Hot-Electron Problem. I. A Unified Formulation

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The fact that both the Boltzmann equation for the hot-electron problem and Schrödinger's equation in quantum mechanics are first order in $\partial/\partial t$ is exploited to develop a formal treatment of the Boltzmann equation that parallels some of the formalism of quantum mechanics. Within this formalism, new methods are proposed and simple derivations of old methods are given both for the time-dependent and steady-state problems. Simple formal treatments of time-independent and time-dependent perturbations from the steady state are also given.

I. INTRODUCTION

Most of the theoretical interest in hot-electron problems is based on the Boltzmann equation or in formalisms that are equivalent to it. The latest efforts were attempts to obtain exact results by numerical methods.

In the work of Price,[1,2] Rees,[3,4] and Budd,[5] particular attention has been paid to the steady-state distribution, the point of departure in each case being a homogeneous integral equation equivalent to the time-independent Boltzmann equation. In all three cases, an iteration procedure is used and the classical paths of accelerated (but not scattered) electrons play a central role. The integral equations differ principally by different groupings of terms in the original differential equation.

The question of convergence of the iterations was first considered by Price. Introducing the notion of "before- and after-distribution functions," which are loosely related to the time evolution, Price showed that the successive before-distribution functions are essentially equal to the successive iterates of his integral equation, providing a heuristic proof that if the system actually evolves toward a steady state, then the iteration procedure for the steady-state equation will converge.

Rees,[3] starting from a stochastic formulation of the hot-electron problem rather than the Boltzmann equation, gave an alternative (but to us less convincing) set of arguments to show essentially the same result. More importantly, Rees also introduced the notion of an additional fictitious scattering called "self-scattering" which has the virtue of allowing the total scattering rate to have a constant value Γ (i.e., independent of $\vec{k}$). The calculations in each iteration of the new steady-state equation are greatly simplified thereby, at the expense of slower convergence of the iterative procedure. Corresponding to Price's relation between successive iterates and the before-distribution functions, Rees showed that as $\Gamma \to \infty$ (for which the convergence becomes infinitely slow), successive iterates would trace out the time-dependent distribution function at time intervals $1/\Gamma$. Rees[4] also applied these ideas to obtain the actual time-dependent properties of certain hot-electron systems.

Budd,[5] less concerned with general proofs of convergence, derived an integral equation. Budd further noted that for certain phonon scattering processes that are isotropic (nonpolar optical and elastic acoustic), this three-dimensional integral equation can be reduced to a one-dimensional integral equation which he then solved numerically by iteration.

In this paper we wish to present a unified formulation of both the transient and steady-state problems. The treatment is based on the application of operator-algebraic techniques, familiar in quantum mechanics, to solving the Boltzmann equation. As a result, we are able to make the previous formulations and their relationships completely transparent, and to propose some new and apparently more efficient methods for solving the problem.

II. ANALOG WITH QUANTUM MECHANICS

The form of the Boltzmann equation we wish to consider is

$$\left(\frac{\partial}{\partial t} + \vec{F}(\vec{k},\vec{r})\cdot\vec{\nabla}_k + \vec{v}(\vec{k})\cdot\vec{\nabla}_r\right) f(\vec{k},\vec{r},t)$$
$$= \int d^3k'\, W(\vec{k},\vec{k}')f(\vec{k}',\vec{r},t)$$
$$- \left(\int d^2k'\, W(\vec{k}',\vec{k})\right) f(\vec{k},\vec{r},t)\,, \qquad (1)$$

i.e., we consider a system of noninteracting electrons moving in a field $\vec{F}$ that can be spatially inhomogeneous ($\vec{r}$ dependent) and can depend on the electron wave vector [e.g., it may include a Lorentz force $\vec{v}(\vec{k})\times\vec{B}$]. We assume for simplicity that all electrons are confined to one band with an energy function $E(\vec{k})$ from which the velocity function $\vec{v}(\vec{k})$ is immediately defined by $\vec{v}(\vec{k}) = \vec{\nabla}E(\vec{k})$. The terms on the right-hand side are the customary

collision terms, the first being the "in scattering" from all other points in the band and the second being the total "out scattering." The transition rate per unit time $W(\vec{k}, \vec{k}')$ from $\vec{k}'$ to $\vec{k}$ is calculated quantum mechanically assuming the scattering system (inpurities, phonons, etc.) to remain in some steady state, not necessarily (but not excluding) thermal equilibrium.

Although the Boltzmann equation, except for the collision terms, is essentially an equation for a classical gas, it strongly resembles the time-dependent Schrödinger equation in one respect: It is first order in the time variable. This similarity suggests the applicability of many of the techniques of quantum mechanics. To make this similarity more apparent, we can rewrite the Boltzmann equation as

$$\frac{\partial}{\partial t} f = (D_0 + D_1) f \,. \tag{2}$$

The operators D_0 and D_1 in the $(\vec{k}, \vec{r})$ representation are

$$\langle \vec{k}\vec{r} | D_0 | \vec{k}'\vec{r}' \rangle = -[\vec{F}(\vec{k}, \vec{r}) \cdot \vec{\nabla}_k + \vec{v}(\vec{k}) \cdot \vec{\nabla}_r] \times \delta(\vec{k} - \vec{k}') \delta(\vec{r} - \vec{r}') \,, \tag{3a}$$

$$\langle \vec{k}\vec{r} | D_1 | \vec{k}'\vec{r}' \rangle = [W(\vec{k}, \vec{k}') - w(\vec{k}) \delta(\vec{k} - \vec{k}')] \delta(\vec{r} - \vec{r}') \,, \tag{3b}$$

with

$$w(\vec{k}) = \int d^3k' \, W(\vec{k}', \vec{k}) \,. \tag{3c}$$

Other representations for D_0 and D_1 are, of course, possible and may even be preferable. The boundary condition one imposes on Eq. (2) is the physical one of requiring f to be normalizable in the following sense: The integral of f over the relevant part of $\vec{k}$ space, which would be the first Brillouin zone in the case of a crystalline solid or the entire $\vec{k}$ space otherwise, must be finite. The normalization in $\vec{r}$ space may be achieved very simply by first introducing an appropriate periodic boundary condition of a convenient nature and then requiring the integral of f over one fundamental domain to be finite. *In this paper only the case of a uniform electric field is considered.* Then one can work exclusively with $\vec{r}$-independent distribution functions provided, of course, that in solving for the time-dependent distribution function one starts with a spatially uniform distribution.

