec{\mathbf{k}}-\vec{\mathbf{k}}')$$

$$\times \exp[-i\epsilon(\vec{\mathbf{k}})(t-t')]. \qquad (3.9)$$

The two changes are the following: (i) the shift in the momentum-conservation law to account for the acceleration due to the electric field, and (ii) the time evolution of the kinetic energy.

The two different expressions derived for the Green function for a uniform electric field [(3.4) and (3.7)] correspond to the same physical situation. It is therefore reasonable to expect that the two expressions (3.4) and

(3.7) be linked in a simple way. The explanation is the following. The labels  $\vec{k}$  and  $\vec{k}'$  in (3.3) and (3.4) refer to the *canonical* momentum, i.e., *not* to the velocity. If one performs a variable change in (3.4) via  $\vec{k} = \vec{v} + \vec{A}(t)$ , i.e., expresses the Green function in the "velocity" basis, the two expressions (3.4) and (3.8) agree. The connection between (3.4) and (3.8) can also be established by a suitable gauge transformation.<sup>5,6</sup>

Consider now external fields which are position dependent. One might hope that a clever choice of gauge renders the mathematics in a tractable form. Unfortunately, this seems unlikely except for some special cases. The reason is that in any gauge the equation of motion always contains a term where the Green function is multiplied by the position-dependent field. One usually Fourier-transforms the equation to simplify the kinetic energy operator, but since a product of two functions does not possess a simple Fourier transform, progress seems difficult. One has to solve a second-order (in the position space) differential equation which is considerably more difficult than the first-order (in the time domain) equations discussed above. It is worth noting that the case of a uniform magnetic field which requires a positiondependent vector potential can be treated along the lines discussed above because the resulting second-order differential equation can be solved in terms of the wellknown Landau states. The case when the external perturbations are slowly varying can be treated within the gradient of expansion and is discussed below.

# C. Spectral density and exact expressions

The spectral density plays a central role in the construction of quantum kinetic equations. It is therefore of interest to derive exact expressions for this quantity, which are then later used in the derivation of transport equations. The spectral density is defined as

$$\begin{aligned} A(\vec{p},\omega;\vec{R},T) &= -\left[G_a(\vec{p},\omega;\vec{R},T) - G_r(\vec{p},\omega;\vec{R},T)\right] \\ &= -i\left[G^{<}(\vec{p},\omega;\vec{R},T) - G^{>}(\vec{p},\omega;\vec{R},T)\right]. \end{aligned}$$
(3.10)

The second line in (3.10) follows from the definitions and we used the Wigner coordinates in anticipation of a gradient expansion. Note that the spectral density satisfies the sum rule

$$\int \frac{d\omega}{2\pi} A(\vec{p},\omega;\vec{R},T) = 1$$
(3.11)

in both equilibrium and nonequilibrium situations. One can say that (3.11) is a restatement of the anticommutation rule for the field operators.

Substituting now the expressions for  $G_r^{\vec{A}}$  and  $G_a^{\vec{A}}$  in (3.10), one obtains

$$A(\vec{p},\omega;\vec{R},T) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \\ \times \exp\left[-i\int_{T-\tau/2}^{T+\tau/2} d\vec{t} \,\epsilon(\vec{p}-\vec{A}(\vec{t}))\right].$$
(3.12)

Note that (3.1) is exact: No gradient expansion has been carried out so far.

It is instructive to derive an equation for the spectral density starting from the basic equation (2.6b). By subtracting the two equations (2.6b) and making use of  $\Sigma = 0$  (the scattering has not yet been turned on) gives

$$[(G^0)^{-1} - U, A] = 0. (3.13)$$

It can be verified by direct calculation that (3.12) indeed satisfies (3.13). Equation (3.13) will be useful in constructing *Ansätze* for the distribution function (see below).

#### D. Gradient expansions

The next step is to derive expressions for the fielddependent Green functions for systems under the influence of time- and position-dependent, but slowly varying, electric and magnetic fields. We will then use the derived Green functions to obtain an expression for the spectral density and to construct the driving terms in the Boltzmann equation.

Note that the driving terms are derived from the *commutators* on the left-hand side of the GKB equations (2.6) or (2.8). From the expansion rule (2.9a) for commutators we observe that the leading term is of the first order with respect to the small gradients  $\partial_T$  and  $\vec{\nabla}_{\vec{R}}$ . Therefore, to apply (2.9a) consistently, we need the quantities "A" and "B" appearing in (2.9a) to zeroth order in the small gradients. Thus instead of the exact equation of motion we are led to consider the first term in its gradient expansion,

$$\left[i\frac{\partial}{\partial\tau}-\epsilon(-i\vec{\nabla}_{\vec{r}}-\vec{A}(\vec{R},T))-\phi(\vec{R},T)\right]G(\vec{r},\tau;\vec{R},T)$$

 $=\delta(\vec{r})\delta(\tau)$ .

(3.14)

In writing (3.14), we used

$$\frac{\partial}{\partial t} \equiv \frac{d\tau}{dt} \frac{\partial}{\partial \tau} + \frac{dT}{dt} \frac{\partial}{\partial T} \rightarrow \frac{\partial}{\partial \tau} ,$$

and analogously for the position variables. Equation (3.14) is readily solved as follows:

$$G_r(\vec{\mathbf{p}},\omega;\vec{\mathbf{R}},T) = [\omega - \epsilon(\vec{\mathbf{p}} - \vec{\mathbf{A}}(\vec{\mathbf{R}},T)) - \phi(\vec{\mathbf{R}},T) + i\eta]^{-1}.$$
(3.15)

The advanced function is obtained from (3.15) by the replacement  $+i\eta \rightarrow -i\eta$ , and the expression for the spectral density becomes

$$A(\vec{p},\omega;\vec{R},T) = 2\pi\delta(\omega - H(\vec{p},\vec{R},T)), \qquad (3.16)$$

where we have defined the classical Hamiltonian function for a charged particle in an electromagnetic field,

$$H(\vec{p},\vec{R},T) = \epsilon(\vec{p} - \vec{A}(\vec{R},T)) + \phi(\vec{R},T) . \qquad (3.17)$$

Equation (3.16) also applies to situations where there is a magnetic field and it is therefore a generalization of Barker's recent result [cf. Eq. (20) in Ref. 7].

Let us now apply (3.16) to derive the driving terms in

the Boltzmann equation. In particular, we will evaluate the piece  $[(G^U)^{-1}, G^<]$  of the GKB equation (2.8) with

$$[G^{U}(\vec{p},\omega;\vec{R},T)]^{-1} = \omega - H(\vec{p},\vec{R},T) . \qquad (3.18)$$

An application of the rule (2.9a) now gives the following expression for the driving terms (equal to  $\mathcal{D}$ ):

$$\mathcal{D} = \{\partial_T + \partial_T H(\vec{p}, \vec{R}, T) \partial_\omega + [\vec{\nabla}_{\vec{p}} H(\vec{p}, \vec{R}, T)] \cdot \vec{\nabla}_{\vec{R}} - [\vec{\nabla}_{\vec{R}} H(\vec{p}, \vec{R}, T)] \cdot \vec{\nabla}_{\vec{p}} \} G^{<}(\vec{p}, \omega; \vec{R}, T) .$$
(3.19)

We now make the following Ansätze for  $G^{<}$  and  $G^{>}$ :

$$G^{<}(\vec{\mathbf{p}},\omega;\vec{\mathbf{R}},T) = iA(\vec{\mathbf{p}},\omega;\vec{\mathbf{R}},T)f(\vec{\mathbf{p}},\vec{\mathbf{R}},T) ,$$

$$(3.20)$$

$$G^{>}(\vec{\mathbf{p}},\omega;\vec{\mathbf{R}},T) = -iA(\vec{\mathbf{p}},\omega;\vec{\mathbf{R}},T)[1-f(\vec{\mathbf{p}},\vec{\mathbf{R}},T)] .$$

The choice (3.20) is by no means unique but it is particularly convenient in this context because (i) the differential operator in (3.19) commutes with the spectral function [this is a consequence of (3.13)], and (ii) Eq. (3.20) satisfies the connection (2.5) between  $G^{<}$  and the Wigner distribution function. By using (3.20) in (3.19) we obtain

$$A(\vec{p},\omega;\vec{R},T)[\partial_{T} + \vec{\nabla}_{\vec{p}}H(\vec{p},\vec{R},T)\cdot\vec{\nabla}_{\vec{R}} - \vec{\nabla}_{\vec{R}}H(\vec{p},\vec{R},T)\cdot\vec{\nabla}_{\vec{p}}]f(\vec{p},\vec{R},T) = I(G^{\leq}),$$
(3.21)

where we denoted the collision term by  $I(G^{\leq})$ .

Let us now work out the explicit form of the driving terms. One would expect to get the ordinary Boltzmann driving terms because we recognize the Hamiltonian equations of classical mechanics in (3.21) as

$$\partial_{p_i} H(\vec{p}, \vec{R}) = \dot{R}_i, \quad -\partial_{R_i} H(\vec{p}, \vec{R}) = \dot{p}_i$$
 (3.22)

Indeed, the first of Eqs. (3.22) yields the velocity, whereas the second gives the Lorentz force.<sup>10</sup> Integrating over frequency, one obtains

$$\{\partial_{T} + \vec{v} \cdot \vec{\nabla}_{\vec{R}} + [\vec{E}(\vec{R},T) + \vec{v} \times \vec{B}(\vec{R},T)] \cdot \partial_{\vec{p}}\} f(\vec{p},\vec{R},T)$$
$$= \int \frac{d\omega}{2\pi} I(G^{\leq}), \quad (3.23)$$

where

$$\vec{\mathbf{E}}(\vec{\mathbf{R}},T) = -\vec{\nabla}\phi(\vec{\mathbf{R}},T) - \frac{\partial}{\partial T}\vec{\mathbf{A}}(\vec{\mathbf{R}},T) ,$$
  
$$\vec{\mathbf{B}}(\vec{\mathbf{R}},T) = \vec{\nabla}\times\vec{\mathbf{A}}(\vec{\mathbf{R}},T) .$$
(3.24)

Some comments are now in order. We have not (until now) discussed the terms on the left-hand side of the GKB equation (2.8) which involve the self-energies. These terms may lead to important renormalization effects of the driving terms [see, e.g., Ref. 2(a)]. Furthermore, no account of interactions has been taken in the expression used for the spectral density. It will be important

#### E. Exact results versus gradient expansion

In this section we develop the techniques to extract gradient-expanded forms from the exact results derived in Sec. III B. The basic quantity we need is the gradient expansion of the time integral appearing in the exponent of (3.4) or (3.12). We find

$$\int_{T-\tau/2}^{T+\tau/2} d\bar{t} \,\epsilon(\vec{p}-\vec{A}(\bar{t})) \simeq \epsilon(\vec{p}-\vec{A}(T))\tau + O(\tau^3) \,. (3.25)$$

By substituting (3.25) in (3.12) we obtain

$$A(\vec{\mathbf{p}},\omega;\mathbf{R},T) = 2\pi\delta(\omega - \epsilon(\vec{\mathbf{p}} - \mathbf{A}(T))) + A_1 , \qquad (3.26)$$

where the correction term  $A_1$  involves Airy functions which are characteristic of the electric field. We recognize (3.26) as a special case (i.e., spatially uniform electric field represented via a vector potential) of the result (3.16) derived in the preceding section.

