Generalized Kadanoff-Baym ansatz for deriving quantum transport equations

P. Lipavský, V. Špička, and B. Velický

Institute of Physics, Czechoslovak Academy of Sciences, Na Slovance 2, 18040 Prague 8, Czechoslovakia

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A systematic and unambiguous method of deriving generalized transport equations, i.e., equations for distribution functions having a single-time structure, on the basis of the nonequilibrium Green function is obtained, if the common Kadanoff-Baym (KB) ansatz is replaced by a modification which we call the generalized KB ansatz. This new ansatz is fully consistent with the dynamical structure of the theory and is independent of any specific representation. The resulting equations appear to be the zeroth-order approximation of a systematic expansion in terms of the collision duration. In the case of the electron transport in a strong homogeneous electric field, the generalized ansatz is shown to be in agreement with the superoperator methods, whereas the KB ansatz is known to fail in this case.

I. INTRODUCTION

A productive approach to the theory of transport phenomena is to view it as a superstructure built above the theory of equilibrium many-particle systems. Already in the early times of applying the quantum field methods to many-body systems, systematic approximation methods, well tested for thermal equilibrium, were used in the theory of transport.

This development, which began in the early 1960's, followed two parallel lines. One of these is based on a generalization of the Matsubara thermodynamic Green functions¹ to nonequilibrium, which is usually identified as the Kadanoff-Baym (KB) method.² The formal clumsiness of the KB formalism was later alleviated by Langreth and Wilkins,³ who reformulated this approach in a simple, very general, algebraic language. This approach is usually termed the generalized Kadanoff-Baym (GKB) formalism.⁴ The alternative theory started from the Bogolyubov real-time Green functions, well known from the Zubarev review,⁵ where a complete set of anticommutator Green functions (GF) was introduced well before it was by Langreth and Wilkins. A corresponding systematic method for deriving approximations based on generalized Feynman diagrams was discovered by Keldysh.⁶ The Keldysh and the GKB formalisms are strictly equivalent; the GKB method is easier for practical applications, however, and this article is based on it.

On a general level, the field theory of nonequilibrium systems achieved its principal goals. The equations for double-time quantities were cast into an algebraic form with simple structure, and they formed a basis for generation of complete equation systems for observable quantities starting from self-consistent diagrammatic expansions. Direct applications to the transport have been rare, because an actual solution of the equations for doubletime correlation functions is extremely demanding.

Nevertheless, the theory proved to be very useful as a starting point for finding transport equations for singletime functions, that is, equations having a structure close to the generalized master equations (GME's) of the projection superoperator methods.^{7,8} The standard way of generating single-time equations within the GF method became an approximate construction proposed by Kadanoff and Baym (KB ansatz). This ansatz is intuitively appealing and easily leads to usable equations. Practically all treatments of transport by the field methods have made use of the KB ansatz or of its equivalent. Nevertheless, the KB ansatz has several important limitations connected with its intuitive background. First, the KB ansatz is bound with the standard Wigner representation and its validity is limited to quasiclassical disturbances of homogeneous systems. More significantly, the KB ansatz enters the structure of the field theory as an alien element, whose utilization breaks up the systematic GF machinery. This hinders the establishment of a criterion of applicability of the KB ansatz, and, still more, its generalization. This contrasts unfavorably with the superoperator techniques, which are usually also employed only to generate the lowest-order approximations for the GME's, but, in principle, could yield results to all orders.

In this paper, the main emphasis will be concentrated on such a generalization of the Kadanoff-Baym construction, to be termed in the rest of the paper the GKB ansatz, which will overcome the difficulties described and will be formally consistent with the GKB formalism. For convenience, Sec. II will be devoted to a summary of this formalism, that is, the KB formalism in the Langreth-Wilkins (LW) dialect. The convenient formal structure of the technique and its immediate connection with the standard equilibrium theory of solids are reviewed in Sec. II A. Furthermore, the structure of the theory is very suggestive for deriving the generalized transport equations as described in Sec. II B. This is followed by an analysis of the KB ansatz in Sec. II C.

Section III is devoted to the derivation and an analysis of the GKB ansatz. In Sec. III A the idea of the GKB ansatz is defined, and several natural physical and formal requirements are listed. Then, in Sec. III B, the GKB ansatz is developed from these requirements, and is shown to be the zeroth-order approximation in the expansion of the correlation functions in terms of the collision duration time. In Sec. III C, the whole expansion is obtained from

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a formally closed equation of motion for the correlation functions. Thus, in agreement with the superprojection theories, the GKB ansatz can be extended to an arbitrary order.

The use of the GKB ansatz is documented in Sec. IV for electron high-field transport in the presence of weak This is the simplest step beyond the scattering. Boltzmann equation, in which an interference between the field and the scattering should manifest itself. The choice of the ansatz thus becomes nontrivial. This problem has been previously treated by the superprojection methods,⁹ and by the GF methods employing the standard KB ansatz.⁴ The results of the two approaches do not agree. The sources of the discrepancy can be traced to the quasiclassical character of the KB ansatz, with which one cannot grasp adequately the gradient corrections. By contrast, the GKB ansatz is nonperturbative in the external field and reproduces the result of the superprojection treatment in full.

II. GREEN FUNCTION APPROACH TO TRANSPORT

A. GKB formalism

First, in this section, the formal framework to be used later is specified. Second, the GKB machinery is given an interpretation, which makes it a powerful heuristic tool for the transport theory.