The operator $D = D_0 + D_1$ is analogous to the Hamiltonian operator in quantum mechanics but with some differences. First of all let us consider D_1. The collision operator $W(\vec{k}, \vec{k}')$ is normally assumed to describe the interaction of the electron with an external reservoir system that is in a certain prescribed steady state unaffected by the fields applied to the electron distribution. Whenever, in this steady state, the principle of detailed balance can be satisfied, the collision operation $W(\vec{k}, \vec{k}')$ has the following structure[6]:

$$W(\vec{k}, \vec{k}') = g(\vec{k}) S(\vec{k}, \vec{k}') \,, \tag{4}$$

where $S(\vec{k}, \vec{k}')$ is symmetric and $g(\vec{k})$ is the steady-state zero-field ($D_0 = 0$) electron distribution function in equilibrium with the external reservoir. One can readily deduce the following properties of D_1 for such a scattering function. D_1 can be made Hermitian (or symmetric since it is real) by the similarity transformation $\tilde{D}_1 = g^{-1/2} D_1 g^{1/2}$, using the fact that g is everywhere positive. Therefore, it has real eigenvalues and, at least when $\vec{k}$ space is a finite set, a complete set of orthonormal left and right eigenvectors. Furthermore, by a simple application of Schwarz's inequality[7] one can show that there is one nondegenerate eigenvalue of D_1 equal to zero and that all the rest are negative. The right eigenvector for the zero eigenvalue is just the function g. The corresponding left eigenvector is easily found to be any nonzero constant C, i.e., $\int d^3k \, C \langle \vec{k} | D_1 | \vec{k}' \rangle = 0$, a simple consequence of particle conservation in the scattering processes. All other right eigenvectors, being orthogonal to this constant left eigenvector, have zero total particle number.

Thus the expansion of any initial distribution in right eigenvectors has a finite contribution from the special eigenvector of zero eigenvalue. For a finite system (hence discrete $\vec{k}$ space) and a single band, the eigenvalues will be finite in number so that only this special eigenvector will survive as $t \to \infty$, demonstrating the approach to steady state. For an infinite set of $\vec{k}$'s, the eigenvalue spectrum may be continuous in some finite neighborhood of zero, in which case the behavior as $t \to \infty$ is not so clear. The situation is quite analogous to the behavior of the canonical ensemble as $T \to 0$ and the question of whether or not the zero-temperature limit is equivalent to the ground state.

If the external field is not zero or the scattering operator does not have the structure (4), then D can no longer be Hermitized. We are unable to make any statement about its eigenvalue spectrum and its eigenvectors except that there is one zero eigenvalue with at least one left eigenvector, a nonzero constant. This means that the time-independent Boltzmann equation $Df_s = 0$ will always admit at least one nontrivial solution (f_s being the corresponding right eigenvector). However, there may be more than one solution as will be the case when the zero eigenvalue is degenerate. Even when the zero eigenvalue is nondegenerate, it does not follow that every initial distribution will converge to a steady-state distribution. The above discussion shows that the operator D is, in general, a much more complicated object to handle than the

Hermitian and usually local Hamiltonians one ordinarily comes across in quantum mechanics.

A second distinguishing feature of D does lead to a substantial simplification in the carrying out of operator-algebraic manipulations. It is the fact that D_0 is linear in the operators $\vec{\nabla}_k$ (in contrast to the usual kinetic-energy operator $-\vec{\nabla}_r^2/2m$ of quantum mechanics which is quadratic). This leads to an extremely simple time-development operator $e^{D_0 t}$ related to the fact that the equations of motion for the Heisenberg operators $\vec{k}(t) = e^{-D_0 t}\vec{k}e^{D_0 t}$, etc., are identical with the classical equations of motion.

III. TIME-DEPENDENT SOLUTIONS: NEW METHODS

Let us now consider the solution of the time-dependent equation (2) for an arbitrary initial ($t=0$) state f_i. Equation (2) has the obvious formal solution

$$f(\vec{k}, t) = e^{(D_0 + D_1)t} f_i(\vec{k}) . \tag{5}$$

The quantum-mechanical analogy immediately suggests some sort of perturbation treatment, if not with D_1 then with some modification $K_1 = D_1 + U$ or $L_1 = R^{-1}D_1 R$, considering $K_0 = D_0 - U$ or $L_0 = R^{-1}D_0 R$ as the "unperturbed" operator. U or R would have to be appropriately chosen to speed convergence while not making K_0 or L_0 too complicated. The difficulty with a perturbative approach is that D_0 does not even have a steady-state solution, only D_1 has. In weak fields D_1 rather than D_0 is the appropriate unperturbed operator, yet it is usually very complicated. Since its steady-state solution may belong to an eigenvalue that is at the top of a continuum, it is by no means clear that a perturbation series in the strength of D_0 (i.e., the field F) even exists.[8] In strong fields, D_0 and D_1 are equally important. Thus, if D_1 or K_1 (or L_1) is to be treated by a perturbation expansion, the expansion must be of infinite order.

On the other hand, what is simple about (2) is the presumed approach to a unique steady-state solution. To make use of this fact, and still be able to treat K_1 in some sense perturbationally, we introduce an iterative procedure by subdividing the time evolution into sufficiently small time intervals Δt so that $K_1 \Delta t$ can be treated as small. Thus, let us write

$$e^{Dt} = (e^{D\Delta t})^n = \{e^{K_0 \Delta t} T \exp[\int_0^{\Delta t} dt' K_1(t')]\}^n , \tag{6}$$

where

$$\begin{aligned} n &= t/\Delta t , \\ K_1(t) &= e^{-K_0 t} K_1 e^{K_0 t} , \end{aligned} \tag{7}$$

and T is the usual time-ordering operator which orders all operators from right to left in order of increasing values of their time arguments. Equation (6) is exact for all Δt. But if Δt is small enough, the operator $T\exp[\int_0^{\Delta t} dt' K_1(t')]$ can be expanded in powers of Δt yielding

$$e^{D\Delta t} = e^{K_0 \Delta t}[1 + K_1 \Delta t + \tfrac{1}{2}(K_1^2 - [K_0, K_1])(\Delta t)^2 + \cdots] . \tag{8}$$

For small enough Δt we may truncate the expansion after $K_1 \Delta t$, because

$$e^{Dt} = [e^{K_0 \Delta t}(1 + K_1 \Delta t)]^n e^{n O(\Delta t)^2} \tag{9}$$

and the correction factor $e^{n O(\Delta t)^2} \to 1$ as $\Delta t \to 0$, $n \to \infty$, $n\Delta t = t$. To speed calculations, it may be desirable to choose a larger Δt in which case second and even higher-order terms in (8) may be retained. The time evolution of $f(t)$ can be obtained from repeated application of the time-evolution operator for a single interval Δt:

$$f(t + \Delta t) = e^{K_0 \Delta t}(1 + K_1 \Delta t) f(t) \quad \text{as } \Delta t \to 0 . \tag{10}$$

What is crucial to the success of this procedure is a choice of K_0 which makes $e^{K_0 \Delta t}$ extremely simple. Choosing $K_0 = D_0$ (i.e., $U = 0$) has this advantage. Taking U equal to a c number is a trivial change and not an improvement, while choosing U to be more complicated destroys the simplicity of $e^{K_0 \Delta t}$.