In the scalar potential gauge the algebra is somewhat more tedious. The first step is to rewrite the exponential in (3.7) in a form symmetric with respect to  $\vec{k}$  and  $\vec{k}$ '; with the aid of the  $\delta$  function, one derives

$$G_{r}^{\phi}(\vec{\mathbf{k}},\vec{\mathbf{k}}';t,t') = -i\Theta(t-t')\delta\left[\vec{\mathbf{k}}-\vec{\mathbf{k}}'-\int_{t'}^{t}d\vec{t}\ \vec{\mathbf{F}}(\vec{t})\right]$$
$$\times \exp\left[-i\int_{t'}^{t}d\vec{t}\ \epsilon(\vec{\mathbf{K}}_{\vec{t}})\right], \qquad (3.27)$$

where

$$\vec{\mathbf{K}}_{\vec{t}} \equiv \frac{1}{2} \left[ \vec{\mathbf{k}} + \vec{\mathbf{k}}' - \int_{\vec{t}}^{t} dt_1 \vec{\mathbf{F}}(t_1) - \int_{\vec{t}}^{t'} dt_1 \vec{\mathbf{F}}(t_1) \right].$$
(3.28)

By transforming the time variables into the Wigner coordinates and evaluating the time integrals in the spirit of (3.25) one obtains

$$\int_{t'}^{t} d\bar{t} \,\epsilon(\vec{\mathbf{K}}_{\bar{t}}) \cong \tau\epsilon(\vec{\mathbf{K}}_{T}) \cong \tau\epsilon(\frac{1}{2}(\vec{\mathbf{k}}+\vec{\mathbf{k}}')+O(\tau^{2})) \,. \tag{3.29}$$

The spectral density is given to leading order in  $\tau$  by

$$A(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; T, \tau) \cong \delta(\vec{\mathbf{k}} - \vec{\mathbf{k}}' - \vec{\mathbf{F}}(T)\tau) \exp\left[-i\tau\epsilon\left(\frac{1}{2}(\vec{\mathbf{k}} + \vec{\mathbf{k}}')\right)\right],$$
(3.30)

or, in terms of Wigner coordinates,

$$A(\vec{\mathbf{r}},\vec{\mathbf{R}};T,\tau) \cong \sum_{\vec{\mathbf{k}}} \exp\{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}+\tau[\vec{\mathbf{R}}\cdot\vec{\mathbf{F}}(T)-\epsilon(\vec{\mathbf{k}})]\}, \quad (3.31)$$

which finally yields

$$A(\vec{\mathbf{p}}, \vec{\mathbf{R}}; \omega, T) \cong 2\pi \delta(\omega - \epsilon_{\vec{\mathbf{p}}} + \vec{\mathbf{R}} \cdot \vec{\mathbf{F}}(T)) . \qquad (3.32)$$

One should keep in mind the physical equivalence of (3.16) and (3.32) as revealed by the general expression (3.16).

This concludes our discussion of the formal properties of the field-dependent free Green functions. Table I summarizes central results obtained in this section.

## IV. RLM IN AN EXTERNAL ELECTRIC FIELD—DYNAMICS

### A. Introduction

We now apply the field-dependent Green functions of the preceding section to study the high-electric-field properties of a system consisting of electrons interacting with a dilute concentration of impurities. The main objectives of this section are (i) to derive a self-energy functional, and (ii) to find expressions for  $G_{r,a}$  which can be used in the GKB equations (2.8) to construct quantum-transport equations for the RLM.

When choosing the model interaction between electrons and impurities we have kept the following considerations in mind. The main emphasis of this study is on the general structure of the nonlinear theory; however, we want to apply the techniques developed in the preceding sections to a model for which explicit, and if possible, analytic, results can be obtained. The elastic impurity problem would be a good candidate for a simple but nontrivial scattering mechanism. Its properties (at least in the lowconcentration limit) have been extensively studied and are in general well understood. However, it has the slightly complicating feature that the single-site T matrix satisfies an equation which is not analytically solvable. Instead of treating the elastic impurity problem in an approximate way (for example, in the Born approximation), we have studied the RLM for which the T-matrix equation is readily solved (see below).

Physically, the RLM [aslo known as the virtual boundstate model (VBM)] describes a localized state in a continuum: The conduction electrons make transitions between the localized level and the conduction band, thus forming a scattering resonance. By varying the parameters of the model, one can adjust the position of the scattering resonance with respect to the Fermi level, thus displaying a variety of physical phenomena. Numerous applications have been found for the RLM;<sup>11-19</sup> from our point of view, the RLM is a model of an energy-dependent 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.

The outline of this section is the following. We briefly review some of the standard results for the single-site RLM, then couple it to a static external field, and finally consider the effects of a dilute concentration of the scatterers. Some of the results of this section have been briefly discussed elsewhere.<sup>8,9</sup>

## B. Single-site results

The RLM Hamiltonian is given by

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$$H^{\text{RLM}} = \sum_{\vec{k}} \epsilon(\vec{k}) c_{\vec{k}}^{\dagger} c_{\vec{k}}$$
$$+ Eb^{\dagger}b + \sum_{\vec{k}} \left[ V(\vec{k}) c_{\vec{k}}^{\dagger} b + V^{*}(\vec{k}) b^{\dagger} c_{\vec{k}} \right].$$

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(4.1)

Equation in text		Comments
(3.7)	$\begin{aligned} G_r^{\phi}(\vec{k},\vec{k}';t,t') \\ &= -i\Theta(t-t')\delta\left[\vec{k}-\vec{k}'-\int_t^t d\vec{t} F(\vec{t})\right] \exp\left[-i\int_t^t d\vec{t} \epsilon\left[\vec{k}-\int_t^t dt_1\vec{F}(t_1)\right]\right] \end{aligned}$	Time-dependent scalar potential, $\phi = -\vec{x} \cdot \vec{F}(t)$
(3.8)	$G_{r}^{\phi}(\vec{k},\vec{k}';t,t') = -i\Theta(t-t')\delta(\vec{k}-\vec{k}'-\vec{F}(t-t'))\exp\left[-i\int_{0}^{t-t'}dt_{1}\epsilon(\vec{k}-t_{1}\vec{F})\right]$	Time-independent scalar potential, $\phi = -\vec{x} \cdot \vec{F}$
	$\begin{aligned} G_{r}^{\phi}(\vec{k},\vec{k}';\omega) \\ = -\frac{i}{F}\Theta(k_{  } - k'_{  })\delta(\vec{k}_{1} - \vec{k}_{1}', )\exp\left[\frac{i}{F}(k_{  } - k'_{  })(\omega - \frac{1}{2}k_{1}^{2} - \frac{1}{6}(k_{  }^{2} + k_{  }k'_{  } + k'_{  }^{2}))\right] \end{aligned}$	Fourier transform of (3.8)
(3.4)	$\begin{aligned} G_r^{\mathcal{A}}(\vec{k}^c,\vec{k}^{c'};t,t') \\ &= -i\Theta(t-t')\delta(\vec{k}^c-\vec{k}^{c'})\exp\left[-i\int_{t'}^{t}d\vec{t}\epsilon(\vec{k}^c-\vec{A}(\vec{t}))\right] \end{aligned}$	Time-dependent, spatially uniform vector potential, $\vec{A}(t) = -\int_0^t dt' \vec{F}(t')$
(3.12)	$A\left(\vec{\mathbf{k}}^{c},\omega,T\right) = \int_{-\infty}^{\infty} d\tau \exp\left[i\left[\omega\tau - \int_{T-\tau/2}^{T+\tau/2} d\vec{t} \epsilon(\vec{\mathbf{k}}^{c} - \vec{\mathbf{A}}(\vec{t}))\right]\right]$	Spectral density in vector potential gauge
	$A(\vec{k}^{c},\omega,T) = 2\pi\delta(\omega - \epsilon(\vec{k}^{c})) - \frac{2\pi}{i\Omega^{2}}\vec{F}(T) \cdot \frac{\partial\epsilon}{\partial\vec{k}} \left[\delta(\omega - \epsilon(\vec{k}^{c}) - \Omega/2) - \delta(\omega - \epsilon(\vec{k}^{c}) + \Omega/2)\right]$	Linear (in $\vec{F}$ ) expansion of (3.12) for harmonic electric field, $\vec{F}(t) = \vec{F}_0 \exp[-i\Omega t]$ (see Ref. 31).
(3.16)	$A\left(\vec{\mathbf{k}}^{c},\omega;\vec{\mathbf{R}},T\right)=2\pi\delta(\omega-\epsilon(\vec{\mathbf{k}}^{c}-\vec{\mathbf{A}}(\vec{\mathbf{R}},T))-\phi(\vec{\mathbf{R}},T))$	Lowest-order gradient expansion of (3.12) generalized to the spatially inhomogeneous case.

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Here  $c_{\vec{k}}$ 's refer to the conduction electrons, and b is the localized-level destruction operator. The energy E gives the position of the localized level and  $V(\vec{k})$  is the hybridization matrix element. We omit all spin indices.

The interaction (4.1) is separable; from this it follows that the Green function corresponding to (4.1) can be evaluated exactly. A straightforward equation-of-motion analysis yields

$$G(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega) = \delta_{\vec{\mathbf{k}}, \vec{\mathbf{k}}} G_0(\vec{\mathbf{k}}, \omega)$$
  
+  $G_0(\vec{\mathbf{k}}, \omega) T(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega) G_0(\vec{\mathbf{k}}', \omega) , \quad (4.2)$ 

where the single-site T matrix is given by

$$T(\vec{k}, \vec{k}'; \omega) = \frac{V(\vec{k})V(\vec{k}')}{g_0^{-1}(\omega) - M_0(\omega)} .$$
(4.3)

The free (retarded) Green functions for the conduction electrons and the localized level are given by

$$G_0(\vec{\mathbf{k}},\omega) = [\omega - \epsilon(\vec{\mathbf{k}}) + i\eta]^{-1}, \quad g_0(\omega) = (\omega - E + i\eta)^{-1},$$
(4.4)

respectively, and finally  $M_0(\omega)$  is defined by

$$M_{0}(\omega) \equiv \sum_{\vec{k}} |V(\vec{k})|^{2} G_{0}(\vec{k},\omega) .$$
(4.5)

The imaginary part of the diagonal piece of the T matrix is closely related to the scattering rate  $1/\tau(\omega)$ , and has the resonant structure

$$\frac{1}{2\tau(\omega)} = c \operatorname{Im} T = \frac{c}{\pi\rho} \frac{\Gamma^2}{(\omega - E)^2 + \Gamma^2} , \qquad (4.6)$$

where  $\Gamma = \pi \rho \langle V^2 \rangle$  is the level width, and c is the concentration of impurities. Below, we will examine the field dependence of  $\Gamma$ .