Consider a system whose initial state ρ was established by contact with a bath up to a time t_0 in a distant past. In the Heisenberg picture, with respect to t_0 and a oneelectron basis labeled by v, the field operator of the electron field will be written as $\psi(t,v)$. We shall also use the notation $(t_1,v_1)\equiv 1$, etc. The full physical information on the one-particle excitations is contained in two correlation functions, $g^{<}$ and $g^{>}$, related, respectively, to the electrons and the holes,

$$g^{<}(1,2) = \operatorname{Tr}[\rho \psi^{\dagger}(2)\psi(1)],$$
 (1)

$$g^{>}(1,2) = \operatorname{Tr}[\rho\psi(1)\psi^{\mathsf{T}}(2)]$$
 (2)

The physical meaning of $g^{<},g^{>}$ is twofold. For equal times, $t_1 = t_2 = t$, (1) and (2) reduce to the one-particle density matrices

$$\rho^{\leq}(t;v_1,v_2) = g^{\leq}(t,v_1;t,v_2) .$$
(3)

Thus, the "time diagonal" $t_1 = t_2$ provides the statistical information on the system, and $\rho^<, \rho^>$ are enough to specify mean values of all one-electron observables. In addition, the full double-time $g^<, g^>$ also contain the dynamical information on the evolution of the one-particle excitations of both types. The double-time struc-

ture of $g^{<},g^{>}$ is essential for developing the full set of equations of motion. Such a set consists of formal equations of motion for $g^{<},g^{>}$ and of a prescription for constructing the self-energy terms appearing in these equations. The KB method solves the double task by extending the concept of the Matsubara temperature Green functions from equilibrium also to arbitrary external fields (analytical in the lower complex time half plane).

The Matsubara GF obeys the causal boundary condition,

$$G(1,2) = -i \operatorname{Tr}[T\rho\psi(1)\psi^{\dagger}(2)], \qquad (4)$$

where the chronological operator T acts along a path connecting the points t_0 and $t_0 - i\beta$, where β is the reciprocal temperature of the bath. Originally, the ordering was along the straight line joining t_0 and $t_0 - i\beta$, but the analytical structure of G allows one to deform this path to a curve, preserving the order of the imaginary parts of the times involved, but coming arbitrarily close to the real axis. Of the useful choices, the Keldysh trajectory extends to infinity and back, while the Kadanoff-Baym path possesses two protuberances to the times t_1 and t_2 , folded according to the order of $Im(t_1)$ and $Im(t_2)$. The realtime functions $g^{<}$ and $g^{>}$ are thus obtained as an analytical continuation of the related part of G to the real-time axis. The causal structure of G permits one to develop the perturbation series for it by standard means, like the functional derivatives, or diagrams. This perturbation series can be continued to the real axis term by term, and this yields the desired perturbation expansion for the selfenergy terms. This completes the KB level.

As a last step, we write down the Dyson equation,

$$G = G_0 + G_0 \Sigma G \quad . \tag{5}$$

The formal multiplications mean matrix multiplication plus integration along the time trajectory. The free GF, G_0 , is conveniently chosen to incorporate the free Hamiltonian H_0 , and nonperturbatively, the external field Uand all mean-field (i.e., time-diagonal and Hermitian) terms of the self-energy combining with U to U_{eff} ,

$$G_0^{-1}(1,2) = \left[\delta(v_1 - v_2) i \frac{\partial}{\partial t_1} - H_0(v_1, v_2) - U_{\text{eff}}(t_1, v_1, v_2) \right] \delta(t_1 - t_2) .$$
(6)

To introduce the LW rules as the basis of the GKB formalism, we write down the analytical continuation of a product of two causal functions,

$$Z(t_1, t_2) = \int_{t_0}^{t_0 - i\beta} d\,\overline{t}\, X(t_1, \overline{t})\, Y(\overline{t}, t_2) \,. \tag{7}$$

The electronlike part for t_1, t_2 on the real axis becomes

$$iz^{<}(t_{1},t_{2}) = \int_{t_{0}}^{t_{1}} d\,\overline{t}\,x^{>}(t_{1},\overline{t})y^{<}(\overline{t},t_{2}) - \int_{t_{1}}^{t_{0}} d\,\overline{t}\,x^{<}(t_{1},\overline{t})y^{<}(\overline{t},t_{2}) - \int_{t_{0}}^{t_{2}} d\,\overline{t}\,x^{<}(t_{1},\overline{t})y^{<}(\overline{t},t_{2}) + \int_{t_{0}}^{t_{0}-i\beta} d\,\overline{t}\,x^{<}(t_{1},\overline{t})y^{>}(\overline{t},t_{2}) .$$

$$(8)$$

This type of expression has two formal disadvantages. It contains a number of integrals over various ranges, and the integrals involve all possible products of $x \leq \text{and } y \leq$. The clumsiness of such expressions would increase with each additional factor. Of the numerous integrals, only the last can be suppressed by the limit $t_0 \rightarrow -\infty$, in which it vanishes due to the Bogolyubov principle of asymptotic vanishing of correlations.¹⁰ In that limit, a substantial formal simplification can be achieved by introducing the anticommutator real-time GF,

$$X_{R}(t_{1},t_{2}) = -i\Theta(t_{1}-t_{2})[x^{>}(t_{1},t_{2})+x^{<}(t_{1},t_{2})], \qquad (9)$$

$$X_{A}(t_{1},t_{2}) = i\Theta(t_{2}-t_{1})[x^{>}(t_{1},t_{2})+x^{<}(t_{1},t_{2})].$$
(10)

With these definitions, the time integrations in (8) extend from $-\infty$ to ∞ and can be understood as a part of a formal (matrix) multiplication. Thus,

$$z^{<} = X_R y^{<} + x^{<} Y_A \quad (11)$$

This is the first of the Langreth-Wilkins (LW) rules. The remaining three read as follows:

$$z^{>} = X_R y^{>} + x^{>} Y_A$$
, (12)

$$Z_R = X_R Y_R , \qquad (13)$$

$$Z_A = X_A Y_A . (14)$$

These rules generate a complete algebra by which an analytical continuation of an arbitrary product of causal functions in the complex-time domain can be continued to the real-time axis in an unambiguous and completely mechanical manner. Of the four quantities $x^{<}$, $x^{>}$, X_R , and X_A , only two are independent. The connecting identities are

$$X_{R}(t_{1},t_{2}) = X_{A}^{\mathsf{T}}(t_{2},t_{1}) , \qquad (15)$$

$$i(X_R - X_A) = x^{>} + x^{<}$$
 (16)

These identities are important for checking the physical consistency of approximations, as well as for rearranging equations (for example, expressing them entirely in terms of $g^{<}$ and $g^{>}$).

This section will be concluded by several comments on the LW rules. These have several formal advantages.

(a) The chain rule resulting from the LW rules permits one to continue analytically a product of any number of causal factors.