Let us consider the meaning of $e^{D\Delta t}$ when applied on some more or less arbitrary function $g(\vec{k})$, assuming a uniform electric field. Then $e^{D_0 t} = e^{-(\vec{F}\cdot\vec{\nabla}_k)t}$ is obviously a translation operator in $\vec{k}$ space in the sense that for any reasonable function $g(\vec{k})$,

$$e^{-(\vec{F}\cdot\vec{\nabla}_k)t} g(\vec{k}) = g(\vec{k} - \vec{F}t) . \tag{11}$$

The time-evolution equation (10) becomes explicitly

$$\begin{aligned} f(\vec{k}, t + \Delta t) &= \int d^3k' [\delta(\vec{k} - \vec{F}t - \vec{k}') \\ &\quad + \Delta t\, D_1(\vec{k} - \vec{F}t, \vec{k}')] f(\vec{k}', t) \quad \text{as } \Delta t \to 0 \\ &= f(\vec{k} - \vec{F}t, t) + \Delta t \int d^3k'\, D_1(\vec{k} - \vec{F}t, \vec{k}') \\ &\quad \times f(\vec{k}', t) \quad \text{as } \Delta t \to 0 . \end{aligned} \tag{12}$$

Since both $f(\vec{k}, t)$ and $D_1(\vec{k}, \vec{k}')$ must be defined on some discrete mesh in $\vec{k}$ space, the operator $e^{D_0 \Delta t}$ will be just a relabeling of the points if Δt is so chosen that $\vec{F}\Delta t$ is a fundamental translation of the mesh, and extremely simple result.

To understand the case of a more general field and spatial inhomogeneity, observe that for a uniform field, $\vec{k} - \vec{F}t$ is the point in $\vec{k}$ space at which a classical particle obeying the classical equation $\dot{\vec{k}}(t) = \vec{F}$ must start, at $t = 0$, to arrive at $\vec{k}$ at time t. In more general fields we let

$$\vec{\kappa}(t - t_0; \vec{k}_0 \vec{r}_0), \quad \vec{\rho}(t - t_0; \vec{k}_0 \vec{r}_0) \tag{13}$$

be the solution of the classical equations of motion

$$\frac{d}{dt}\vec{\kappa}(t)=\vec{F}(\vec{\kappa}(t),\vec{\rho}(t))\,;\quad \frac{d}{dt}\vec{\rho}(t)=\vec{v}(\vec{\kappa}(t)) \tag{14}$$

passing through $(\vec{k}_0, \vec{r}_0)$ at t_0. Then the point at time $t=0$ leading to $\vec{k}$, $\vec{r}$ at time t is just $\vec{\kappa}(-t;\vec{k}\vec{r})$, $\vec{\rho}(-t;\vec{k}\vec{r})$. We show in the Appendix that the expected generalization of (11) holds:

$$e^{D_0 t}\,g(\vec{k},\vec{r})=g(\vec{\kappa}(-t;\vec{k}\vec{r}),\ \vec{\rho}(-t;\vec{k}\vec{r}))\,, \tag{15}$$

or, considered as an integral operator,

$$\langle\vec{k}\vec{r}\,|\,e^{D_0 t}\,|\,\vec{k}'\vec{r}'\rangle=\delta(\vec{k}'-\vec{\kappa}(-t;\vec{k}\vec{r}))\,\delta(\vec{r}'-\vec{\rho}(-t;\vec{k}\vec{r}))\,.$$

We thus have the general time-evolution equation

$$f(\vec{k}\vec{r},\,t+\Delta t)=f(\vec{\kappa}(-t;\vec{k}\vec{r}),\ \vec{\rho}(-t;\vec{k}\vec{r}),\,t)+\Delta t\int d^3k'$$

$$\times\,D_1(\vec{\kappa}(-t;\vec{k}\vec{r}),\vec{k}')f(\vec{k}',\vec{r},\,t)\ \text{ as }\Delta t\to 0\,. \tag{16}$$

In case D_0 or $\vec{F}$ depends on time, the formalism of this paper also applies, although the exact and approximate time-development operators from t' to t cannot be written simply as $e^{D(t-t')}$ and $e^{D_0(t-t')}$ but depend on t and t' separately. Replacing $e^{D_0(t-t')}$ is a propagation operator $u_0(t,t')$. Again only the classical orbits are needed but instead of (15) one has the equation

$$u_0(t,t')\,g(\vec{k},\vec{r})=g(\vec{\kappa}(t';\vec{k}\vec{r}t),\ \vec{\rho}(t';\vec{k}\vec{r}t))\,, \tag{15'}$$

where $(\vec{\kappa}(t';\vec{k}\vec{r}t),\ \vec{\rho}(t';\vec{k}\vec{r}t))$ is the position at t' of an orbit passing through $(\vec{k},\vec{r})$ at time t. In general, only if D_0 is time independent, is $\vec{\kappa}(t';\,\vec{k}\vec{r}t)=\vec{\kappa}(t'-t;\vec{k}\vec{r})$, etc.

The time-evolution equation used by Rees can be derived from (10) by making the approximation

$$e^{D_0\Delta t}\simeq(1-D_0\Delta t)^{-1}\,, \tag{17}$$

which is consistent with the approximation that Δt be small, underlying (10). Letting $\Gamma=1/\Delta t$ and using the representation

$$(\Gamma-D_0)^{-1}=\int_0^\infty dt'\,e^{-\Gamma t'}\,e^{D_0 t'}\,, \tag{18}$$

we have

$$f(t+1/\Gamma)=\int_0^\infty dt'\,e^{-\Gamma t'}\,e^{D_0 t'}\,(\Gamma+D_1)f(t)\ \text{ as }\Gamma\to\infty \tag{19}$$

or in the $\vec{k}$ representation,

$$f(\vec{k},\,t+1/\Gamma)=\int_0^\infty dt'\,e^{-\Gamma t'}\,[\Gamma f(\vec{k}-\vec{F}t',\,t)+\int d^3k'$$

$$\times\,D_1(\vec{k}-\vec{F}t',\vec{k}')f(\vec{k}',\,t)]\ \text{ as }\Gamma\to\infty \tag{20}$$

which is just Rees's time-evolution formula and is to be contrasted with (12).

Now the approximation (17) is consistent with neglecting terms of order $(\Delta t)^2$ (but, of course, it cannot be made consistently if higher-order terms in Δt are kept in the expansion of $T\{\exp[\int_0^\Delta K_1(t')dt']\}$). However, it is clear that the right-hand side of (20) is considerably more complicated than the right-hand side of (12), involving as it does one additional integration and the positions along the path that ends at $\vec{k}$ for all previous times.