Let us now consider the effects of a uniform static electric field. The Hamiltonian acquires an additional term (we use here the scalar potential gauge; see Sec. III B),

$$U = -i\vec{\mathbf{F}} \cdot \vec{\nabla}_{\vec{\mathbf{V}}} \,. \tag{4.7}$$

The equation-of-motion analysis leading to (4.2) can be repeated, essentially unchanged, with the result

$$G(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega) = G^{\phi}(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega)$$

$$+ \sum_{\vec{q}_1, \vec{q}_2} G^{\phi}(\vec{\mathbf{k}}, \vec{\mathbf{q}}_1; \omega) T^{\phi}(\vec{\mathbf{q}}_1, \vec{\mathbf{q}}_2; \omega)$$

$$\times G^{\phi}(\vec{\mathbf{q}}_2, \vec{\mathbf{k}}'; \omega), \qquad (4.8)$$

where the field-dependent free Green function  $G^{\phi}$  is defined in (3.8), and the field-dependent T matrix is given by

$$T^{\phi}(\vec{q}_1, \vec{q}_2; \omega) = \frac{V(\vec{q}_1)V^*(\vec{q}_2)}{\omega - E - M^{\phi}(\omega)}, \qquad (4.9)$$

with

$$M^{\phi}(\omega) = \sum_{\vec{p}_1, \vec{p}_2} V^*(\vec{p}_1) G^{\phi}(\vec{p}_1, \vec{p}_2; \omega) V(\vec{p}_2) .$$
(4.10)

The field-dependent level width  $\Gamma^{\phi}(\omega)$  [i.e., the imaginary part of  $M^{\phi}(\omega)$ ] for a Gaussian model  $V(k) = V_0 \exp(-\lambda^2 k^2/2)$  ( $\lambda$  is a parameter describing the range of the interaction) is calculated as follows:

$$\Gamma^{\phi}(\omega) = \operatorname{Im} \left[ -i \int_{0}^{\infty} dt \, e^{i\omega t} \sum_{\vec{p}} V(\vec{p} - \frac{1}{2}t\vec{F}) V(\vec{p} + \frac{1}{2}t\vec{F}) \exp\{-i[\epsilon(\vec{p})t + F^{2}t^{3}/24]\} \right]$$
  
=  $-\frac{1}{2} V_{0}^{2} \rho \int_{-\infty}^{\infty} dt \int_{0}^{\infty} d\epsilon_{\vec{p}} \exp\{-i[\epsilon(\vec{p}) - \omega]t - iF^{2}t^{3}/24 - \frac{1}{4}\lambda^{2}F^{2}t^{2} - \lambda^{2}p^{2}\}$   
=  $-\Gamma(\omega) \exp(\frac{2}{3}\lambda^{6}F^{2}) \int_{-\infty}^{\alpha(F)} dx \operatorname{Ai}(-x) ,$  (4.11)

where  $\Gamma(\omega) = \pi \rho V_0^2 \exp(-2\lambda^2 \omega)$  is the zero-field level width. Here  $\alpha(F) = 2\omega/F^{2/3} - \lambda^4 F^{4/3}$ , and Ai(x) is the Airy function. A numerical evaluation of (4.11), with parameter values  $\lambda = 20$  Å and  $\omega = 0.01$  eV, yields the result shown in Fig. 1(a). We distinguish three regions: (i) lowfield regime where the level width retains approximately its zero-field value, (ii) transitional regime where the level width is a decreasing function of the electric field, and (iii) high-field regime where the level width is very small, thus indicating decoupling of the conduction electrons from the resonant level. Figure 1(b) shows these three regimes for general values of energy and electric field. The most important conclusions obtained from Fig. 1 are (i) the coupling between the conduction electrons and the resonant level [which is characterized by the level width  $\Gamma^{\phi}(\omega)$ ] vanishes for very high fields, and (ii) it approaches its zero-field value as the energy is increased. We will make use of these observations below, where we construct a field-dependent Green function including the effects of impurity scattering. Reference 8 gives a more detailed discussion on (4.11).

## C. Dilute concentration of resonant scatterers

We follow the standard procedure:<sup>20</sup> The Dyson equation for a fixed configuration of impurities is iterated and averaged term by term, and, finally, a partial infinite resummation is carried out to construct a self-energy functional. One has to bear in mind, however, that the impurity averaging takes place with the external field turned on, and that some care must be exercised when generalizing the zero-field results. Specifically, consider the Dyson equation

$$G(\vec{k},\vec{k}';\omega,\{\vec{R}_{\alpha}\}) = G^{\phi}(\vec{k},\vec{k}';\omega) + \sum_{\substack{\vec{q}_{1},\vec{q}_{2},\\ \{\vec{R}_{\alpha}\}}} G^{\phi}(\vec{k},\vec{q}_{1};\omega) \exp[-i(\vec{q}_{1}-\vec{q}_{2})\cdot\vec{R}_{\alpha}]V(\vec{q}_{1},\vec{q}_{2};\omega)G(\vec{q}_{2},\vec{k}';\omega,\{\vec{R}_{\alpha}\}), \quad (4.12)$$

where we explicitly indicate that the Green function depends on the sites of the impurity locations. In (4.12) we have introduced a generalized scattering vertex  $V(\vec{q}_1, \vec{q}_2; \omega)$  because this will allow us to treat both the RLM and the elastic impurity problem on equal footing; for RLM we have

$$V^{\text{RLM}}(\vec{q}_1, \vec{q}_2; \omega) = V(\vec{q}_1) V(\vec{q}_2) g_0(\omega) ,$$

and for the elastic impurity case

$$V^{\text{imp}}(\vec{q}_1, \vec{q}_2; \omega) = V(\vec{q}_1 - \vec{q}_2)$$

respectively. We neglect impurity-impurity correlations and calculate the averaged Green function  $\overline{G}$  with the prescription

$$\overline{G} \equiv \langle G(\{\vec{R}\}) \rangle_{av} = \prod_{\alpha} \int \frac{d^3 R_{\alpha}}{\Omega} G(\{\vec{R}_{\alpha}\}), \qquad (4.13)$$



FIG. 1 (a) Level width for a Gaussian-model interaction for  $\lambda = 20$  Å and  $\omega = 0.01$  eV. The field strengths  $F_{12}$  and  $F_{23}$  mark the transitions between low-field, transitional, and high-field regimes (see text). (b) Three regimes for general values of  $\omega$ . The line  $\omega = \omega_0$  denotes the energy which was used while constructing (a).

where  $\Omega$  is the volume of the system.

Sum now all scattering events at a given site  $\vec{R}_{\alpha}$ . This procedure replaces the matrix element V in (4.12) by the single-site T matrix

$$G(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega, \{\vec{\mathbf{R}}_{\alpha}\}) = G^{\phi}(\vec{\mathbf{k}}, \vec{\mathbf{k}}'; \omega)$$

$$+ \sum_{\vec{\mathbf{q}}_{1}, \vec{\mathbf{q}}_{2}, \atop \{\vec{\mathbf{R}}_{\alpha}\}} G^{\phi}(\vec{\mathbf{k}}, \vec{\mathbf{q}}_{1}; \omega) T^{\vec{\mathbf{R}}} \alpha(\vec{\mathbf{q}}_{1}, \vec{\mathbf{q}}_{2}; \omega)$$

$$\times G(\vec{\mathbf{q}}_{2}, \vec{\mathbf{k}}'; \omega, \{\vec{\mathbf{R}}_{\alpha}\}) . \quad (4.14)$$

The prime in the summation indicates that the  $\mathbf{R}_{\alpha}$  label is not allowed to be the same twice in succession when (4.14) is iterated because, by definition, the *T* matrix contains all scattering events at a given site. The site-dependent *T* matrix in (4.14) satisfies

$$T^{\vec{R}} (\vec{q}_{1}, \vec{q}_{2}; \omega) = e^{-i(\vec{q}_{1} - \vec{q}_{2}) \cdot \vec{R}} V(\vec{q}_{1}, \vec{q}_{2}; \omega) + \sum_{\vec{p}_{1}, \vec{p}_{2}} V(\vec{q}_{1}, \vec{p}_{1}; \omega) e^{-i(\vec{q}_{1} - \vec{p}_{1}) \cdot \vec{R}} \times G^{\phi}(\vec{p}_{1}, \vec{p}_{2}; \omega) T^{\vec{R}} (\vec{p}_{2}, \vec{q}_{2}; \omega) .$$
(4.15)

Note that the T matrix defined according to (4.15) is a functional of the free field-dependent Green function,  $T^{\vec{R}}{}_{\alpha} = T^{\vec{R}}{}_{\alpha}[G^{\phi}].$ 

We now iterate (4.14) and calculate the average term by term with (4.13). One obtains terms such as

$$\overline{G} = \cdots + \langle G^{\phi}T^{\overrightarrow{R}}{}^{\alpha}[G^{\phi}]G^{\phi}T^{\overrightarrow{R}}{}^{\beta}[G^{\phi}]G^{\phi}T^{\overrightarrow{R}}{}^{\alpha}[G^{\phi}]G^{\phi}\rangle_{av}$$

$$+ \cdots + \langle G^{\phi}T^{\overrightarrow{R}}{}^{\alpha}[G^{\phi}]G^{\phi}T^{\overrightarrow{R}}{}^{\beta}[G^{\phi}]G^{\phi}T^{\overrightarrow{R}}{}^{\gamma}[G^{\phi}]$$

$$\times G^{\phi}T^{\overrightarrow{R}}{}^{\alpha}[G^{\phi}]G^{\phi}\rangle_{av} + \cdots . \qquad (4.16)$$

When carrying out the impurity averaging, one can commute the  $\vec{R}_i$  integrals in such a way that the innermost integrals are always done first. For example, in (4.16) the  $\vec{R}_{\beta}$  (in the first term) and  $\vec{R}_{\beta}$  and  $\vec{R}_{\gamma}$  (in the second term) integrals are done first. The effect of this procedure is to build in parts of the impurity-averaged Green function as an *internal* line. It is easy to convince oneself that this part of the analysis is entirely equivalent to the standard one for vanishing external fields. The net result is that terms such as the ones in (4.16) can all be collected together by choosing a self-energy functional which equals the single-site T matrix averaged over its site label,

$$\Sigma[\overline{G}] = c \int \frac{d^3 R}{\Omega} T^{\vec{R}}[\overline{G}] . \qquad (4.17)$$

Note that the argument of the T matrix is the full impurity-averaged Green function.

The choice (4.17) does not, however, reproduce all the terms generated by iterating (4.14). Consider, for example, structures such as

$$\overline{G} = \cdots + \langle G^{\phi} T^{\overrightarrow{R}} {}^{\alpha} [G^{\phi}] G^{\phi} T^{\overrightarrow{R}} {}^{\beta} [G^{\phi}] G^{\phi} T^{\overrightarrow{R}} {}^{\alpha} [G^{\phi}]$$

$$\times G^{\phi} T^{\overrightarrow{R}} {}^{\beta} [G^{\phi}] G^{\phi} \rangle_{av} + \cdots .$$
(4.18)

These terms correspond to the so-called crossed diagrams. Conventionally, these terms are neglected due to a phase-space argument,<sup>20</sup> but it is not necessarily obvious that the argument holds in the nonequilibrium situation. However, the crossed diagrams will always lead to a contribution to the self-energy which is of second or higher order in the concentration, and we use this as a formal justification for omitting them in subsequent discussion.