(b) In the product chain of the GF, the correlation functions appear only once. That means that the equations for correlation functions necessarily have the character of linear superoperator equations provided the propagators G^A and G^R are known.

(c) In particular, the LW rules separate the electron and the hole correlation functions—in distinction to both the original KB and the Keldysh formalism. The form of the equations is identical for both $g^{<}$ and $g^{>}$.

(d) The LW rules are representationless.

(e) G^R and G^A have, over $g^<$ and $g^>$, the advantage of having a specified boundary condition (retarded or advanced), which is crucial for constructing the equations of motion and for the spectral structure.

The expressions structured according to the LW rules

can be given a suggestive interpretation, important for the transport equations. It reads as follows.

(a) Separation of quasiparticle statistics and dynamics: The LW rules separate to the maximum extent the quasiparticle propagation described by the retarded and advanced quantities⁵ from the particle statistical distribution reflected explicitly by the correlation functions.

(b) Causal structure: The invariable order of factors retarded, correlation, advanced—reflects explicitly the causality of the evolution of the correlation functions. In addition, the time integrations select by themselves the limits specified by the causality requirements.

B. Quantum transport equations

A prototype transport equation is the Boltzmann equation, which describes the time evolution of the singleparticle distribution function f,

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$$\frac{\partial}{\partial t}f(t) = \left|\frac{\partial}{\partial t}f(t)\right|_{\text{drift}} = [f(t)]_{\text{backscattering}} - [f(t)]_{\text{direct scattering}}, \quad (17)$$

The left-hand side (lhs) of (17) corresponds to the drifting of free particles with the Hamiltonian $H_0 + U_{eff}$. The right-hand side (rhs) contains the scattering terms. In particular, the back scattering has an integral character and, as a rule, is a nonlinear function of f. The parameters of this functional dependence are the differential scattering cross sections, which, with respect to the Boltzmann equation, represent input parameters independent of the external fields. The drift, as well as the scattering, depend only on the instantaneous values of the distribution function. The evolution described by such an equation is strictly Markovian.

To derive such equations by means of any of number of methods, it is necessary to assume the scattering to be weak in the sense of a low collision frequency, and the external fields moderately strong and, in particular, smooth in time and space. With these assumptions, a physically significant time interval exists, in which the equation of the type (17) holds true.¹¹

The Boltzmann equation can be generalized to a quantum transport equation for the time evolution of the single-particle density matrix (3) by relaxing some of the requirements on the physical processes in the system. This will lead to various corresponding types of quantum coherence. For example, for an increased frequency of collisions, these will not be mutually incoherent. In Sec. IV we shall treat the case of strong fields, which is manifested by the coherence of the external field and of the collisions. Such quantum coherence will render the Markov approximation invalid. In other words, the collision term will have some memory. The locality in time is generalized to a causal dependence of the collision term on $\rho^{<}$ for all preceding times,

$$\frac{\partial}{\partial T}\rho^{<}(T) - \left| \frac{\partial}{\partial T}\rho^{<}(T) \right|_{\text{drift}} = \int_{-\infty}^{T} d\,\overline{t} [\rho^{<}(\overline{t})]_{\text{backscattering}} - \int_{-\infty}^{T} d\,\overline{t} [\rho^{<}(\overline{t})]_{\text{direct scattering}}.$$
(18)

Kadanoff and Baym proposed a method for the transition from the field formalism to the quantum transport equations. Their approach will now be described in paraphrase suitable for further modifications and extensions.

The Dyson equation (5), when continued analytically to the real-time axis, becomes a set of two couples of equivalent equations. The first pair has the form of the Dyson equations for retarded and advanced quantities,

$$G_{R,A} = G_{R,A}^0 + G_{R,A}^0 \Sigma_{R,A} G_{R,A} .$$
⁽¹⁹⁾

The key relations for $g^{<}$ or $g^{>}$ can be formally cast into an explicit integral form, ^{12,13}

$$g^{\varsigma} = G_R \sigma^{\varsigma} G_A + (1 + G_R \Sigma_R) g_0^{\varsigma} (1 + \Sigma_A G_A) . \qquad (20)$$

In relations (19) and (20), the G^0 plays the role of the boundary condition specifying G as a functional of the external field at fixed initial statistical conditions. The Dyson equations (19) are apparently independent from (20). In fact, these equations are independent only exceptionally. In general, the full self-energy having four parts—retarded, advanced, and two correlation—is a functional of the full Green function also having four such parts. This functional interrelation specifies the internal dynamics of the system, and, at the same time, mediates the coupling of the quasiparticle propagation (19) with the evolution of the distribution function (20).

To obtain universal dynamic equations, freed from the boundary conditions, we shall bring (20) to a differential form. This is possible in two ways:

$$G_R^{-1}g^{\S} = \sigma^{\S}G_A , \qquad (21)$$

$$g^{\varsigma}G_A^{-1} = G_R \sigma^{\varsigma} . \tag{22}$$

The free GF disappeared because of the obvious identities,

$$G_0^{-1}g_0^{\leq} = 0 , \qquad (23)$$

$$g_0^{\leq} G_0^{-1} = 0 . (24)$$

A more meaningful set of equations is obtained by adding and subtracting Eqs. (21) and (22). In particular, the subtraction yields the GKB equation,

$$-i(G_{R}^{-1}g^{<}-g^{<}G_{A}^{-1})=i(G_{R}\sigma^{<}-\sigma^{<}G_{A}), \qquad (25)$$

a double-time precursor of transport equations. The "Liouvillian" on the lhs describes a nonunitary propagation of quasiparticles including renormalizations and damping; the rhs compensates for the successive dying out of quasiparticles and thus has the meaning of a generalized backscattering.

The evolution of the density matrices ρ^{\leq} follows from (25), if $G_{R,A}^{-1}$ are replaced by $G_0^{-1} - \Sigma_{R,A}$ from the Dyson equation, all quantities are reduced to g^{\leq} and σ^{\leq} using the definition identities (9) and (10); finally, the two times are set equal, $t_1 = t_2 = T$. The result is

$$-i\left[G_{0}^{-1},\rho^{<}\right](T) = \int_{-\infty}^{T} d\,\overline{t}\left[\sigma^{>}(T,\overline{t})g^{<}(\overline{t},T) + g^{<}(T,\overline{t})\sigma^{>}(\overline{t},T)\right] - \int_{-\infty}^{T} d\,\overline{t}\left[\sigma^{<}(T,\overline{t})g^{>}(\overline{t},T) + g^{>}(T,\overline{t})\sigma^{<}(\overline{t},T)\right] \,. \tag{26}$$

This identity⁴ will be called the GBE, although it cannot be considered an equation for $\rho^{<}$, because it is not closed.