We wish to discuss another approach suggested naturally by quantum mechanics, the use of the interaction picture. We define a new distribution $f^I(t)$ by

$$f^I(t)=e^{-K_0 t}f(t)\,. \tag{21}$$

In this picture the Boltzmann equation is just

$$\frac{\partial}{\partial t}f^I(t)=e^{-K_0 t}\,K_1\,e^{K_0 t}f^I(t)\,. \tag{22}$$

If we let $U=0$ so that $K_0=D_0$ and $K_1=D_1$ and write this explicitly in the $\vec{k}$ representation, we have

$$\frac{\partial}{\partial t}f^I(\vec{k},\,t)=\int d^3k'\,D_1(\vec{k}+\vec{F}t,\vec{k}'+\vec{F}t)f^I(\vec{k}',\,t)\,. \tag{23}$$

The generalization to include spatial variation and arbitrary fields is straightforward. Instead of $\vec{k}+\vec{F}t$ we have $\vec{\kappa}(t;\vec{k}\vec{r})$, etc. The integration over $\vec{k}'$, $\vec{r}'$ can be directly replaced by an integration over $\vec{\kappa}'=\vec{\kappa}(-t;\vec{k}'\vec{r}')$, $\vec{\rho}'=\vec{\rho}(-t;\vec{k}'\vec{r}')$, etc., because the Jacobian of this transformation, being a Poincaré invariant, is always unity. For this choice of K_0 and K_1, it is also useful to point out, from Eq. (21), that

$$f^I(\vec{k},\,t)=f(\vec{k}+\vec{F}t,\,t)=f(\vec{\kappa}(t,\vec{k}),\,t)\,, \tag{24}$$

where $\vec{\kappa}(t,\vec{k})=\vec{k}+\vec{F}t$ is just the classical path starting at $\vec{k}$. Boltzmann's equation is then just

$$\left(\frac{\partial}{\partial t}f(\vec{\kappa}(t,\vec{k}),\,t)\right)_{\vec{k}}=\int d^3\vec{\kappa}'\,D_1(\vec{\kappa}(t,\vec{k}),\,\vec{\kappa}')f(\vec{\kappa}',\,t)\,, \tag{25}$$

i.e., the interaction picture is essentially equivalent to writing the Boltzmann equation for the distribution function $f(\vec{k},\,t)$ in terms of "path variables."

The advantage of this equation, as has been pointed out by Williams of this laboratory, is that it is especially suitable for using Hamming's higher-order formulas for numerical integration of differential equations,[9] because it is first order in time, and in contrast to the original Boltzmann equation (the Schrödinger picture), the operator on the right-hand side, being an integral operator, has a smoothing effect. But for the Boltzmann equation, where the solutions $f(t)$ are assumed to approach a steady state f^s, the solution in the interaction picture $f^{s,I}=\exp(-K_0 t)f^s$ is still a function of time, being appreciable over a set of points that are moving along the classical orbits. Thus, many trajectories must be calculated for appreciable time intervals into regions of $\vec{k}$ space that are not really of interest. For a uniform field $\vec{F}$, this is no problem because one has the orbits analytically,

so the method may give the most rapid convergence, an approach under investigation by Marcus and Lebwohl of this laboratory.

Finally, just as in quantum mechanics, a Green's-function approach is possible that converts the Boltzmann equation from a differential to an integral equation in the time variable. Thus, if we define a retarded Green's-function operator[10] $P_0(t-t')$ by

$$\left(\frac{\partial}{\partial t} - K_0\right) P_0(t-t') = \delta(t-t') , \tag{26}$$

then we have explicitly

$$\begin{aligned} P_0(t-t') &= e^{K_0(t-t')} , \quad t > t' \\ &= 0 , \quad t < t' \end{aligned} \tag{27}$$

and Boltzmann's equation becomes

$$\begin{aligned} f(t) &= e^{K_0 t} f_0 + \int_0^t dt'\, e^{K_0(t-t')} K_1 f(t') \\ &= P_0(t) f_0 + \int_0^\infty dt'\, P_0(t-t') K_1 f(t') . \end{aligned} \tag{28}$$

The term $P_0(t)f_0$ is a solution of the "homogeneous" equation

$$\left(\frac{\partial}{\partial t} - K_0\right) P_0(t) f_0 = 0$$

that must be added to satisfy the initial condition. This integral equation can easily be "solved" with Laplace transforms and also converted to an interaction picture.

If $K_0 = D_0$, we have already exhibited the operator $P_0(t-t')$ in the $\vec{k}$ representation. If instead we choose $K_0 = D_0 - U$, where U may depend on $\vec{k}$ but is diagonal in the $\vec{k}$ representation, P_0 can still be calculated explicitly using ordered operators:

$$e^{K_0 t} = e^{(D_0 - U)t} = e^{D_0 t}\, T \exp\left[-\int_0^t dt'\, U(\vec{k}, t')\right] , \tag{29}$$

where

$$U(\vec{k}, t) = e^{-D_0 t}\, U(\vec{k})\, e^{D_0 t} = U(\vec{\kappa}(t, \vec{k})) . \tag{30}$$

Since both $U(\vec{k}, t')$ and $U(\vec{k}, t'')$ are functions only of $\vec{k}$ and not of $\nabla_{\vec{k}}$, they commute and time ordering in (29) is unnecessary. We find that

$$e^{K_0 t} = e^{D_0 t} \exp\left[-\int_0^t dt'\, U(\vec{\kappa}(t', \vec{k}))\right] , \quad t > 0 \tag{31}$$

so that, as an integral operator,

$$\begin{aligned} P_0(\vec{k}, \vec{k}', t) &= \delta(\vec{k}' - \vec{\kappa}(-t, \vec{k})) \\ &\quad \times \exp\left[-\int_0^t dt'\, U(\vec{\kappa}(t', \vec{k}))\right] , \quad t > 0 . \end{aligned} \tag{32}$$

If we take $U(\vec{k}) \equiv w(\vec{k})$ (in which case $K_1 = W$), then $P_0(\vec{k}, \vec{k}', t-t')$ is exactly the kernel used by Price and Budd, and the integral equation (28) has a simple stochastic interpretation: $P_0(\vec{k}, \vec{k}', t)$ is the probability that a particle goes from $\vec{k}'$ to $\vec{k}$ in time t without suffering a scattering, so that in (28), the term $P_0(t)f_0$ is the contribution to $f(t)$ of particles having suffered no scattering, and

$$P_0(t-t')\, K_1 f(t')dt' = P_0(t-t')\, W f(t')\, dt'$$

is the contribution to $f(t)$ of particles having suffered their last scattering in the time interval $(t', t'+dt')$.

If instead of $U = w$, one takes $U = \Gamma$, so that $K_1 = W + (\Gamma - w)$, one then has the P_0 used by Rees.[3] P_0 still has the stochastic interpretation of being the probability of propagation without scattering. Now, however, the concept of scattering must be enlarged to include not only the physical scattering W but also a self-scattering rate $\Gamma - w$. To make this notion of self-scattering probability both mathematically and physically acceptable, it must be, respectively, non-negative and diagonal in $\vec{k}$.