The result (4.17) holds both for elastic impurity scattering and for the RLM. However, only in the RLM case is the *T*-matrix equation (4.15) explicitly solvable, and we find

$$\Sigma^{\text{RLM}}[\overline{G}] = c \int \frac{d^3 R}{\Omega} \frac{e^{-i(\vec{q}_1 - \vec{q}_2) \cdot \vec{R}} V(\vec{q}_1) V(\vec{q}_2)}{\omega - E - \overline{M}^{\vec{R}}(\omega)} , \quad (4.19)$$

where

$$\overline{M}^{\vec{\mathsf{R}}}(\omega) = \sum_{\vec{p}_1, \vec{p}_2} e^{i(\vec{p}_1 - \vec{p}_2) \cdot \vec{\mathsf{R}}} V(\vec{p}_1) \overline{G}(\vec{p}_1, \vec{p}_2; \omega) V(\vec{p}_2) .$$
(4.20)

Let us now make a connection to the equilibrium case. For vanishing external fields the impurity-averaged Green function is diagonal in its momentum labels,  $\overline{G}(\vec{p}_1, \vec{p}_2) \rightarrow \delta_{\vec{p}_1, \vec{p}_2} \overline{G}(\vec{p}_1)$ , and the  $\vec{R}$  integration in (4.19) is trivial with the result

$$\Sigma_{\text{equil}}^{\text{RLM}}[\overline{G}] = \frac{c |V(\vec{q})|^2}{\omega - E - \overline{M}(\omega)}, \qquad (4.21)$$

where

$$\overline{M}(\omega) = \sum_{\vec{k}} |V(\vec{k})|^2 \overline{G}(\vec{k},\omega) . \qquad (4.22)$$

The coherent potential approximation self-energy for the RLM (Ref. 19) reduces to (4.21) in the limit of a dilute impurity concentration.

The explicit  $\hat{R}$  dependence in the denominator of (4.19) complicates the mathematical structure considerably, and we have only been able to find an approximate, but physically motivated, solution to the self-consistent problem defined by the Dyson equation and the self-energy (4.19).

# D. Approximate solution for the field-dependent impurity-averaged Green function

We use the results obtained for equilibrium<sup>20</sup> as a guideline in constructing an approximate solution for the impurity-averaged field-dependent Green function. In equilibrium, it is found<sup>19,20</sup> that the self-consistent solution of (4.21) and (4.22) is  $\overline{M}(\omega) = -i\Gamma$ , with  $\Gamma = \pi \rho \langle V^2 \rangle$ . The crucial observation is that the same solution would have emerged even with the free Green function  $G_0(\vec{k},\omega)$ in (4.22); in other words one could equally well have used  $M_0$  (4.5) instead of  $\overline{M}$  (4.22). We use this piece of information in making our first approximation: It is assumed that  $\overline{M} \stackrel{\vec{R}}{=} (4.20)$  can be evaluated with the field-dependent free Green function  $G^{\phi}$ . The calculation is similar to the one performed in the evaluation of (4.11), and the result is

$$\overline{M}^{\vec{R}}(\omega) = i\Gamma^{\phi}(\omega + \vec{F} \cdot \vec{R}), \qquad (4.23)$$

where  $\Gamma^{\phi}$  is defined in (4.11) and we suppress the real part. Using (4.23) in the expression for the self-energy (4.19), we get the following equation for the Green function:

$$\overline{G}(k_{||},k_{||},\vec{k}_{\perp};\omega) = G^{\phi}(k_{||},k_{||},\vec{k}_{\perp};\omega) + \int_{0}^{L} \frac{dR_{||}}{L} \sum_{q_{1}^{||},q_{2}^{||}} G^{\phi}(k_{||},q_{1}^{||},\vec{k}_{\perp};\omega) \\
\times \frac{ce^{-i(q_{1}^{||}-q_{2}^{||})R_{||}}V(q_{1}^{||},\vec{k}_{\perp})V(q_{2}^{||},\vec{k}_{\perp})}{\omega - E - i\Gamma^{\phi}(\omega + FR_{||})} \overline{G}(q_{2}^{||},k_{||},\vec{k}_{\perp};\omega) .$$
(4.24)

In writing (4.24) we have defined a coordinate system where the electric field defines a parallel direction, and the two other directions are referred to as perpendicular directions.

The physical interpretation of (4.24) is the following. We imagine the charge carrier entering from a field-free region to a region of space  $0 \le R \le L$  where there is a uniform electric field.  $\overline{G}(k_{||},k'_{||};\vec{k}_{\perp};\omega)$  then describes the propagation of a charge carrier from a state  $(k_{||},\vec{k}_{\perp};\omega)$  to a state  $(k'_{||},\vec{k}_{\perp},\omega)$  under the influence of a constant electric field and the resonant interaction with impurities.

This interpretation implies that a new approximation

has been made. In the calculation of  $G^{\phi}$  it was not taken into account that the electric field extends over a finite region in space. Allowing for this would have complicated the analysis enormously and analytic progress would hardly have been possible. When writing (4.24) we assume that the boundary effects do not play an important role and that the physics is run by the "bulk" properties.

As it stands, (4.24) still seems impossible to solve analytically. However, a numerical solution may well be possible: One can evaluate the  $R_{||}$  integral once and for all and then proceed by some suitable iterative technique. Instead of pursuing this line further in the present context, we introduce yet another approximation which is motivated by our numerical experience for the field-dependent level width (4.11); see the discussion below (4.11) and especially Fig. 1. There we found that increasing the energy brings the level width closer to its zero-field value. For example, for  $F = 10^6$  V/m and  $R_{\parallel} = 100$  Å the shift in the energy argument [see (4.23)] is sufficient to reduce the level width to essentially its zero-field value. Thus only the first few scatterings have a width which significantly differs from the zero-field value. Since we are neglecting boundary effects anyway, we assume that the significant contribution to the integral in (4.24) comes from the region where the level width has relaxed to its zerofield value. In what follows, we approximate  $\Gamma^{\phi}(\omega + FR_{\parallel}) \simeq \Gamma(\omega)$ . But now a major simplification occurs: The remaining  $R_{\parallel}$  dependence is trivial, and the integration is readily performed. One obtains

$$\overline{G}(k_{||},k_{||},\vec{\mathbf{k}}_{\perp};\omega) = G^{\phi}(k_{||},k_{||},\vec{\mathbf{k}}_{\perp};\omega) + \sum_{q_{||}} G^{\phi}(k_{||},q_{||},\vec{\mathbf{k}}_{\perp};\omega) \frac{cV(q_{||},\vec{\mathbf{k}}_{\perp})^{2}}{\omega - E - i\Gamma(\omega)} \times \overline{G}(q_{||},k_{||}',\vec{\mathbf{k}}_{\perp};\omega) .$$
(4.25)

Equation (4.25) is now in a form which can be solved exactly.

Before turning to the solution of (4.25), we mention that the above approximations have resulted in a self-energy which does not depend explicitly on the external field. The functions  $G^{\phi}$  take into account the effects of the field between the collisions exactly, and to our knowledge this problem has not been treated in the literature. We will show below that the solutions of the approximate equation (4.25) in a certain sense also constitute a self-consistent solution to the *full* equations (4.19) and (4.20).

Let us now solve (4.25). Introducing a shorthand notation, we rewrite it as

$$\overline{G}(k,k') = G^{\phi}(k,k') + \sum_{q} G^{\phi}(k,q) \Sigma(q) \overline{G}(q,k') . \quad (4.26)$$

The *n*th iterate of (4.26) is

$$\overline{G}_{n}(k,k') = \left[-\frac{i}{F}\right]^{n+1} \exp\left[-\frac{i}{6F}\left[k^{3}-(k')^{3}\right] + \frac{i}{F}(\omega-\frac{1}{2}k_{\perp}^{2})(k-k')\right] \times \sum_{q_{1},\ldots,q_{n}} \Theta(k-q_{1})\cdots\Theta(q_{n}-k')\Sigma(q_{1})\cdots\Sigma(q_{n}),$$
(4.27)

where we used the time Fourier transform of (3.8) for  $G^{\phi}$  (see Table I). The  $q_i$  integrals can be manipulated to yield

$$\overline{G}(k,k') = G^{\phi}(k,k') \sum_{n=0}^{\infty} \left[ -\frac{i}{F} \right]^n I_n(k,k') , \qquad (4.28)$$

where

$$I_{n}(k,k') = \int_{k'}^{k} dq_{1} \int_{k'}^{q_{1}} dq_{2} \cdots \int_{k'}^{q_{n-1}} dq_{n} \Sigma(q_{1}) \cdots \Sigma(q_{n}) .$$
(4.29)

 $I_n(k,k')$  satisfies the boundary conditions

$$I_n(k,k) = 0, \ I_1(k,k') = \int_{k'}^{k} dq \ \Sigma(q) ,$$
 (4.30)

and the difference equation

$$\frac{dI_n(k,k')}{dk} = \Sigma(k)I_{n-1}(k,k') .$$
(4.31)

By using (4.30) and (4.31) and inductive reasoning, it is seen that  $I_n(k,k')$  is given as

$$I_n(k,k') = \frac{1}{n!} \left[ \int_{k'}^k dq \, \Sigma(q) \right]^n, \qquad (4.32)$$

and we obtain the final result

$$\overline{G}(k_{||},k_{||},\overline{k}_{\perp};\omega) = G^{\phi}(k_{||},k_{||},\overline{k}_{\perp};\omega)$$

$$\times \exp\left[-\frac{i}{F}\int_{k_{||}}^{k_{||}}dq_{||}\frac{cV(q_{||},\overline{k}_{\perp})^{2}}{\omega-E-i\Gamma(\omega)}\right].$$
(4.33)

Equation (4.33) is an important result: To our knowledge it is the first explicit solution to a fielddependent Dyson equation, and, in addition, it forms an essential ingredient for the GKB transport equations to be constructed in the next section.

## E. Consistency of the solution (4.33)

The first thing one has to check is that the solution (4.33) reduces to the correct zero-field limit as  $F \rightarrow 0$ . The limiting process is nontrivial, and one has to interpret (4.33) as a generalized function to obtain a meaningful result. In Appendix B we show that

$$\lim_{F \to 0} [\Theta(x)(1/F)e^{-\eta(x/F)}e^{i(x/F)g(x)}] = i \frac{\delta(x)}{g(x=0) + i\eta} .$$
(4.34)

Making the identifications

$$x = k_{||} - k'_{||},$$
  

$$g(x) = \omega - \frac{1}{6} [(x + k'_{||})^{2} + k'_{||}(x + k'_{||}) + k'_{||}^{2}]$$
  

$$- \frac{1}{x} \int_{k'_{||}}^{k'_{||} + x} dq_{||} \frac{cV(q_{||}, \vec{k}'_{\perp})^{2}}{\omega - E - i\Gamma(\omega)} + \frac{1}{2}k_{\perp}^{2},$$
  
(4.35)

one verifies that

$$\lim_{F \to 0} \overline{G}(k_{\parallel}, k_{\parallel}', \vec{k}_{\perp}; \omega) = \frac{\delta(\vec{k} - \vec{k}')}{\omega - \epsilon(\vec{k}) - c [V(\vec{k})]^2 / (\omega - E - i\Gamma)},$$
(4.36)

which is the correct result. Thus our approximate solution satisfies the correct boundary condition.