The lhs of (26) has precisely the meaning of a timediagonal drift in the mean field. On the right-hand side, by contrast, the double-time structure is still preserved and essential, because the correlation functions are spread over a strip around the time diagonal of the width of quasiparticle lifetime.

C. Kadanoff-Baym ansatz

Kadanoff and Baym proposed to convert the GBE into a closed equation by expressing approximately the correlation functions g^{\leq} through their time diagonals ρ^{\leq} . In other words, they search for an approximate functional dependence $g^{\leq} [\rho^{\leq}]$. For a weak scattering homogeneous system in equilibrium, the lifetime is long and the quasiparticles spend most of their time in a state with a sharp energy. This free propagation is infrequently interrupted by collisions, whose duration is short. In the presence of an external field smoothly changing in space and time, this picture is locally correct, and represents the physical basis of the approximation known as the KB ansatz. This ansatz emerges as an outgrowth of a physical picture already visualized by Boltzmann and developed by Bogoljubov, van Hove, and others, as reviewed in Ref. 14. The formal expression of the KB ansatz has been developed using a gradient expansion around equilibrium. The natural representation is then the mixed Wigner representation, in which the two times t_1 and t_2 are replaced by T and ω , where $T = (t_1 + t_2)/2$ and energy ω is the Fourier conjugate to $(t_1 - t_2)$; the same is done for the momenta and coordinates.

For a homogeneous equilibrium system, the correlation function can be expressed employing the Fermi-Dirac distribution function,²

$$g^{<}(\omega,p) = f_{\rm FD}(\omega)i \left[G_R(\omega,p) - G_A(\omega,p) \right].$$
⁽²⁷⁾

The spectral function, defined as

$$a(\omega,p) = i \left[G_R(\omega,p) - G_A(\omega,p) \right], \qquad (28)$$

has, in the weak scattering limit, a δ -like character,

$$a(\omega,p) \approx 2\pi \delta(\omega - \epsilon(p))$$
 (29)

This permits us to relate the Fermi-Dirac distribution to the density matrix $\rho^{<}$,

$$\rho^{<}(p) \equiv g^{<}(t_1, t_2, p) \mid_{t_1 = t_2}$$
$$= \int \frac{d\omega}{2\pi} g^{<}(\omega, p) \approx f_{\rm FD}(\epsilon(p)) . \tag{30}$$

With this correspondence, the approximate functional

dependence $g < [\rho^{<}]$ is

$$g^{<}(\omega,p) \approx \rho^{<}(p)a(\omega,p)$$
 (31)

Kadanoff and Baym assumed this relation to be locally valid also in the case of weak nonequilibrium. This yielded the KB ansatz as

$$g^{<}(\omega, T, p, R) \approx \rho^{<}(T, p, R) a(\omega, T, p, R) .$$
(32)

This ansatz solves the task of converting the GBE (26) into a closed equation for the distribution $\rho^{<}$, at least if the propagation factor *a* depends on the distribution at most through the mean field. Such separation of the statistical aspect from the dynamics is strictly valid only for the Boltzmann assumption of instantaneous local collisions. In addition, this assumption is utilized in an intuitive manner when generalizing (31), justified in homogeneous equilibrium systems, to the KB ansatz (32). The accent on the near equilibrium leading to the use of the mixed representation masks somewhat the circumstance that (32) does not satisfy the requirement of the causal time evolution.

This is harmless in the true Boltzmann limit. The problem emerges when corrections for gradient, renormalization, or interference effects are required. The GBE contains all this, but when combined with the KB ansatz, it may include the corrections in an incomplete or inconsistent way. This has been suspected for some time,¹⁵ and was pointed out specifically in Ref. 16. Finally, the intuitive character of the KB ansatz was an obstacle to deriving its validity criterion, so that the resulting equations could be checked only against the results of independent studies employing alternative techniques of nonequilibrium statistics, while it was clear that the fundamental assumption about the collisions should provide the starting point for judging the theory with the use of its intrinsic means.

III. BACK CONSTRUCTION OF TWO-TIME CORRELATION FUNCTIONS FROM DISTRIBUTION FUNCTIONS

A. General considerations

In this section, which is central to the entire paper, we shall develop further the idea of reconstructing the total correlation function $g^{<}$ from its time-diagonal element $\rho^{<}$. The construction of the functional $g^{<}[\rho^{<}]$ will be attempted on two levels. First, an approximation on the physical level of the KB ansatz will be constructed and will be called the GKB ansatz to indicate that it is fully consistent with the exact framework of the GKB formalism. Next, we shall obtain an exact closed functional equation from which the functional $g^{<}[\rho^{<}]$ can be constructed to any order of approximation. It is important that such a relation exists, because an approximation can be judged against it. An approximation for $g^{<}[\rho^{<}]$ fitting into the GKB scheme should obey the following conditions.

(1) The structure of the approximate g^{\leq} should explicitly reflect the requirement of causal time evolution.

(2) The expressions should have a full electron-hole symmetry.

(3) For equal times, $t_1 = t_2$, the identity (3) must hold.

(4) For $|t_1-t_2|$ sufficiently large (this will be quantified below), g^{\leq} should satisfy the homogeneous equations,

$$G_R^{-1}g^{\leq} \approx 0 , \qquad (33)$$

$$g^{\leq}G_A^{-1}\approx 0, \qquad (34)$$

which are the asymptotic limit of the exact equations of motion, Eqs. (21) and (22).

(5) The correlation function should satisfy the spectral identity (16).

In addition to these conditions, we shall attempt not to use any specific representation. The formal conditions define the natural class of admissible functionals $g^{\leq} [\rho^{\leq}]$ entirely by their dynamical properties. Any particulars of the physical system, and/or an approximation for the self-energy are secondary. The class is rather wide, but not wide enough to contain the $g^{<}$ specified by the KB ansatz.