We see that neither of these restrictions on $\Gamma - w$ appears to be required when we view an equation like (28) from the more formal point of view of this paper rather than the stochastic viewpoint of Rees. Whether necessarily approximate calculations of the time evolution employing the idea of self-scattering are stable for self-scattering operators that are not diagonal or not positive semi-definite is, of course, another matter. In the following paper we present soluble models in which a self-scattering operator that is not positive semi-definite still leads to a stable approximation scheme.

Let us now consider the closely related question of the iterative approach to the steady-state solution.

IV. TIME-INDEPENDENT STEADY-STATE SOLUTION

The obvious approach to the steady-state solution f^s, based on our discussion of the time-dependent problem, is just to calculate the time-dependent solution for sufficiently many intervals Δt. Errors will in general be made at each step, but if these errors are small enough, the sequence of functions $f(\vec{k}, n\Delta t)$ should still converge to the steady state because any function will start evolving towards the steady state. By contrast, Price, Rees, and Budd have been concerned with procedures for finding f^s more directly. It may be useful to see their approaches from a simple and unified viewpoint. The problem is to solve the time-independent equation

$$Df^s = (D_0 + D_1) f^s = (K_0 + K_1) f^s = 0 \tag{33}$$

or equivalently

$$f^s = -K_0^{-1} K_1 f^s \tag{34}$$

assuming that K_0^{-1} exists. This equation is to be solved by interactions, the sequence of iterates $f_0^s, f_1^s, f_2^s, \ldots$ satisfying the equation

$$f^s_{n+1} = -K_0^{-1} K_1 f^s_n = (U - D_0)^{-1} (D_1 + U) f^s_n \ . \qquad (35)$$

Formally we may represent K_0^{-1} by

$$K_0^{-1} = -\int_0^\infty dt\, e^{K_0 t} \ , \qquad (36)$$

obtaining the homogeneous equation

$$f^s = \int_0^\infty dt\, e^{(D_0 - U)t} (D_1 + U) f^s \ . \qquad (37)$$

If $U = \Gamma$, a c number, then in the $\vec{k}$ representation this is precisely Rees's equation

$$f^s(\vec{k}) = \int_0^\infty dt\, e^{-\Gamma t} [\Gamma f^s(\vec{k} - \vec{F}t)$$

$$+ \int d^3k'\, D_1(\vec{k} - \vec{F}t, \vec{k}') f^s(\vec{k}')] \ . \qquad (38)$$

When solved by iteration, this equation is formally identical with (20). Thus, as Rees has importantly observed, the successive iterations of the time-independent equation with $U = \Gamma$ approximate the time-dependent solution at time intervals $1/\Gamma$ if Γ is large. Thus, as $\Gamma \to \infty$, the convergence of the iterations to the time-independent equation becomes infinitely slow.

If we take $U = w(\vec{k})$, then we can make use of (31) and obtain essentially the integral equation considered by Price:

$$f^s(\vec{k}) = \int_0^\infty dt \int d^3k'\, \delta(\vec{k} - \vec{F}t - \vec{k}')$$

$$\times \exp[-\int_0^t dt'\, w(\vec{k} + \vec{F}t')] \int d^3k''\, W(\vec{k}', \vec{k}'') f^s(\vec{k}'')$$

$$= \int_0^\infty dt \exp[-\int_0^t dt'\, w(\vec{k} - \vec{F}(t - t'))]$$

$$\times \int d^3k'\, W(\vec{k} - \vec{F}t, \vec{k}') f^s(\vec{k}') \ . \qquad (39)$$

Obviously the successive iterations of Rees's equation are less difficult to compute. But since for sufficiently large Γ the iterations of Rees's equation converge arbitrarily slowly, what must be determined is the optimum choice for Γ and how the Rees procedure then compares with that of Price. In seeking the optimum Γ we are not constrained, *a priori*, by the requirement that $\Gamma - w(\vec{k})$ be nonnegative, as we have remarked earlier.

For completeness we may remark that Budd also considered the integral equation corresponding to $U = w(\vec{k})$, i.e., $f^s = (w - D_0)^{-1} W f^s$. He noted that this is a particularly convenient form for the steady-state equation when one is dealing with spherically symmetric energy surfaces and scattering by nonpolar optical modes and/or very low-energy acoustic modes, for which the scattering operator $W(\vec{k}, \vec{k}')$ is a function only of E_k and $E_{k'}$, not the directions of $\vec{k}$ and $\vec{k}'$. Then, if $f^s(\vec{k})$ is decomposed into a spherically symmetric part $S_0(E_k)$ and an anisotropic part $A(\vec{k})$, such a scattering operator annihilates the anisotropic part, i.e., $WA = 0$, so that, integrating over the direction of $\vec{k}$, Budd obtained the one-dimensional integral equation

$$S_0(E) = \int dE'\, K(E, E') S_0(E') \ , \qquad (40)$$

where

$$K(E_k, E') \propto \int d\Omega_k \int d^3k'' \langle \vec{k} | (w - D_0)^{-1} | \vec{k}'' \rangle$$

$$\times\ W(E_{k''}, E') \ , \qquad (41)$$

and Ω_k is the direction of $\vec{k}$. The function $A(\vec{k})$ can be constructed later from $S_0(E_k)$. We observe that to preserve this "reducibility," any choice of U other than $w(\vec{k})$ would have to differ from $w(\vec{k})$ by an operator also annihilating A, and hence nondiagonal. Such a U would make $(U - D_0)^{-1}$ intractable.

For a general understanding of the convergence of any of these iteration procedures, the most useful insight, we believe, comes from Price.[2] Price showed that the successive iterates of the time-independent equation are related to the time evolution, but in a very subtle way. Considering any scattering operator W, Price considered the sequence of distributions $f^b_1, f^b_2, f^b_3, \ldots$, of particles each immediately before its own first, second, third, etc., scattering (and hence, in general, each distribution function refers to all particles at different times). Price has shown that these unusual distribution functions satisfy the recursion relation

$$f^b_{n+1} = w(w - D_0)^{-1} W w^{-1} f^b_n \ . \qquad (42)$$

Furthermore, the distribution function just before the first scattering, f^b_1, is related to the initial distribution function by the equation

$$f^b_1 = w(w - D_0)^{-1} f_i \ . \qquad (43)$$

Comparison of Eqs. (40) and (35) will show that the successive iterates of the time-independent equation, $f^s_1, f^s_2, \ldots$, are related to the successive before-distribution functions of an actual system developing in time by the simple equation

$$f^s_n = w^{-1} f^b_n \ , \qquad (44)$$

provided (i) we take $U = w$ in the iteration scheme and (ii) the initial distribution f_i and the initial trial f^s_1 are related by the condition $f_i = (w - D_0) f^s_1$.