Let us now turn to the consistency of our solution. The result (4.33) was obtained for a self-energy which did not depent explicitly on the Green function itself [see (4.25)]. However, in constructing transport equations one needs a self-energy which is an explicit functional of the Green function. Therefore, we must now find a self-energy functional which (i) explicitly involves  $\overline{G}$ , and (ii) yields (4.33) as a self-consistent solution to the Dyson equation. We shall now show that neglecting the  $\overline{R}$  dependence of  $\overline{M}^{\overline{R}}$  [see (4.20)], i.e., using  $\overline{M}^{\overline{R}=\overline{0}}$ , leads to a self-energy which satisfies both of the above criteria. Consider now

$$\Sigma(\vec{q},\omega) = \frac{c [V(\vec{q})]^2}{\omega - E - \overline{M} \vec{R} = \vec{0}(\omega)} , \qquad (4.37)$$

where

$$\overline{M}^{\vec{R}=\vec{0}}(\omega) = \sum_{\vec{p}_1, \vec{p}_2} V(\vec{p}_1) \overline{G}(\vec{p}_1, \vec{p}_2; \omega) V(\vec{p}_2) , \quad (4.38)$$

and where  $\overline{G}$  is given by (4.33). The consistency requirements are satisfied if one can show that

$$\overline{M}^{\mathbf{R}=0}(\omega) = i\Gamma(\omega) . \tag{4.39}$$

The proof of (4.39) is a direct calculation. We consider here only the case for which the momentum dependence of the hybridization matrix element  $V(\vec{q})$  is so weak that it can be neglected, i.e., we choose  $V(\vec{q}) \simeq V_0$ . Equation (4.39) then becomes

$$\overline{M} \ \overline{R} = \vec{0}(\omega) = V_0^2 \sum_{\vec{p}_1, \vec{p}_2} \left[ -\frac{i}{F} \right] \Theta(p_1^{||} - p_2^{||}) \delta(\vec{p}_1^{||} - \vec{p}_2^{||}) \\ \times \exp\left[ -\frac{i}{6F} (p_1^{||} - p_2^{||}) (p_1^{||^2} + p_1^{||} p_2^{||} + p_2^{||^2}) - \frac{i}{F} (p_1^{||} - p_2^{||}) \left[ \frac{1}{2} p_1^{||^2} - \omega - i \frac{c}{\rho \pi} \frac{\Gamma_0^2}{(\omega - E)^2 + \Gamma_0^2} \right] \right],$$
(4.40)

where  $\Gamma_0 = -\rho \pi V_0^2$  (this sign choice corresponds to the retarded function) and we only consider the imaginary part of the self-energy. The sum in (4.40) is conveniently evaluated by defining new variables via

$$\vec{\mathbf{k}} = \vec{\mathbf{p}}_1 - \vec{\mathbf{p}}_2, \ \vec{\mathbf{Q}} = \frac{1}{2} (\vec{\mathbf{p}}_1 + \vec{\mathbf{p}}_2),$$
(4.41)

when (4.40) transforms into

$$\overline{M}^{\vec{R}=\vec{0}}(\omega) = V_0^2 \sum_{\vec{Q},k_{||}} \left[ -\frac{i}{F} \right] \Theta(k_{||}) \exp\left[ i \frac{k_{||}}{F} \left[ \omega + i \frac{c}{\rho \pi} \frac{\Gamma_0^2}{(\omega - E)^2 + \Gamma_0^2} - \epsilon(\vec{Q}) \right] - \frac{i}{24F} k_{||}^3 \right].$$

$$(4.42)$$

The calculation of the  $\vec{Q}$  sum is straightforward,

$$\sum_{\vec{Q}} \exp\left[-i\frac{k_{||}}{F}\epsilon(\vec{Q})\right] \simeq \rho \int d\epsilon(\vec{Q}) \exp\left[-i\frac{k_{||}}{F}\epsilon(\vec{Q})\right] = 2\pi\rho\delta\left[\frac{k_{||}}{F}\right], \qquad (4.43)$$

and we obtain

$$\overline{M}^{\overrightarrow{R}=\overrightarrow{0}}(\omega) = 2\pi\rho V_0^2 \sum_{k_{||}} \left[ -\frac{i}{F} \right] \delta \left[ \frac{k_{||}}{F} \right] \Theta(k_{||}) \exp \left[ -\frac{i}{24F} k_{||}^3 + \frac{i}{F} k_{||} \left[ \omega + i \frac{c}{\rho \pi} \frac{\Gamma_0^2}{(\omega - E)^2 + \Gamma_0^2} \right] \right].$$
(4.44)

In (4.44) one uses  $\Theta(x=0)=\frac{1}{2}$  and finally obtains

$$\overline{M}^{\overline{R}=\overline{0}}(\omega) = i\pi\rho V_0^2 \equiv i\Gamma_0 , \qquad (4.45)$$

which is the desired result (4.39). Thus the approximate solution (4.33) is also a self-consistent solution if one (i) suppresses the  $\vec{R}$  dependence in  $\overline{M}^{\vec{R}}$  (which seems plausible according to our numerical experience), and (ii) considers only interactions which are weakly dependent on the momentum (which is almost invariable done).

This concludes our discussion on the dynamics (single-particle properties) of the RLM in an external field; in the next section we discuss kinetic equations derived with the aid of the main results of this section.

# **V. QUANTUM KINETIC EQUATIONS FOR THE RLM**

# A. Analytic continuation of the self-energy

In the GKB kinetic equation one needs the analytic continuations  $\Sigma^{\gtrless}$  of the self-energy [cf. (2.8)]. This is achieved by repeated applications of the following "theorems."<sup>2</sup> If

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$$D(t,t') = \int dt_1 A(t,t_1) B(t_1,t') , \qquad (5.1)$$

then

$$D^{\gtrless}(t,t') = \int dt_1 [A_r(t,t_1)B^{\gtrless}(t_1,t') + A^{\gtrless}(t,t_1)B_a(t_1,t')] .$$
(5.2)

The self-energy functional of Sec. IV was

$$\Sigma(\vec{q}_{1},\vec{q}_{2};\omega) = c \int \frac{d^{3}R}{\Omega} \frac{\exp[-i(\vec{q}_{1}-\vec{q}_{2})\cdot\vec{R}]V(\vec{q}_{1})V(\vec{q}_{2})}{\omega - E - \sum_{\vec{p}_{1},\vec{p}_{2}} V(\vec{p}_{1})\vec{G}(\vec{p}_{1},\vec{p}_{2};\omega)V(\vec{p}_{2})},$$
(5.3)

and  $\Sigma^{\stackrel{>}{\leq}}$  can be obtained from (5.3) with a straightforward series expansion. The *n*th-order expansion of (5.3) reads, in time space (we suppress here all inessential variables),

$$\Sigma^{(n)}(t,t') = \int dt_1 \cdots dt_{2n} g_0(t-t_1) G(t_1-t_2) g_0(t_2-t_3) \cdots G(t_{2n-1}-t_{2n}) g_0(t_{2n}-t') .$$
(5.4)

Applying (5.2) repeatedly, one obtains

$$\Sigma^{(n)}(t,t')^{\gtrless} = \int dt_1 \cdots dt_{2n} [g_0'(t-t_1)G'(t_1-t_2)\cdots g_0^{\gtrless}(t_{2n}-t') + g_0'(t-t_1)\cdots G^{\gtrless}(t_{2n-1}-t_{2n})g_0^a(t_{2n}-t') + \cdots + g_0^{\gtrless}(t-t_1)G^a(t_1-t_2)\cdots g_0^a(t_{2n}-t')].$$
(5.5)

The series can be resummed, and the final result in  $\omega$  space is (note V's are suppressed)

$$\Sigma^{\gtrless}(\omega) = \sum_{n=0}^{\infty} \Sigma^{(n)}(\omega)^{\gtrless} = \frac{1}{g_0^{-1}(\omega) - G^r(\omega)} G^{\gtrless}(\omega) \frac{1}{g_0^{-1}(\omega - G^a(\omega))} + \frac{1}{1 - g_0(\omega)G^r(\omega)} g_0^{\gtrless}(\omega) \frac{1}{1 - g_0(\omega)G^a(\omega)} .$$
(5.6)

The second term in (5.6) vanishes because  $g_0^{-1}(\omega)g_0^{\gtrless}(\omega) \equiv 0$ . Reintroducing the momentum variables, we identify  $T^{\vec{R}}[\vec{G}_{a,r}]$  in (5.6) and have therefore obtained

$$\Sigma^{\gtrless}(\vec{q}_{1},\vec{q}_{2};\omega) = c \sum_{\vec{p}_{1},\vec{p}_{2}} \int \frac{d^{3}R}{\Omega} T^{\vec{R}}_{\vec{q}_{1},\vec{p}_{1}}[\vec{G}'] \vec{G}^{\gtrless}(\vec{p}_{1},\vec{p}_{2};\omega) T^{\vec{R}}_{\vec{p}_{1},\vec{q}_{2}}[\vec{G}''].$$
(5.7)

This is an important result: Among other things it can be used to derive a Boltzmann equation with the full T matrix rather than the Born approximation for the scattering probability, which is what the standard derivations usually lead to. We also note that the above derivation is valid for cases where the T matrix is not explicitly solvable (for example, for the elastic impurity case) and that it can be extended to the case where the Green functions depends separately on two time labels, i.e., to the case of time-dependent external fields.

## B. Quantum kinetic equations for the RLM

Using the notation of the preceding section, we can state the GKB kinetic equations for the RLM [cf. (2.8)],

$$\overline{G}_{r,a}(\vec{k},\vec{k}';\omega) = G_{r,a}^{\phi}(\vec{k},\vec{k}';\omega) + c \int \frac{d^{3}R}{\Omega} \sum_{\vec{q}_{1},\vec{q}_{2}} G^{\phi}(\vec{k},\vec{q}_{1};\omega) T_{\vec{q}_{1},\vec{q}_{2}}^{\vec{R}}[\bar{G}_{r,a}] \overline{G}_{r,a}(\vec{q}_{2},\vec{k}';\omega), \qquad (5.8a)$$

$$\left[ G^{\phi^{-1}} - \frac{1}{2}c \int \frac{d^{3}R}{\Omega} (T^{\vec{R}}[\bar{G}_{r}] + T^{\vec{R}}[\bar{G}_{a}]), G^{\gtrless} \right] - \left[ c \int \frac{d^{3}R}{\Omega} (T^{\vec{R}}[\bar{G}_{r}]G^{\gtrless}T^{\vec{R}}[\bar{G}_{a}]), \frac{1}{2}(\bar{G}_{a} + \bar{G}_{r}) \right]$$

$$= -\frac{1}{2}c \int \frac{d^{3}R}{\Omega} \{T^{\vec{R}}[\bar{G}_{r}]G^{\lhd}T^{\vec{R}}[\bar{G}_{a}], G^{\gt}\} + \frac{1}{2}c \int \frac{d^{3}R}{\Omega} \{T^{\vec{R}}[\bar{G}_{r}]G^{\gt}T^{\vec{R}}[\bar{G}_{a}], G^{<}\}. \qquad (5.8b)$$

In Eq. (5.8b) we have suppressed the intermediate position and time integrations. The extremely nonlinear character of these equations has been stressed by explicitly indicating how the various self-energy terms depend on the retarded and advanced Green functions. Equations (5.8) also clearly indicate the two-step structure inherent in all (nonlinear) nonequilibrium calculations: The expressions for the retarded and advanced Green functions are needed as an input to the kinetic equation.

In the derivation of (5.8) the only approximation made is that in the construction of the self-energy functional only terms linear in the concentration were accounted for. Other than that, Eqs. (5.8) give an exact prescription for determining the transport properties of a system consisting of noninteracting electrons coupled to a dilute concentration of resonant scatterers under the influence of an arbitrarily strong static field.

One should note, however, that in the electron-impurity system there is no mechanism to dissipate the energy fed in by the electric field. Thus if one were to use Eqs. (5.8) to determine the nonlinear current, for example, singularities may arise due to Joule heating. One should add terms to (5.8) which would allow the dissipation of the Joule heat. This could be done, for example, by coupling the system to a phonon bath. An even more ambitious approach would be to consider simultaneously the nonequilibrium phonon system as well. In our opinion the most important feature of Eqs. (5.8) is that they allow an explicit study of how the conventional impurity Boltzmann equation is modified by an arbitrarily strong electric field. To solve Eqs. (5.8) we use the approximate, but consistent, solutions for  $G^{a,r}$  obtained in the preceding section. In particular, in the expression for  $T^{\vec{R}}$  [cf. (4.17) and (4.19)],  $\overline{M}^{\vec{R}}(\omega)$  is replaced by  $i\Gamma_0$ ; see (4.45) and the discussion following it.