B. Zeroth order: GKB ansatz

The GKB ansatz will be developed considering the same kind of physical situation as the original KB ansatz, namely the case of a weak scattering in the system, when the individual collisions are not very frequent, while the quasiparticle lifetimes are long. Each scattering event can then be understood as being a very fast transition between two quasiparticle asymptotic states. This regime permits us to transform the description of the time development of $g^{<}$ in a physically important manner directly leading to the GKB ansatz. The integral form of the Dyson equation (20) for $g^{<}$ selects the appropriate solution of the differential GKB equation (25) after the boundary condition specified by the "free" $g_0^{<}$. This can be transformed to a form containing only the full quantities $g^{>}$, simultaneously replacing the boundary condition by an initial condition locally valid at each moment on the time diagonal. The initial condition will be given by the particle density matrix $\rho^{<}$ just before the collision. In this formulation, there is no need to explicitly recall the quasiparticle incoming states, and thus, any specific representation (like the momentum representation for homogeneous case). After these comments, we shall derive the GKB ansatz in two ways, based on purely heuristic considerations.

First, the exact equation (20) can be, with the use of (19), written as

$$g^{\leq} = G_R (G_{0r}^{-1} g_0^{\leq} G_{0A}^{-1} + \sigma^{\leq}) G_A , \qquad (35)$$

The KB ansatz (32), when transformed to the time domain, reads

$$g^{<}(t_{1},t_{2}) = i\rho^{<} \left(\frac{t_{1}+t_{2}}{2}\right) G_{R}(t_{1},t_{2})$$
$$-i\rho^{<} \left(\frac{t_{1}+t_{2}}{2}\right) G_{A}(t_{1},t_{2}) .$$
(36)

Transition from (35) to (36) formally represents a transformation from the boundary condition to the local initial conditions; it is not possible in this form, because

(36) evidently violates two of the conditions of Sec. III A, namely conditions 1 and 4. We shall arrive at the GKB ansatz by improving (36) ad hoc to the form

$$g^{\S} = -i(G_R f^{\S} - f^{\S} G_A), \qquad (37)$$

where we have denoted

$$f^{\leq}(t_1, t_2) = \rho^{\leq}(t_1)\delta(t_1 - t_2) , \qquad (38)$$

to keep the two-time form. This approximation for g^{\leq} automatically satisfies the formal conditions of Sec. III A, and is thus consistent with the GKB framework. The innocent change in the order of two factors leading to (36) in fact makes deep changes in the structure of g^{\leq} . This emerges when trying to determine under what conditions Eqs. (37) and (36) might be equivalent. For this, (i) the time ordering should be unessential-equilibrium or near-equilibrium state; (ii) $G_{R,A}$ and ρ^{\leq} should commute as operators. This is automatic only if the system has a natural representation-practically a homogeneous system. Thus, the equivalence is limited to the original KB assumptions, and allows no straightforward generalization.

The second derivation of the GKB ansatz will be based on the use of two characteristic times, the quasiparticle lifetime τ , and τ_c , which is customarily called the collision time and should measure the time span over which the quantum coherence, many-particle correlation, and similar phenomena decay. The presently considered regime is characterized by the inequality $\tau_c \ll \tau$: beyond τ_c the system behaves as if it were composed of a gas of quasiparticles damped with the lifetime τ and the condition (4) above becomes $|t_1 - t_2| \gg \tau_c$. We want to give the GKB ansatz a physical interpretation by showing that Eq. (37) follows from Eq. (35) under the model assumption $\tau_c = 0$; it is appropriate to call this the Wigner-Weisskopf (WW) model.¹⁷ Then the self-energy will be local in time, that is, all four components σ^{\leq} , $\Sigma_{R,A}$ will contain the factor $\delta(t_1 - t_2)$. This leads, in the first place, to the "semigroup property" of the quasiparticle propagation,

$$G_R(t,t') = iG_R(t,t'')G_R(t'',t'), \quad t \ge t'' \ge t' .$$
(39)

Second, in (35), the highly singular term $G_{0R}^{-1}g_0^{\leq}G_{0A}^{-1}$ is

concentrated to the time diagonal in any case. In the WW model, σ^{\leq} also behaves that way. If now, say, $t_1 > t_2$, then the first term of (37) results, and for $t_1 < t_2$, the other one results. This derivation indicates the meaning of the GKB ansatz, but is not truly satisfactory: it replaces the condition $\tau_c/\tau \ll 1$ by $\tau_c = 0$. This degenerate case does not allow us to consider the physical consequences of nonzero, even if small, collision times.

C. Complete iterative reconstruction of g^{\leq} from ρ^{\leq}

The feasibility of an exact building up of the full correlation functions from their time-diagonal sections can be motivated on physical grounds resembling somewhat the reasoning leading to the Kohn-Hohenberg theory.¹⁸ The behavior of the system is completely specified by the indication of the external field, which is a function of a single time variable. If now a functional substitution is intended to replace the external field by a response of the system as an independent variable, it should be expected that it will again be represented by a function of a single time. Then arbitrarily complex characteristics of the system, including the full correlation function as a special case, must be completely specified by the fundamental response function.

A procedure for this goal can be developed starting from another set of four basic GF equations,

$$g_{R}^{\leq}(t_{1},t_{2}) = -i\Theta(t_{1}-t_{2})g^{\leq}(t_{1},t_{2}) , \qquad (40)$$

$$g_{A}^{\geq}(t_{1},t_{2}) = i\Theta(t_{2}-t_{1})g^{\geq}(t_{1},t_{2}) .$$
(41)

These functions are easily related to $G_{R,A}, g^{\leq}$ and have the property that the discontinuity in their time derivative contains the distribution function ρ^{\leq} (see Ref. 5). This allows us to write expressions for these quantities which explicitly separate the equal-time initial conditions,

$$g_R^{\S} = G_R f^{\S} - i G_R \delta F_R^{\S} , \qquad (42)$$

$$g_A^{\S} = f^{\S} G_A + i \delta F_A^{\S} G_A .$$
(43)

Combining these two equations, the correlation functions are obtained as

$$g^{\$} = i \left(G_R f^{\$} - f^{\$} G_A \right) + G_R \delta F_R^{\$} + \delta F_A^{\$} G_A \quad . \tag{44}$$

If the correction terms δF could be neglected, the GKB ansatz for g^{\leq} would be immediately recovered.