Thus the sequence of iterates of the steady-state equation converges if the sequence of before distributions converges. It is intuitively appealing (though not proved) that the convergence of the before distributions is in turn assured by the approach to a steady state of the time-developing distribution function. If one believes that, for long times, the distribution of nth collision times sampled in the nth before distribution becomes

sufficiently sharply peaked, then one has a heuristic proof of convergence of the iteration scheme. We have not supplied the mathematical details.

The advantage of Price's formulation is that it is not restricted to just physical scattering operators. Thus, if instead of W we take $W_G \equiv W + (\Gamma - w)$ to be the collision operator, the same arguments can be made – the nth iterate is simply related to the distribution just before the nth scattering W or self-scattering $\Gamma - w$. It now appears that the number of generalized scatterings that is required to describe a certain time interval increases monotonically with Γ (provided $\Gamma - w \geq 0$); i.e., the sequence of before distributions (and hence time-independent iterates) converges more slowly the larger Γ is.

Unfortunately these arguments, also being stochastic in nature, do not apply to negative self-scattering probabilities. For this reason, among others, we have investigated some soluble models in the following paper.

V. PERTURBATIONS ON STEADY STATE

Perturbations on the steady state that are both time independent and time dependent have been discussed by Price[2] and by Rees.[11] In our formulation both problems are easily given formal solutions. Consider a time-independent change in the field or the scattering operator from a situation for which the steady state has already been found. Thus, let

$$D \to D + D' , \tag{45}$$

where D' represents a change in D_0, D_1 or both, and is assumed linear in some small parameter ϵ. Then, if $f^{s\prime}$ is the first-order change in the steady-state solution, it is determined by an inhomogeneous equation

$$Df^{s\prime} = -D'f^s . \tag{46}$$

A formal solution to this equation is

$$f^{s\prime} = \beta f^s + (\eta - D)^{-1} D' f^s , \tag{47}$$

where it is understood that η, a positive infinitesimal, is included to make the operator D^{-1} well defined. The term βf^s may be added because $Df^s = 0$. We determine β by requiring that the norm of $f^{s\prime}$ be zero. Thus

$$\beta = \int d^3k\, (\eta - D)^{-1} D' f^s . \tag{48}$$

To evaluate this expression for β, we use the integral representation $(\eta - D)^{-1} = \int_0^\infty dt\, e^{-\eta t}\, e^{Dt}$ and the fact that e^{Dt} is norm conserving. Thus, because $D'f^s$ has zero norm, so does $e^{Dt}D'f^s$ and hence $\beta = 0$.[12]

We can evaluate $(\eta - D)^{-1}$ in at least two different ways:

$$(\eta - D)^{-1} = \int_0^\infty dt\, e^{-\eta t}\, e^{Dt} \tag{49a}$$

and

$$\frac{1}{\eta - D} = \frac{1}{\eta - K_0 - K_1} = \sum_{m=0}^{\infty} \left(\frac{1}{\eta - K_0}\, K_1\right)^m \frac{1}{\eta - K_0} . \tag{49b}$$

The first expression, when applied to $D'f^s$, would involve evaluation of $e^{Dt}D'f^s$ for *all* $t > 0$ and an integration over this whole range which is clearly undesirable. The second expression, when applied to the state $D'f^s$, gives a sum of terms which, for $K_0 = D_0 - w(\vec{k})$ or $K_0 = D_0 - \Gamma$, can be considered the successive before distributions [modified with a factor $w(\vec{k})$ or Γ] if we start with the particleless distribution $f_0 = (\eta - K_0)^{-1} D'f^s$. Presumably after a certain number of collisions, such distributions are approximated by zero everywhere, suggesting that for evaluating $(\eta - D)^{-1}$, the series expression is much superior, a conclusion stressed by Rees.

The conclusion that $\beta = 0$ depends on the way we defined D^{-1}, as $\lim(\eta - D)^{-1}$ as $\eta \to 0+$. Another definition of D^{-1} which is more useful in computation leads to a different value for β as we now show.

Instead of $\lim(\eta - D)^{-1}D'f^s$ as $\eta \to 0+$ we now propose to define $D^{-1}D'f^s$ by taking the limit $\eta \to 0+$ in each term of the infinite series (49b). The result, as Rees has shown,[11] is the first-order term in the expansion in primed quantities of

$$\lim_{n\to\infty}\left[\frac{1}{w + w' - D_0 - D_0'}\,(W + W')\right]^n f^s \equiv (1 - \beta)\,(f^s + f^{s\prime}) , \tag{50}$$

where $f^{s\prime}$ is uniquely defined by requiring that it have norm zero. Equating first-order terms of (50) we obtain an equation for $f^{s\prime}$ and β:

$$P_0 \sum_{m=0}^{\infty} (WP_0)^m\, D'f^s = (1 - \beta)\,(f^s + f^{s\prime}) - f^s = -\beta f^s + f^{s\prime} , \tag{51}$$

where

$$P_0 = (w - D_0)^{-1} . \tag{52}$$

In general, the quantity β, though well defined by (51), is not equal to zero, contrary to an assertion by Rees,[11] because the operator P_0W for any W is not norm conserving. β can be determined by simply requiring the norms of both sides to be the same:

$$\beta = -\int d^3k\, P_0 \sum_{m=0}^{\infty} (WP_0)^m\, D'f^s . \tag{53}$$

The fact that $\beta \neq 0$ demonstrates that the limit $\eta \to 0+$ and the infinite summation over m cannot be interchanged without affecting the result; i.e.,

$$\lim_{\eta\to 0+} P_0(\eta)\sum_{m=0}^{\infty}[WP_0(\eta)]^m D'f^s \neq P_0\sum_{m=0}^{\infty}(WP_0)^m D'f^s , \tag{54}$$

where

$$P_0(\eta)\equiv(\eta+w-D_0)^{-1} . \tag{55}$$

We can understand the source of the discrepancy between the two expressions in (54), if we assume that $WP_0(\eta)$ can be written in terms of its right and left eigenvectors, defined by

$$\begin{aligned} WP_0(\eta)\,|r_i\rangle_\eta &= \gamma_i(\eta)\,|r_i\rangle_\eta , \\ {}_\eta\langle l_i|\,WP_0(\eta) &= \gamma_i(\eta)\,{}_\eta\langle l_i| . \end{aligned} \tag{56}$$

Then

$$[WP_0(\eta)]^m = \textstyle\sum_i |r_i\rangle_\eta\,(\gamma(\eta_i))^m\,{}_\eta\langle l_i| . \tag{57}$$