Consider now the terms which involve  $T[\overline{G}_{r,a}]$ . In Secs. IV D and IV E it was shown that the solutions of (5.8a), when substituted in the expression for the self-energy, lead to the simple result

$$\Gamma_{\vec{q}_{1},\vec{q}_{2}}^{\vec{R}}[\vec{G}_{r}] = \frac{V(\vec{q}_{1})V(\vec{q}_{2})\exp[-i(\vec{q}_{1}-\vec{q}_{2})\cdot\vec{R}]}{\omega - E + i\Gamma_{0}} .$$
(5.9)

 $T^{\vec{R}}[\vec{G}_a]$  is obtained from (5.9) by setting  $i\Gamma_0 \rightarrow -i\Gamma_0$ . The use of (5.9) in the self-energy part of the collision integral of (5.8b) yields

$$\Sigma^{\gtrless}(\vec{k},\vec{k}';\omega) = c \sum_{\vec{q}_{1},\vec{q}_{2}} \int \frac{d^{3}R}{\Omega} \frac{1}{(\omega-E)^{2} + \Gamma_{0}^{2}} \exp[-i(\vec{k}-\vec{q}_{1}+\vec{q}_{2}-\vec{k}')\cdot\vec{R}] V(\vec{k}) V(\vec{q}_{1}) V(\vec{q}_{2}) V(\vec{k}') G^{\gtrless}(\vec{q}_{1},\vec{q}_{2};\omega) .$$
(5.10)

We recognize in (5.10) the resonant prefactor which is reminiscent of the energy-dependent relaxation time used in the Boltzmann equation for the RLM.<sup>21</sup> The energy-dependent prefactor in (5.10) will give rise to interesting additional structure even in the Boltzmann limit, as compared to the elastic impurity problem, and we will now discuss this limit where the physics is more transparent than in the cumbersome equations (5.8) or (5.10).

# C. RLM transport equation in the limit of slow spatial and temporal variations

In order to use the gradient-expansion technique described in Sec. II, we transform the self-energy into the Wigner coordinates. After some algebra one obtains

$$\Sigma(\vec{p},\vec{R};\omega) = \frac{8c}{(\omega-E)^2 + \Gamma_0^2} \int d^3R' \sum_{\vec{q},\vec{p}'} V(\vec{p}+\vec{q})V(\vec{p}'+\vec{q})G(\vec{p}',\vec{R}')V(\vec{p}'-\vec{q})V(\vec{p}-\vec{q})\exp[2i\vec{q}\cdot(\vec{R}-\vec{R}')].$$
(5.11)

To appreciate the consequences of (5.11) let us make, once again, a connection with the more familiar elastic impurity case. The prescription of obtaining the elastic impurity result from (5.11) is to replace  $V(\vec{k})V(\vec{k}')$  by  $V(\vec{k}-\vec{k}')$  (and suppress the resonant prefactor which resulted from using the T matrix instead of the Born approximation),

$$\Sigma^{\rm imp}(\vec{p},\vec{R};\omega) = 8c \int d^3R' \sum_{\vec{q},\vec{p}} |V(\vec{p}-\vec{p}')|^2 G(\vec{p}',\vec{R}') \exp[2i\vec{q}\cdot(\vec{R}-\vec{R}')].$$
(5.12)

The  $\vec{q}$  summation can be performed to give  $\frac{1}{8}\delta(\vec{R}-\vec{R}')$ ; hence, (5.12) is identical to the conventional result (A15). There is a fundamental difference between (5.11) and (5.12): The collision integral resulting from (5.11) is *nonlocal* in the *R* variables (because the summation variable  $\vec{q}$  appears explicitly in the scattering matrix elements). To be explicit, the collision integral for the elastic impurity case is (within the gradient approximation)

$$I^{\text{imp}}[G] = -c \sum_{\vec{p}\,'} |V(\vec{p} - \vec{p}\,')|^2 [G^{<}(\vec{p}\,',\omega;\vec{R},T)G^{>}(\vec{p},\omega;\vec{R},T) - G^{>}(\vec{p}\,',\omega;\vec{R},T)G^{<}(\vec{p},\omega;\vec{R},T)], \qquad (5.13)$$

whereas for the RLM it is given by

$$I^{\text{RLM}}[G] = -\frac{8c}{(\omega - E)^2 + \Gamma^2} \int d^3R' \sum_{\vec{q}, \vec{p}'} \exp[2i\vec{q} \cdot (\vec{R} - \vec{R}')] V(\vec{p} + \vec{q}) V(\vec{p}' + \vec{q}) V(\vec{p}' - \vec{q}) V(\vec{p} - \vec{q}) \times [G^{<}(\vec{p}', \omega; \vec{R}', T)G^{>}(\vec{p}, \omega; \vec{R}, T) - G^{>}(\vec{p}', \omega; \vec{R}', T)G^{<}(\vec{p}, \omega; \vec{R}, T)].$$
(5.14)

To simplify (5.14) further (and to include the driving terms as well), we use the Ansatz (3.20) for the Green functions; the spectral density is given by (3.32). Note that it would be inconsistent to use here a spectral density which includes scattering because we are working in the lowest order in the concentration, and (5.14) already is of the first order in c. By putting all the pieces together, and specializing to the Gaussian-model interaction discussed in Sec. IV C, (5.14) reduces to

(5.15)

$$\begin{bmatrix} \vec{\nabla}_{\vec{p}} \epsilon(\vec{p}) \cdot \vec{\nabla}_{\vec{R}} + \vec{F} \cdot \vec{\nabla}_{\vec{p}} \end{bmatrix} f(\vec{p},\vec{R}) = \frac{c}{[\epsilon(\vec{p}) - \vec{F} \cdot \vec{R} - E]^2 + \Gamma_0^2} \sum_{\vec{p}'} \int d^3 R' \frac{\exp[-(\vec{R} - \vec{R}')^2/2\lambda^2]}{(2\pi\lambda^2)^{3/2}} V^2(\vec{p}) V^2(\vec{p}') \times \delta(\epsilon(\vec{p}) - \epsilon(\vec{p}') - \vec{F} \cdot (\vec{R} - \vec{R}')) [f(\vec{p},\vec{R}) - f(\vec{p}',\vec{R}')].$$

Equation (5.15) contains the following important features. (i) Nonlocality in space. This is due to the finite range of the model interaction. (ii) Field dependence in the collision integral. This is a consequence of the energydependent prefactor characteristic of the RLM. For elastic impurity scattering, no such field dependence would occur. The field-dependent energy shifts in (5.15) are easily understood if one recalls that the potential energy is position dependent as a result of the applied electric field. (iii) Equation (5.15) cannot be reduced to a relaxation-time form as is the case with the ordinary impurity Boltzmann equation. (iv) Equation (5.15) is consistent with the continuity equation only when coarse-grained over a distance several times the range of the Gaussian-model interaction. Accordingly, in the next section we consider a localized interaction for which the continuity equation is explicitly satisfied.

# D. Special case: A localized interaction

In the limit  $\lambda \rightarrow 0$ , the exponential factor in (5.15) becomes a representation of a  $\delta$  function and further simplification can be achieved. For  $\lambda \rightarrow 0$ , we have

$$[\nabla_{\vec{p}}\epsilon(\vec{p})\cdot\nabla_{\vec{R}} + F\cdot\nabla_{\vec{p}}]f(\vec{p},R)$$

$$= -\frac{cV_0^4}{[\epsilon(\vec{p}) - \vec{F}\cdot\vec{R} - E]^2 + \Gamma_0^2}$$

$$\times \sum_{\vec{p}'} \delta(\epsilon(\vec{p}) - \epsilon(\vec{p}'))[f(\vec{p},\vec{R}) - f(\vec{p}',\vec{R})].$$
(5.16)

This form is exactly the RLM Boltzmann equation, apart from the field dependence of the resonant prefactor. Equation (5.16) can be transformed into

$$\left| \vec{\nabla}_{\vec{p}} \epsilon(\vec{p}) \cdot \vec{\nabla}_{\vec{R}} + F \left| \cos\theta \frac{\partial}{\partial p} - \frac{1}{p} \sin\theta \frac{\partial}{\partial \theta} \right| \right| f(p, \theta, \vec{R})$$
$$= \frac{1}{\tau(\epsilon(\vec{p}) - \vec{F} \cdot \vec{R})} [f(p, \theta, \vec{R}) - \bar{f}(p, \vec{R})], \quad (5.17)$$

where  $\overline{f}$  is the angular average of f,

$$\bar{f}(p,\vec{\mathbf{R}}) = \int \frac{d\Omega}{4\pi} f(p,\theta,\vec{\mathbf{R}}) , \qquad (5.18)$$

and

 $\rightarrow \rightarrow$ 

$$\frac{1}{\tau(\epsilon)} = \frac{c\rho V_0^4}{(\epsilon - E)^2 + \Gamma_0^2} .$$
 (5.19)

In obtaining (5.17) we changed variables via  $\vec{p} \rightarrow (p \equiv |\vec{p}|, \theta)$  and used the constant-density-of-states

approximation.

Equation (5.17) is not a relaxation-time Boltzmann equation in the usual sense: The nonequilibrium distribution function  $f(p,\theta,\vec{R})$  relaxes towards its angular average rather than towards a local equilibrium distribution function. This point was incorrectly formulated in the recent Letter<sup>9</sup> by the present authors. The angular average  $\bar{f}$ does not relax at all: This behavior is a reflection of the lack of dissipation (i.e., no inelastic scattering mechanisms are included) in the system under study.

The lack of dissipation makes it meaningless to try to evaluate a nonlinear current from (5.17). To clarify the issue let us consider a simplified case where spatial variations can be suppressed and where the relaxation time can be viewed as a constant. In one dimension, where the variable  $\theta$  acquires only values  $\pm 1$ , (5.17) reduces to

$$F\frac{\partial}{\partial p}f(p) = -\frac{1}{2\tau}[f(p)-f(-p)]. \qquad (5.20)$$

It is not difficult to see<sup>22(a)</sup> that (5.20) has *no* solutions (apart from f = const, which is a trivial one and leads to a vanishing current), even though it does have a well-defined *linear* (in F) solution in agreement with the Boltzmann theory.

One might attempt to transform (5.17) into a more tractable form with the substitution

$$f(\vec{\mathbf{p}}) = f^{0}(\boldsymbol{\epsilon}(\vec{\mathbf{p}})) - \vec{\mathbf{F}} \cdot \vec{\mathbf{p}} \frac{\partial f^{0}(\boldsymbol{\epsilon}(\vec{\mathbf{p}}))}{\partial \boldsymbol{\epsilon}(\vec{\mathbf{p}})} \chi(\boldsymbol{\epsilon}(\vec{\mathbf{p}})) , \qquad (5.21)$$

which is very useful in ordinary Boltzmann theory. Substituting (5.21) in (5.17), one finds (we consider again only the spatially homogeneous case)

$$Fp \cos\theta - F^{2} \left[ \chi(\epsilon(\vec{p})) + p^{2} \cos^{2}\theta \frac{\partial \chi(\epsilon(\vec{p}))}{\partial \epsilon(\vec{p})} \right]$$
$$= -\frac{1}{\tau} Fp \cos\theta \chi(\epsilon(\vec{p})) . \quad (5.22)$$

However, (5.22) is a well-defined equation only in *linear* theory when the quantity in brackets can be neglected; otherwise, the  $\theta$  dependence does not cancel, which is an inconsistency because  $\chi$  is assumed to be independent of  $\theta$ . Therefore, contrary to the arguments put forward in our Letter,<sup>6</sup> it is *not* possible to transform the high-field RLM Boltzmann to a form where a local equilibrium function appears.