The correction terms have an explicit form, which we write here for electronlike $\delta F_R^{<}$, $\delta F_A^{<}$

$$\delta F_{R}^{<}(t_{1},t_{2}) = -i\Theta(t_{1}-t_{2})\int_{-\infty}^{t_{2}} \left[\sigma^{<}(t_{1},\overline{t})g^{>}(\overline{t},t_{2}) - \sigma^{>}(t_{1},\overline{t})g^{<}(\overline{t},t_{2})\right]d\overline{t} , \qquad (45)$$

$$\delta F_{A}^{<}(t_{1},t_{2}) = i\Theta(t_{2}-t_{1})\int_{-\infty}^{1} \left[g^{>}(t_{1},\overline{t})\sigma^{<}(\overline{t},t_{2}) - g^{<}(t_{1},\overline{t})\sigma^{>}(\overline{t},t_{2})\right]d\overline{t} , \qquad (46)$$

which can be found by applying G_R^{-1} to (42) or G_A^{-1} to (43). Equations (44), together with (45) and (46) clearly represent a set of linear integral equations for g^{\leq} provided G_R , G_A , and the functional $\sigma^{\leq} [g^{\leq}]$ are known. Before discussing the meaning of this result, it is useful to perform certain transformations using Eqs. (9) and (10).

Then, for example $g < \text{ for } t_1 > t_2$ is given by

$$g^{<}(t_1,t_2) = G_R(t_1,t_2) f^{<}(t_2) + \int_{t_2}^{t_1} d\,\overline{\overline{t}} G_R(t_1,\overline{\overline{t}}) \int_{-\infty}^{t_2} d\,\overline{t} \,\sigma^{<}(\overline{\overline{t}},\overline{\overline{t}}) G_A(\overline{t},t_2) + \int_{t_2}^{t_1} d\,\overline{\overline{t}} G_R(t_1,\overline{\overline{t}}) \int_{-\infty}^{t_2} d\,\overline{\overline{t}} \,\Sigma_R(\overline{\overline{t}},\overline{\overline{t}}) g^{<}(\overline{t},t_2) \,.$$

$$\tag{47}$$

In this form, $g^{<}$ and $g^{>}$ are formally decoupled, and a direct comparison with (35) is possible. The first term of $g^{<}$ according to (35) (the boundary condition) is replaced in (47) by the term representing the gliding initial condition. This replacement is not exact, and the difference is transferred to the correction terms. These are, in either case, formally of the order of the scattering strength, and iteration of both (35) and (47) can thus be interpreted as an expansion in the powers of the scattering interactions, with the external field incorporated nonperturbatively in each successive term, including, in particular, the zeroth order of (47) (the GKB ansatz).

The correction terms in (47) have the general form of the back scattering $G_R \sigma^{<} G_A$ term of (35); the integration limits are different, however. Namely, the outer integration extends only from t_2 to t_1 in contrast to the $-\infty$ lower limit in (35). By this, the integration variables in (47) satisfy the inequalities $t_1 > \overline{t} > t_2 > \overline{t}$. It is this separation of ranges of \overline{t} and $\overline{\overline{t}}$ that makes the inner integrals negligible, once \overline{t} exceeds t_2 by more than a characteristic time by which the self-energy is already small. For the second term of (47), this is the decay time of the manyparticle correlations in the Bogolyubov sense, while for the third one it is the characteristic time for the quasiparticle formation. Both correction terms thus appear for t_1 sufficiently later than t_2 to function as a renormalization of the GKB ansatz term by amounts expressing an explicit memory of times before t_2 , and reflecting the time spread of the collision around t_2 . Similar interpretation can be given to other time combinations, and to $g^>$.

This analysis shows that iteration of the integral equation (47) for g < around the GKB ansatz should be understood rather as an expansion in terms of the short relaxation times in the system ("the collision duration times"), than in terms of the scattering strength. At the same time, the notion of the collision time τ_c was not needed during the derivation. With this interpretation, (47) operationally replaces the definition of the collision time. The present method of deriving the quantum transport equations thus appears to have the physical background identical with the approaches based on the superoperator techniques.

IV. HIGH-FIELD ELECTRON DRIFT: A TEST EXAMPLE

A. Importance of the example

Our general analysis will now be illustrated by the example of electrons drifting in a single band under the influence of a strong homogeneous electric field. If the scattering is weak, there is no formal obstacle against using the usual Boltzmann equation. At the same time, deviations form the purely Markovian character of the transport are to be expected, because the electric field can produce sizable effects upon the collision process itself. This interference effect is the simplest quantum correction to the Boltzmann equation. It is so simple that the corresponding GBE can be obtained in an explicit form, which opens the path to a full numerical solution. Because of all these advantages, this example was previously treated by several authors using various approaches including the superoperator formalism^{9,19} and the GKB formalism.⁴ The first attempt to combine GKB with the KB ansatz was made by Barker,²⁰ who seems to have believed that there is complete agreement with the superoperator results.9 More recent work by Jauho and Wilkins⁴ discovered that a straightforward application of the KB ansatz to GKB produces in the final equations retardations which are halved, in places, compared to superoperator results which are undoubtedly correct. As pointed out already,⁴ in the GF procedure, which is formally impeccable, some physical ingredient must be wrong and the most suspicious among the candidates is the KB ansatz itself. In the following, we shall replace the KB ansatz by the GKB ansatz, repeat the derivation, and then make the comparison.