As $\eta\to 0+$, the interesting behavior is in the largest eigenvalue $\gamma_1(\eta)$ and the corresponding left eigenvector ${}_\eta\langle l_1|$. When $\eta=0$, ${}_0\langle l_1|D'f^s\rangle=0$ (because ${}_0\langle l_1|$ is a constant) so we get no contribution to any term of the sum from the eigenvalue γ_1. However, if $\eta\neq 0$, then $\gamma_1=1-O(\eta)$ and ${}_\eta\langle l_1|D'f^s\rangle=O(\eta)$ so that, when summing on m, this eigenvalue gives

$$|r_1\rangle_\eta\{1-[1-O(\eta)]\}^{-1}O(\eta) \underset{\eta\to 0+}{=} |r_1\rangle_\eta O(1) , \tag{58}$$

i.e., the summation is not uniformly convergent in η, so that the limit and summation cannot be exchanged. In fact we see that

$$\begin{aligned} &\lim_{\eta\to 0+} P_0(\eta)\sum_{m=0}^{\infty}[WP_0(\eta)]^m D'f^s \\ &\quad = P_0|r_1\rangle_0 \lim_{\eta\to\infty}\frac{{}_\eta\langle l_1|D'f^s\rangle}{1-\gamma_1(\eta)} + P_0\sum_{m=0}^{\infty}(WP_0)^m D'f^s . \end{aligned} \tag{59}$$

Now the state $P_0|r_1\rangle_0$ obeys the equation

$$P_0WP_0|r_1\rangle_0 = P_0|r_1\rangle_0 ,$$

i.e., $P_0|r_1\rangle_0$ is the right eigenvector of P_0W belonging to the eigenvalue unity and hence is proportional to f^s. Thus

$$\begin{aligned} &\lim_{\eta\to 0+} P_0(\eta)\sum_{m=0}^{\infty}[WP_0(\eta)]^m D'f^s \\ &\quad = \beta f^s + P_0\sum_{m=0}^{\infty}(WP_0)^m D'f^s , \end{aligned} \tag{60}$$

where β is obtained by equating the norms of the first terms on the right-hand side of (59) and (60):

$$\beta = \langle 1|P_0|r_1\rangle_0 \lim_{\eta\to 0+}\frac{{}_\eta\langle l_1|D'f^s\rangle}{1-\gamma_1(\eta)} , \tag{61}$$

an alternative to evaluating (53). For actual calculation, the eigenvalue $\gamma_1(\eta)$ and the states $|r_1\rangle_0$ and ${}_\eta\langle l_1|$ will not be known, so that (61) is inconvenient. The series in (51) and (53) should converge rapidly, however.

In the following paper, a soluble model is introduced for which the calculations involved in (51) and (53) are carried out explicitly, and the two apparently different expressions for β, (53) and (61), are shown to yield identical results.

In all the above, we can, of course, replace W and P_0 by $W+(\Gamma-w)$ and $(\Gamma-D_0)^{-1}$, which simplifies the calculations. With a proper choice of Γ, the convergence may not be seriously impeded.

For a time-dependent perturbation $D'(t)$, the Boltzmann equation for the first-order change in $f(t)$ is just

$$\frac{\partial}{\partial t}f'(t) - Df'(t) = D'(t)f^s , \tag{62}$$

which has the formal solution

$$f'(t) = \int_{t_0}^{t} dt'\, e^{D(t-t')}\,D'(t)f^s , \tag{63}$$

assuming that

$$D'(t)\equiv 0 , \quad t<t_0 . \tag{64}$$

A generalized response operator can be defined by

$$\chi_{f,D'}(t,t') = \delta f(t)/\delta D'(t') = e^{D(t-t')}\,D'(t') . \tag{65}$$

In Eq. (63), with finite t, there is no simple rapidly converging sum to replace the integral. The operator $e^{D(t-t')}$ must be constructed as discussed in Sec. III. If $D'(t)$ has some simple periodic behavior like $D'(t)=D'_\omega e^{i\omega t}$, then $f'(t)=f'_\omega e^{i\omega t}$ and the amplitudes f'_ω and D'_ω are simply related by

$$f'_\omega = (i\omega - D)^{-1}\,D'_\omega f^s . \tag{66}$$

In this case, as long as $\omega\neq 0$, the series expansion

$$\frac{1}{i\omega - D} = P_0(i\omega)\sum_{m=0}^{\infty}[WP_0(i\omega)]^m \tag{67}$$

can probably be truncated effectively. Simpler to evaluate, again, but possibly requiring more terms, would be the analogous expansion in which self-scattering is introduced:

$$\frac{1}{i\omega - D} = P_0(i\omega+\Gamma-w)\sum_{m=0}^{\infty}[(W+\Gamma-w)P_0(i\omega+\Gamma-w)]^m . \tag{68}$$

The effect of introducing a finite frequency ω on the range of possible choices for Γ must be investigated.

VI. SUMMARY

We have formally exploited the fact that the Boltzmann equation, neglecting electron-electron collisions, is a first-order differential equation in $\partial/\partial t$ and also in $\vec{\nabla}_k$ and $\vec{\nabla}_r$. This allows a simple formal solution of the time-dependent equation which suggests various calculational schemes for finding the time-dependent solution. One of the more complicated of these, due to Rees, is readily

derived. Other schemes, which proceed in a simpler stepwise manner with time, have also been proposed. The time-independent equation is shown always to have a solution, and various known iteration procedures for finding it are shown to be special cases of a general approach. It is also shown that the notion of self-scattering, introduced by Rees in a stochastic formulation of the problem, can be generalized to nondiagonal negative "self-scattering probabilities," and it is suggested that the optimum self-scattering for some problems may be of such a nature. The effects of both time-independent and time-dependent perturbations on an unperturbed steady state are also derived very simply within the formalism.

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APPENDIX

The $(\vec{k}\vec{r})$ representation of $e^{D_0 t}$ is $\langle \vec{k}\vec{r} \mid e^{D_0 t} \mid \vec{k}'\vec{r}' \rangle$. To evaluate this, consider the state

$$\langle \vec{k}\vec{r}t \mid \equiv \langle \vec{k}\vec{r} \mid e^{D_0 t} \, . \tag{A1}$$

Applying the operator $\vec{k}_{op}$ to this state we see that

$$\langle \vec{k}\vec{r}t \mid \vec{k}_{op} = \langle \vec{k}\vec{r} \mid (e^{D_0 t} \vec{k}_{op} e^{-D_0 t}) e^{D_0 t} \, . \tag{A2}$$

But the operator $\vec{k}_{op}(t) \equiv e^{-D_0 t} \vec{k}_{op} e^{D_0 t}$ obeys the classical equation of motion because

$$\frac{d}{dt} \vec{k}_{op}(t) = e^{-D_0 t} [-D_0 , \vec{k}_{op}] e^{D_0 t}$$

$$= \vec{F}(\vec{k}_{op}(t), \vec{r}_{op}(t)) \, , \tag{A3}$$

with the solution $\vec{\kappa}(t; \vec{k}_{op}\vec{r}_{op})$. Thus

$$\langle \vec{k}\vec{r}t \mid \vec{k}_{op} = \langle \vec{k}\vec{r}t \mid \vec{\kappa}(-t; \vec{k}\vec{r}) \tag{A4}$$

and similarly

$$\langle \vec{k}\vec{r}t \mid \vec{r}_{op} = \langle \vec{k}\vec{r}t \mid \vec{\rho}(-t; \vec{k}\vec{r}) \, . \tag{A5}$$