Arai<sup>22(b)</sup> has recently discussed a model system where the electrons scatter off from (i) elastic impurities, and (ii) phonons. The latter scattering mechanism is modeled by a relaxation-time approximation. Owing to the presence of dissipation, this model is well defined even in the nonlinear regime, and its behavior is quite interesting. However, a microscopical justification for Arai's model (in the sense of our treatment of the RLM) has not yet been given.

To summarize, the specific example of RLM must be viewed as a partial description of any realistic high-field transport situation; what we have done in Secs. IV and V is to apply the general techniques developed in Secs. II and III to give a rigorous description of an energydependent impurity scattering mechanism under highfield conditions.

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# APPENDIX A: HIGH-FIELD COLLISION INTEGRALS FOR ELECTRON-PHONON AND ELECTRON-ELASTIC IMPURITY SCATTERING

## 1. Introduction

In recent years a number of quantum-transport equations with explicitly field-dependent collision integrals have been reported. These include (i) Barker's early work based on a superoperator technique,<sup>23,24</sup> (ii) his more recent calculations with the Kadanoff-Baym formalism,<sup>7,25</sup> (iii) the extensive series of papers by Seminozhenko, Yatsenko, and collaborators (see Seminozhenko's review article<sup>26</sup> for references to original papers), and (iv) Calecki's and Pottier's<sup>6,27</sup> further developments of Levinson's<sup>5</sup> classic work. Many of the results quoted above are partially overlapping though obtained with different formalisms; the details of the calculations are, however, not always easily reconstructed, and the aim of this appendix is to present a unified, simple, and fully selfcontained derivation of what seems to be an accepted form for the high-field electron-phonon and electronelastic impurity collision integrals. Our derivation is based on the GKB formalism introduced in Sec. II of this report, and serves as an illustration of the utility of the field-dependent Green functions discussed in Sec. III.

## 2. General form of the collision integral

The form (2.6b) of the GKB quantum kinetic equation is well suited for studies where one performs a gradient expansion in the slowly varying variables. For example, the Boltzmann equation follows from (2.6b) as the lowest-order term in the gradient expansion if one discards the terms  $[\Sigma, G^{\geq}]$  and  $[\Sigma^{\geq}, G]$  on the left-hand side of (2.6b). This omission is consistent if the selfenergy contains a small parameter (the electron-phonon coupling, the impurity concentration, etc.), because in that case these terms are of second order in small quantities [see the gradient-expansion rules for commutators and anticommutators (2.9)]. In cases where one wants to retain the full time dependence, the omission is not permissible and the terms  $[\Sigma, G^{\gtrless}]$  and  $[\Sigma^{\gtrless}, G]$  must be included in the analysis. We move these two terms to the right-hand side of the GKB kinetic equation and obtain the following collision integral:

$$I[G^{\stackrel{>}{<}}] = [\Sigma, G^{\stackrel{>}{<}}] + [\Sigma^{\stackrel{>}{<}}, G] - \frac{1}{2} \{\Sigma^{<}, G^{>}\} + \frac{1}{2} \{\Sigma^{>}, G^{<}\}.$$
(A1)

For  $G^{<}$ , (A1) assumes the following explicit form:

$$I(G^{<}) = -\int_{-\infty}^{t'} d\bar{t} \Sigma^{<}(t,\bar{t})G^{>}(\bar{t},t') - \int_{-\infty}^{t} d\bar{t} G^{>}(t,\bar{t})\Sigma^{<}(\bar{t},t') + \int_{-\infty}^{t} d\bar{t} \Sigma^{>}(t,\bar{t})G^{<}(\bar{t},t') + \int_{-\infty}^{t'} d\bar{t} G^{<}(t,\bar{t})\Sigma^{>}(\bar{t},t') + \int_{t'}^{t} d\bar{t} [G^{<}(t,\bar{t})\Sigma^{<}(\bar{t},t') - \Sigma^{<}(t,\bar{t})G^{<}(\bar{t},t')] .$$
(A2)

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In the derivation of (A2) we made use of the following identities valid both for G and  $\Sigma$ :

$$A(t,t') = \frac{1}{2} [A_a(t,t') + A_r(t,t')],$$
  

$$A_a(t,t') = \Theta(t'-t) [A^{<}(t,t') - A^{>}(t,t')],$$
  

$$A_r(t,t') = \Theta(t-t') [A^{>}(t,t') - A^{<}(t,t')].$$
  
(A3)

The result recently reported by Barker [Ref. 9, Eq. (7)] contains a typographical error in which the last line of (A2) is missing. However, in the construction of the Wigner function one requires the equal time piece of  $G^{<}$  [see (2.5)], and this missing term vanishes. The equal time piece of (A2) is

$$I(G^{<}(t,t)) = -\int_{-\infty}^{t} d\bar{t}(\{\Sigma^{<}, G^{>}\} - \{\Sigma^{>}, G^{<}\}) . \quad (A4)$$

The important point to note about (A2) is that the collision integral is explicitly time dependent, and hence the Boltzmann picture with completed collisions is no longer valid. In other words, neglecting the commutator terms in

(A1) and performing the lowest-order gradient expansion amounts to making the classic Stosszahlansatz.

In the next two sections, we will work out the explicit form of (A4) for electron-phonon and electron-elastic impurity scattering.

## 3. Electron-phonon collision integral

In what follows we perform a gradient expansion in the position variables while keeping the complete time dependence in its exact form. In the evaluation of (A4) we need an expression for the electron-phonon self-energy; we choose

$$\Sigma^{\gtrless}(\vec{p},\vec{R};t,t') = \sum_{\vec{q}} |V(\vec{q})|^2 G^{\gtrless}(\vec{p}-\vec{q};\vec{R};t,t')$$
$$\times D_0^{\gtrless}(\vec{q},t-t') , \qquad (A5)$$

where we used the analytic continuation theorem for

"parallel" functions<sup>2(a)</sup> and assume, for simplicity, that the phonons are in thermal equilibrium. We make the ansatz (3.20) for the nonequilibrium electron Green function,

$$G^{<}(\vec{p},\vec{R};t,t') = iA(\vec{p},\vec{R};t,t')f(\vec{p},\vec{R};(t+t')/2),$$
(A6)  

$$G^{>}(\vec{p},\vec{R};t,t') = -iA(\vec{p},\vec{R};t,t')[1-f(\vec{p},\vec{R};(t+t')/2)],$$

where

$$A(\vec{p},\vec{R};t,t') = \exp\left[-i\int_{t'}^{t} d\vec{t}\,\epsilon(\vec{p}-\vec{A}(\vec{t}))\right]$$
(A7)

(see Sec. III C). Since we assume that the phonon matrix element  $|V(\vec{q})|^2$  is small, it is consistent to use the form

(A7) in the collision integral.

For completeness we also quote the standard expressions for the equilibrium phonon Green functions,

$$D_{0}^{>}(\vec{k},t) = \sum_{\eta=\pm 1}^{\infty} (N_{\eta\vec{k}} + \frac{1}{2}\eta + \frac{1}{2})\exp(-i\eta\omega_{k}t) ,$$
(A8)
$$D_{0}^{<}(\vec{k},t) = \sum_{\eta=\pm 1}^{\infty} (N_{-\eta\vec{k}} + \frac{1}{2}\eta + \frac{1}{2})\exp(i\eta\omega_{k}t) .$$

In (A8),  $\eta = +1$  (-1) corresponds to phonon emission (absorption), respectively.

We now substitute (A5) and (A6) in the collision integral (A4); after some simplification one obtains, using the shorthand  $f(\vec{p}) \equiv f(\vec{p}, \vec{R}; \frac{1}{2}(t+\vec{t}))$ ,

$$I[f] = -\int_{-\infty}^{t} d\bar{t} \sum_{\vec{p}\,'} |V(\vec{p}-\vec{p}\,')|^{2} f(\vec{p}\,')[1-f(\vec{p}\,)] 2 \operatorname{Re}[A(\vec{p}\,',t,\bar{t})A(\vec{p},\bar{t},t)D_{0}^{<}(\vec{p}-\vec{p}\,',t-\bar{t})] + \int_{-\infty}^{t} d\bar{t} \sum_{\vec{p}\,'} |V(\vec{p}-\vec{p}\,')|^{2} [1-f(\vec{p}\,')] f(\vec{p}\,) 2 \operatorname{Re}[A(\vec{p}\,',t,\bar{t})A(\vec{p},\bar{t},t)D_{0}^{>}(\vec{p}-\vec{p}\,',t-\bar{t})].$$
(A9)

Use of (A8) in (A9) allows us to write

$$I[f] = -\int_{-\infty}^{t} d\bar{t} \sum_{\vec{p}\,'} S^{\text{in}}(\vec{p},\vec{p}\,';t,\bar{t}) f(\vec{p}\,') [1 - f(\vec{p}\,)] + \int_{-\infty}^{t} d\bar{t} \sum_{\vec{p}\,'} S^{\text{out}}(\vec{p},\vec{p}\,';t,\bar{t}) [1 - f(\vec{p}\,')] f(\vec{p}\,) , \qquad (A10)$$

where the incoming and outgoing scattering kernels are given by

$$S^{\text{in}}(\vec{p},\vec{p}\,';t,\vec{t}) = \sum_{\substack{\vec{q},\\\eta=\pm 1}} |V(\vec{q})|^{2} \operatorname{Re}\left[\exp\left[-i\int_{\vec{t}}^{t} dt_{1}\left[\epsilon(\vec{p}\,') - \epsilon(\vec{p}) - \eta\omega_{q}\right]\right]\right] (N_{\vec{q}} + \frac{1}{2} + \frac{1}{2}\eta)\delta_{\vec{p}\,',\vec{p}\,+\eta\vec{q}},$$

$$S^{\text{out}}(\vec{p},\vec{p}\,';t,\vec{t}) = \sum_{\substack{\vec{q},\\\eta=\pm 1}} |V(\vec{q})|^{2} \operatorname{Re}\left[\exp\left[-i\int_{\vec{t}}^{t} dt_{1}\left[\epsilon(\vec{p}\,') - \epsilon(\vec{p}) + \eta\omega_{q}\right]\right]\right] (N_{\vec{q}} + \frac{1}{2} + \frac{1}{2}\eta)\delta_{\vec{p}\,',\eta\vec{q},\vec{p}},$$
(A11)

respectively, and where

$$\vec{\tilde{p}} = \vec{p} - \vec{A}(t_1)$$
,  $\vec{\tilde{p}}' = \vec{p}' - \vec{A}(t_1)$ . (A12)

We note that the scattering kernels satisfy  $S^{\text{in}}(\vec{p}, \vec{p}'; t, t) = S^{\text{out}}(\vec{p}', \vec{p}; t, t)$ .