B. Procedure

The GKB ansatz, although it appears in the course of general considerations, cannot be applied consistently before a specific approximate description of the considered system is selected. Thus, to employ its advantages in full, the following procedure should be followed: (1) At the Matsubara level, the Dyson equation $G[\Sigma]$ is supplemented by a specific functional $\Sigma[G]$ defining the interactions involved, and the physical approximation used. Here, experience with the equilibrium situation can be transferred to the nonequilibrium. (2) At the GKB level, the LW rules are used to convert these relations into the pair $g^{[\sigma]}[\sigma^{[g]}], \sigma^{[g]}[g^{[s]}]$ valid for the correlation functions. In parallel, the equations for the quasiparticle propagation as given by $G_{R,A}$ and $\Sigma_{R,A}$ can be developed. (3) All these relations are combined into the GBE equation (26), which thus acquires an explicit form specific to the given physical situation. (4) Only at this stage is the GKB ansatz for $g^{>}[\rho^{>}]$ employed, and the correlation functions are replaced by the distribution functions. The generalized transport equation results.

C. Model

The system is formed by noninteracting electrons moving in a single band with the dispersion law $\epsilon(p)$ under the influence of a homogeneous electrical field E(t), which may depend on time. To keep the spatial homogeneity, the gauge

$$\phi = 0, \quad A(t) = -\int^{t} d\overline{t} E(\overline{t})$$
(48)

is used. Then the momentum p^{F} , the free Hamiltonian, and the free field-dependent GF are given by,²¹

$$p^{F} = -i\nabla + eA , \qquad (49)$$

$$H(t) = \epsilon(p^F - eA) , \qquad (50)$$

$$G_0^{-1}(t_1, t_2, p^F) = \left| i \frac{\partial}{\partial t_1} - H(t_1, p^F) \right| \delta(t_1 - t_2) .$$
 (51)

The scattering mechanism will be represented by an interaction of the electrons with a single branch of phonons. It will be assumed that the phonons are not brought out of their equilibrium by the interaction. The approximation for the electron self-energy will be taken in the form of the self-consistent Tamm-Dankoff²² approximation (i.e., the vertex is taken to be bare in the spirit of the Migdal theory). The Dyson equation and the $\Sigma[G]$ functional then become



$$\sigma^{\leq}(t_1,t_2;p^F) = \sum_{q} |V_q|^2 d^{\leq}(t_1,t_2,q)g^{\leq}(t_1,t_2,p^F-q) ,$$



with the standard meaning of all graphical symbols.

D. GBE and transport equation

The LW rules are trivial for the present self-energy and yield it as

where the form of the interaction element V_q need not be specified, and the phonon correlation function is that of free phonons, see (58) below. Introducing this into the GBE, Eq. (26), it becomes

(52)

$$\frac{\partial}{\partial T}\rho^{<}(T,p^{F}) = \sum_{q} |V_{q}|^{2} \int_{-\infty}^{T} d\overline{t}[g^{>}(T,\overline{t},p^{F})d^{<}(\overline{t},T,q)g^{<}(\overline{t},T,p^{F}-q) + d^{<}(T,\overline{t},q)g^{>}(\overline{t},T,p^{F}) - g^{<}(T,\overline{t},p^{F}) - g^{<}(T,\overline{t},p^{F}) + d^{<}(\overline{t},T,q)g^{>}(\overline{t},T,q)g^{>}(\overline{t},T,p^{F}-q) - d^{>}(T,\overline{t},q)g^{>}(\overline{t},T,p^{F})].$$

$$(55)$$

Now the GKB ansatz (37) can be applied, and (55) becomes

$$\frac{\partial}{\partial T}\rho^{<}(T,p^{F}) = \int_{-\infty}^{T} d\,\overline{t} \sum_{q} S^{<}(T,\overline{t},p^{F},p^{F}-q)[1-\rho^{<}(\overline{t},p^{F})]\rho^{<}(\overline{t},p^{F}-q) -\int_{-\infty}^{T} d\,\overline{t} \sum_{q} S^{>}(T,\overline{t},p^{F}-q,p^{F})[1-\rho^{<}(\overline{t},p^{F}-q)]\rho^{<}(\overline{t},p^{F}), \qquad (56)$$

with the transition probabilities (the "memory functions") given by

$$S^{\leq}(T,\overline{t},p_{1}^{F},p_{2}^{F}) = |Vp_{1}^{F}-p_{2}^{F}|^{2} (G_{R}(T,\overline{t},p_{1}^{F})G_{A}(\overline{t},T,p_{2}^{F})) \\ \times d^{\leq}[\overline{t},T,\pm(p_{1}^{F}-p_{2}^{F})] + G_{R}(T,\overline{t},p_{2}^{F})G_{A}(\overline{t},T,p_{1}^{F})d^{\leq}[\overline{t},T,\mp(p_{1}^{F}-p_{2}^{F})]) .$$
(57)

These equations have the standard form of the generalized master equation,^{7.8} and should be considered the final product of the GKB formalism.

E. Explicit relations for the transition probabilities

In general, the GF g^{\leq} and $G_{R,A}$ entering Eq. (57) depend on the electron distribution and are to be determined in the course of the self-consistent process of solving the transport equation (56). This dependence is usually weak and in certain physically important situations, it can be neglected. Then the Dyson equations for $G_{R,A}$ decouple from the transport equations and can be solved as a separate problem. This happens, in particular, for a quasielastic scattering, or in the limit of a low electron concentration, as will be assumed here.

The phonon correlation function is simply

$$d^{>}(t_{1},t_{2},q) = (N_{q}+1)e^{-i\omega_{q}(t_{1}-t_{2})} + N_{-q}e^{i\omega_{q}(t_{1}-t_{2})}$$

$$d^{<}(t_{1},t_{2},q) = N_{q}e^{-i\omega_{q}(t_{1}-t_{2})} + (N_{-q}+1)e^{i\omega_{q}(t_{1}-t_{2})},$$
(58)

with N_a the Bose-Einstein distribution coefficient.

The self-energy entering the Dyson equation (19) could, in principle, be calculated to the end, because it is the same as it is for an isolated polaron. We shall not need this presently, because we shall resort to the Wigner-Weisskopf approximation. As already pointed out in Sec. III B, this approximation is compatible with the GKB ansatz, and it was also employed in the work of Barker.²⁰ In the present context, the WW approximation means that self-energy is to be taken without retardations, in other words, as being local in time,

$$\Sigma_{R,A}(t_1, t_2, p^F) \approx \frac{\overline{+i}\delta(t_1 - t_2)}{2\tau[p^F - eA(t_1)]} .$$
(59)

In mixed representation, it may be said that the model self-energy is energy independent. Therefore, the real part of Σ means only a shift of the quasiparticle energy and can be adsorbed in the (possibly strong) dependence of the quasiparticle state on the momentum.

The explicit solution of (19) for $G_{R,A}$ in dependence on

time τ is

an arbitrary external field and for any quasiparticle life-

$$G_{R}(t_{1},t_{2},p^{F}) = -i\Theta(t_{1}-t_{2}) \times \exp\left[i\int_{t_{1}}^{t_{2}}d\overline{t}\eta[p^{F}-eA(\overline{t})]\right], \quad (60)$$

where $\eta = \epsilon - i/2\tau$. Introducing (58) and (60) into (57) we obtain the promised explicit form for S^{\leq} .

We shall rewrite the transport equation in an explicit form by inserting the S^{\leq} and returning to the scalar gauge A = 0, $\phi = -Ex$, see Ref. 21. With the notation

$$\begin{split}
\rho(t) &= p - e \int_{t}^{T} E(t'') dt'', \\
\mathscr{I}_{\pm} &= \exp\left[i \int_{\overline{t}}^{T} dt' \{\eta^{*}[\overline{\rho}(t')] - \eta[\rho(t')] \pm \omega_{q}\}\right], \\
\frac{\partial}{\partial T} \rho^{<}(p,T) + e E(T) \frac{\partial}{\partial p} \rho^{<}(p,T) &= 2 \int \frac{dq}{(2\pi)^{3}} \operatorname{Re} |V_{q}|^{2} \\
&\times \int \frac{d\overline{p}}{(2\pi)^{3}} \delta(q - p - \overline{p}) \int_{-\infty}^{T} d\overline{t} \\
&\times \{ [(N_{q} + 1)\mathscr{I}_{+} + N_{-q}\mathscr{I}_{-}][1 - \rho^{<}(\rho(\overline{t}),\overline{t})] \rho^{<}(\overline{\rho}(\overline{t}),\overline{t}) \\
&- [N_{q}\mathscr{I}_{+} + (N_{-q} + 1)\mathscr{I}_{-}][1 - \rho^{<}(\overline{\rho}(\overline{t}),\overline{t})] \rho^{<}(\rho(\overline{t}),\overline{t}) \}.
\end{split}$$
(61)

F. Discussion

The transport equation (61) can be identified with Eq. (22) of Ref. 20. It transcends the BE primarily by the memory character of the collision term, which allows us to take into account the field dependence of the scattering.⁹ This was not prevented by the use of the GKB ansatz, because even for very short collision times the field dependence of the quasiparticle scattering states, as described by the retarded and advanced GF, persists. When this dependence can be neglected, that is, in the limit of slowly varying perturbations, the rhs of the present transport equation reduces to the standard collision term of the Boltzmann equation (17).

A more explicit form is obtained in two limits. The first is for a stationary electric field. Secondly, a fully explicit form is obtained for the linear response, which represents a generalization of the Boltzmann equation to fields with "arbitrarily" high frequencies.

It is in these two limits that a meaningful comparison of the GKB ansatz (37) with the KB ansatz (36) is made possible because of the work of Jauho and Wilkins⁴ who treated the present model applying systematically the KB ansatz. These authors found that the KB ansatz produces an equation for the stationary transport formally identical with (61), but with the time retardations reduced at places by a factor of $\frac{1}{2}$. More drastic effects were found in the high-frequency limit of the linear response, which, with the use of the KB ansatz, displayed unphysical resonances at half the frequency of the external field.²³ Presently, we can give a direct explanation for this. As discussed in Sec. III B, for homogeneous systems the KB ansatz and the GKB ansatz appear in very similar forms, because the operators involved, ρ^{\leq} and $G_{R,A}$ commute. We repeat here for clarity the explicit expressions for $t_1 < t_2$,

$$g^{<}(t_1, t_2, p^F) = -i\rho^{<}(t_1, p^F)G_A(t_1, t_2, p^F)$$
(62)

representing the GKB ansatz, and

$$g^{<}(t_1, t_2, p^F) = -i\rho^{<} \left[\frac{t_1 + t_2}{2}, p^F \right] G_A(t_1, t_2, p^F) , \qquad (63)$$

representing the KB ansatz. The difference between the two ansatzes in this case reduces to the differences in the time arguments of the distribution functions. The mean time appearing in the KB ansatz as a consequence of quasiclassical manipulations is responsible for the abovementioned one-half-factor discrepancies. This can be seen explicitly, if our procedure leading to (61) is repeated, but the step from GBE to the final transport equation (56) is made under the use of the KB ansatz.

V. CONCLUSIONS

The questions addressed in this paper were not connected with a specific system, although we had in mind the electron dc-transport in a single band as a prototype case. The first question we asked was how to find a method of obtaining quantum transport equations, which would be a natural and consequent extension of the nonequilibrium Green-function technique. The central result of this paper is the GKB ansatz (37), which, to our mind, answers this question in full.

In addition to the basic compatibility with the GF approach, the GKB ansatz has several important features, namely a nonperturbative and representationless form, which guarantees that the GKB ansatz can be applied in a wide range of situations including discrete dynamical variables. The GKB ansatz is also not necessarily quasiclassical, as it is not connected with a WKB expansion of the Wigner function.

All these gratifying features do not determine the validity of the GKB ansatz. This must be checked in each specific situation; the second question analyzed in this paper is the general approach to deriving an appropriate criterion. This question is answered by the integral equations (47), which indicate in a closed form the corrections to the GKB ansatz. As mentioned in several places in the paper, the usual discussion of the range of validity of the transport equations is based on the comparison of characteristic times for the quasiparticle formation and the quasiparticle decay. These times are usually called the collision time τ_c and the lifetime τ ; and they have a suitable definition, e.g., under the conditions consistent with the Boltzmann equation. A satisfactory, truly general, definition most probably cannot be given, because such

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times are in general dependent not only on the underlying equilibrium system but also on the strong nonequilibrium process driven by the external field. Our integral equations written in the time domain, and explicitly dependent on the time structure of the self-energy, replace the immediate comparison of characteristic times, whose meaning and magnitude may conversely result from the analysis of a given physical problem based on these equations. It is this direction of investigations which poses many new questions.

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