It is interesting to compare our result to those obtained in the literature. In Refs. 7 and 23-25, the external field is turned on at the time t = 0, and the time integrals in expressions analogous to (A10) run from 0 to t. This appears very natural; before the external field is turned on the system is in thermal equilibrium and the collision integral should vanish. It is, therefore, an important consistency check to verify that our results meet this requirement. In equilibrium the distribution functions do not depend on time, and for *any* time  $t_0$  before t = 0 the time integrals reduce to the form

$$J(t_0) = \int_{-\infty}^{t_0} d\bar{t} \cos\{(\bar{t} - t_0)[\epsilon(\vec{p}') - \epsilon(\vec{p}) + \eta \omega_q]\} \times e^{(\bar{t} - t_0)\delta}, \qquad (A13)$$

where we inserted a factor  $\exp[(t - t_0)\delta]$ ,  $\delta \rightarrow 0$ , to ensure convergence. Equation (A13) is readily evaluated as

$$J(t_0) = \pi \delta(\epsilon(\vec{p}) - \epsilon(\vec{p}') + \eta \omega_q) . \qquad (A14)$$

Thus when the external fields are turned off we recover

the conventional energy-conserving  $\delta$  function and the collision integral vanishes by the same argument as in ordinary Boltzmann theory.

On comparing our results with Barker's results,<sup>7,24</sup> we find a discrepancy in the time arguments of the Wigner functions: We have  $\frac{1}{2}(t+\overline{t})$ , whereas Barker has  $\overline{t}$ . Elsewhere in the literature, Calecki and Pottier<sup>6,27</sup> agree with Barker, whereas Seminozhenko's and Yatsenko's<sup>26</sup> results coincide with ours. In practice, this difference may not be very significant because the time dependence of the scattering kernel S(t,t') dominates that of the slowly varying Wigner function and one may well approximate  $f(\frac{1}{2}(t+\bar{t})) \simeq f(\bar{t})$ . Theoretically, it would be interesting to understand the origin of this difference. While we cannot offer a definite explanation of this point, we speculate that it arises from the nonuniqueness of the Wigner function: It is possible to construct several different "distribution" functions from the density matrix which satisfy the same relations to expectation values as our choice (2.5). Also our specific Ansatz (A6) for  $G^{\stackrel{>}{<}}$  may play a role in

this curious phenomenon. We refer the reader to Ref. 28 for a further discussion on the different representations of the Wigner function.

Finally, the scattering kernel reported by Barker<sup>7,23,24</sup> contains an exponential damping term  $\exp[(t-t)/\tau]$ ,

where  $1/\tau$  represents the "joint collision broadening of states  $\vec{p}, \vec{p}'$  against all scattering processes." In the next section we give an explicit derivation of such a damping term.

## 4. Electron-elastic impurity collision term

In the dilute concentration limit we may use the Born approximation to the self-energy

$$\Sigma^{\gtrless}(\vec{p},\vec{R};t,t') = c \int \frac{d^3p'}{(2\pi)^3} |V(\vec{p}-\vec{p}')|^2 G^{\gtrless}(\vec{p}';t,t') .$$
(A15)

The self-energy (A15) leads to the following collision integral:

$$I(f) = \int_{-\infty}^{t} d\bar{t} \int \frac{d^{3}p'}{(2\pi)^{3}} c |V(\vec{p} - \vec{p}')|^{2} [A(\vec{p}', t, \bar{t})A(\vec{p}, \bar{t}, t) + A(\vec{p}, t, \bar{t})A(\vec{p}', \bar{t}, t)] [f(\vec{p}, \frac{1}{2}(t + \bar{t})) - f(\vec{p}', \frac{1}{2}(t + \bar{t}))]$$
  
$$= \int_{-\infty}^{t} d\bar{t} \int \frac{d^{3}p'}{(2\pi)^{3}} |V(\vec{p} - \vec{p}')|^{2} 2 \cos \left[ \int_{\bar{t}}^{t} dt_{1} [\epsilon(\vec{p} - \vec{A}(t_{1})) - \epsilon(\vec{p}' - \vec{A}(t_{1}))] \right]$$
  
$$\times [f(\vec{p}, \frac{1}{2}(t + \bar{t})) - f(\vec{p}', \frac{1}{2}(t + \bar{t}))].$$
(A16)

Equation (A16) is analyzed in detail in Seminozheko's review article.<sup>26</sup> For dc fields and in the limit of large times, the field dependence of the collision integral (A16) can be analyzed in terms of Fresnel integrals.<sup>26,29</sup>

Let us now turn to the evaluation of the damping term  $\exp[(t-\bar{t})/\tau]$  mentioned in the preceding section. Clearly, this additional term must arise from the spectral functions. In other words, one has to solve the Dyson equations for the retarded and advanced Green functions including impurity scattering, and then construct the spectral function according to the prescription  $A = -i(G_a - G_r)$ . For the impurity problem, the Dyson equation reads

$$G(\vec{\mathbf{p}},t,t') = G^{A}(\vec{\mathbf{p}},t,t') + \int dt_{1}dt_{2}G^{A}(\vec{\mathbf{p}},t,t_{1})$$

$$\times \Sigma(\vec{\mathbf{p}},t_{1},t_{2})G(\vec{\mathbf{p}},t_{2},t'),$$
(A17)

where we use the field-dependent Green function in vector potential gauge (3.4) and make use of the fact that since we are dealing with a uniform system all quantities are independent of  $\vec{R}$ . Finally, the self-energy is given by (A15).

As it stands, (A17) is a nonlinear integral equation (because  $\Sigma$  involves G) and its exact solution seems difficult. However, in *equilibrium* the solution of (A17) is well known (see, for example, Ref. 20) and it leads to the following self-consistently determined self-energy:

$$\Sigma_{r,a}^{\text{equil}}(\vec{\mathbf{p}},t,t') = \mp \frac{i}{2\tau} \delta(t-t') , \qquad (A18)$$

where

$$1/\tau = c \pi \rho \langle V^2 \rangle . \tag{A19}$$

In (A19),  $\rho$  is the free-electron density of states at the Fermi surface and the angular brackets stand for an angular average. We now assume that (A18) *also* holds in the nonequilibrium situation. This assumption can be characterized by saying that instead of the normal elastic impurity problem one considers the so-called Gaussian whitenoise problem (GWN). GWN has recently been studied extensively by Hänsch and Mahan.<sup>30</sup> The explicit solution of (A17) with the assumption (A18) is a straightforward calculation. Consider, for example, the first iterate of (A17). For definiteness, let us first calculate the retarded function. One finds

$$G_{r}^{1}(\vec{p},t,t') = -\frac{i}{2\tau} \int_{-\infty}^{\infty} dt_{1} G_{r}^{\vec{A}}(\vec{p},t,t_{1}) G_{r}^{\vec{A}}(\vec{p},t_{1},t')$$
$$= -\frac{t-t'}{2\tau} G_{r}^{\vec{A}}(\vec{p},t,t') .$$
(A20)

The iteration can easily be repeated and the resulting series summed to give

$$G_r(\vec{\mathbf{p}},t,t') = G_r^{\vec{\mathbf{A}}}(\vec{\mathbf{p}},t,t') \exp\left[-\frac{t-t'}{2\tau}\right].$$
(A21)

A similar calculation for  $G_a$  yields

$$G_{a}(\vec{\mathbf{p}},t,t,') = G_{a}^{\vec{\mathbf{A}}}(\vec{\mathbf{p}},t,t') \exp\left[-\frac{t'-t}{2\tau}\right], \qquad (A22)$$

and one finally obtains the spectral function

$$A(\vec{p},t,t,') = \exp\left[-i\int_{t'}^{t} dt_1 \epsilon(\vec{p} - \vec{A}(t_1))\right]$$
$$\times \exp\left[-\frac{|t-t'|}{2\tau}\right].$$
(A23)

The use of (A23) in the collision (A4) leads to an exponential damping term as introduced by Barker.<sup>7,23,24</sup> One may also include a finite width in the phonon Green functions (A8); a straightforward calculation then leads to the "joint width"

$$\frac{1}{\tau_{\rm eff}} = \frac{1}{\tau} + \frac{1}{\tau_{\rm ph}}$$

in the exponential damping term. It should be noted, however, that the above solution depends crucially on the assumption (A18) made on the self-energy. In the main body of the text, we perform a similar calculation for the **RLM** with less restrictive assumptions (see discussion in Sec. IV D).

#### THEORY OF HIGH-ELECTRIC-FIELD QUANTUM TRANSPORT ...

# APPENDIX B: ZERO-FIELD LIMITS OF FIELD-DEPENDENT GREEN FUNCTIONS

The frequency representations of the free field-dependent Green function (3.8) and the Green function of Sec. IV D are formally divergent in the limit  $F \rightarrow 0$ . We show now how the correct zero-field limit can be obtained if these functions are interpreted in the distribution sense.

Consider a generalized function D(x) defined as

$$D(x) = \lim_{F \to 0} \left[ \Theta(x) \frac{1}{F} e^{-\eta(x/F)} e^{i(x/F)g(x)} \right], \quad (B1)$$

where  $\eta$  is a positive infinitesimal. We want to show that

$$D(x) = i \frac{\delta(x)}{g(x=0) + i\eta} .$$
 (B2)

Consider now the effect of D(x) on a suitable test function f(x),

$$d \equiv \int_{-\infty}^{\infty} dx \, D(x) f(x) \,. \tag{B3}$$

If we can show that

$$d = i \frac{f(0)}{g(0) + i\eta}$$
, (B4)

the proof is complete. The proof proceeds by a direct calculation:

$$d = \lim_{F \to 0} \int_0^\infty dx \, \frac{1}{F} e^{-\eta(x/F)} e^{i(x/F)g(x)} f(x)$$
$$= \lim_{F \to 0} \left[ \left( \frac{e^{-\eta t + itg(Ft)} f(Ft)}{-\eta + ig(Ft) + itFg'(Ft)} \right)_0^\infty - \int_0^\infty dt \, e^{-\eta t + itg(Ft)} \frac{\partial}{\partial t} \left( \frac{f(Ft)}{-\eta + ig(Ft) + itFg'(Ft)} \right) \right]. \tag{B5}$$

Upon arriving at the second line of (B5) we changed the variables via x/F = t and integrated by parts. The first term in (B5) leads to the desired final result (B4) and the second term vanishes, which can be seen by the following reasoning: Consider the derivative of the term in the square brackets. The differentiation produces a multipli-

- cative factor of F which can be moved outside the integral. The remaining integral is convergent [note the importance of the convergence factor  $\exp(-\eta t)$ ], and hence a zero net result is obtained as the external field tends to zero. This completes the proof of (B2).
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$$\frac{1}{i} [G^{0^{-1}} - U - \Sigma, G^{\gtrless}] - \frac{1}{i} [\Sigma^{\gtrless}, G]$$
  
=  $-\{\Sigma^{\gtrless}, G^{\gtrless}\}/2 + \{\Sigma^{\gtrless}, G^{\gtrless}\}/2$ .

If one now replaces  $G^{<} \rightarrow iG^{<}$  and  $G^{>} \rightarrow -iG^{>}$ , (2.56) follows.

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$$\dot{\vec{v}} = \frac{d}{dT} (\vec{p} - \vec{A}(\vec{R}, T)) = -\vec{\nabla}_{\vec{R}} H(\vec{p}, \vec{R}, T)$$
$$-\frac{\partial \vec{A}}{\partial T} - \vec{v} \cdot \vec{\nabla}_{\vec{R}} \vec{A}(\vec{R}, T)$$

In calculating the gradient, the vector identity

$$\frac{1}{2} \nabla (\vec{u}^2) = \vec{u} \times (\nabla \times \vec{u}) + (\vec{u} \cdot \nabla) \vec{u}$$

is useful.

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