Thus

$$\langle \vec{k}\vec{r}t \mid = \langle \vec{\kappa}(-t; \vec{k}\vec{r}), \ \vec{\rho}(-t; \vec{k}\vec{r}) \mid \tag{A6}$$

and so

$$\langle \vec{k}\vec{r} \mid e^{D_0 t} \mid \vec{k}'\vec{r}' \rangle = \delta(\vec{k}' - \vec{\kappa}(-t; \vec{k}\vec{r})) \, \delta(\vec{r}' - \vec{\rho}(-t; \vec{k}\vec{r})) \, . \tag{A7}$$

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[1] P. J. Price, Bull. Am. Phys. Soc. 4, 129 (1959); in *Proceedings of the Ninth International Conference on the Physics of Semiconductors*, edited by S. M. Ryvkin (Nauka Publishing House, Leningrad, 1968), Vol. II, p. 753 ff.

[2] P. J. Price, IBM J. Res. Develop. 14, 12 (1970).

[3] H. D. Rees, Phys. Letters 26A, 416 (1968); J. Phys. Chem. Solids 30, 643 (1969).

[4] H. D. Rees, Solid State Commun. 7, 267 (1969); IBM J. Res. Develop. 13, 537 (1969).

[5] H. F. Budd, J. Phys. Soc. Japan Suppl. 21, 420 (1966); Phys. Rev. 158, 798 (1967).

[6] By detailed balance one means that the electron distribution and the collision operator are such that the total rate of scattering from $\vec{k}'$ to $\vec{k}$ equals that from $\vec{k}$ to $\vec{k}'$, i.e., $W(\vec{k}, \vec{k}')g(\vec{k}') = W(\vec{k}', \vec{k})g(\vec{k})$. In such a case, if we define $S(\vec{k}, \vec{k}') = W(\vec{k}, \vec{k}')/g(\vec{k})$, we see that $S(\vec{k}, \vec{k}') = S(\vec{k}', \vec{k})$.

[7] The eigenvalues of D_1 and $\tilde{D}_1$ are the same because the two operators are related by a similarity transformation. Now if we take the "average" of $\tilde{D}_1$ in an arbitrary state $\phi(\vec{k})$, then the first term

$$\int\int d^3k \, d^3k' \, \phi(\vec{k}) [g(\vec{k})]^{1/2} S(\vec{k}\vec{k}') [g(\vec{k}')]^{1/2} \phi(\vec{k}')$$

can be viewed as the inner product in the space of functions $\vec{k}$ *and* $\vec{k}'$ of two functions:

$$\phi(\vec{k}) \, [S(\vec{k}, \vec{k}')]^{1/2} [g(\vec{k}')]^{1/2}$$

and

$$[g(\vec{k}')]^{1/2} \, [S(\vec{k}, \vec{k}')]^{1/2} \phi(\vec{k}') .$$

By Schwarz's inequality, this term is less than or equal to

$$\int\int d^3k \, d^3k' \mid \phi(\vec{k}) \mid^2 S(\vec{k}, \vec{k}') g(\vec{k}'),$$

which is just minus the average of the second term $\int d^3k \mid \phi(\vec{k}) \mid^2 w(\vec{k})$. Thus,

$$\int\int d^3k \, d^3k' \, \phi(\vec{k}) \, \tilde{D}_1(\vec{k}\vec{k}') \phi(\vec{k}') \leq 0.$$

Furthermore, for the equality to hold, these two functions of $\vec{k}$ and $\vec{k}'$ must be proportional to one another implying that the eigenvector of $\tilde{D}_1$ belonging to the eigenvalue zero is $\phi_1(\vec{k}) \propto [g(\vec{k})]^{1/2}$ and the corresponding right eigenvector of D_1 is just $g(\vec{k})$.

[8] After these papers were prepared, a paper by P. M. Bakshi and E. P. Gross, Ann. Phys. (N. Y.) 49, 513 (1968), was called to our attention by Dr. P. J. Price. Bakshi and Gross, considering models that generalize the first model of the following paper by choosing $W(\vec{k}, \vec{k}')$ to have the structure $s(\vec{k})\, r(\vec{k}')$, are interested in the detailed dependence on F of the steady-state distribution function and steady-state current. They demonstrate how these dependences may differ from simple power-series expansions.

[9] R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1962), pp. 177 and 196.

[10] For positive time differences $t - t'$, the retarded Green's function $P_0(t - t')$ and the propagation function $u_0(t - t')$, of course, agree; and for time-dependent fields the same generalization that was discussed in Sec. III for $u_0(t, t')$ also defines $P_0(t, t')$.

[11] H. D. Rees, J. Phys. C 3, 965 (1970).

[12] Actually we wish to prove that

$$\beta \equiv \int d^3k \lim_{\eta \to 0+} \int_0^\infty dt \, e^{-\eta t} e^{Dt} D' f^s = 0,$$

but we have observed only that $\int d^3k \, e^{Dt} D' f^s = 0$. Our "proof" has therefore implicitly assumed that the $\vec{k}$ integration could be exchanged with the limit $\eta \to 0+$

and $\int_0^\infty dt$. Since we shall be concerned below with the fact that certain other limits cannot be interchanged without affecting the results, a comment about this particular interchange seems necessary. We shall assume that $\vec{k}$ space is finite (say, one Brillouin zone) and that the functions we consider like $e^{Dt}D'f^s$ are continuous in $\vec{k}$. Under these assumptions, the interchange of $\int d^3k$ with the limit $\eta \to 0+$ and $\int_0^\infty dt$ is justifiable.

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Hot-Electron Problem. II. Two Soluble Models

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Two exactly soluble models for the hot-electron problem are introduced. The models are used to illustrate and gain insight into various approaches to the time-dependent and steady-state problems and to the perturbation theory from a known steady state. For one of the models it is shown that the optimum choice for a generalized self-scattering rate violates Rees's condition (that the self-scattering rate be positive) everywhere.

I. INTRODUCTION

In the preceding paper,[1] we have presented an operator formulation of the hot-electron problem that is developed in analogy with the operator formulation of quantum mechanics. The analogy rests on the fact that both the Boltzmann equation and the time-dependent Schrödinger equation are first order in $\partial/\partial t$.

In the present paper we wish to gain further insight into hot-electron problems and mathematical techniques for their solution by introducing two soluble models. We shall derive and discuss their exact behavior (time development, steady state, linear response) and also some of the approximation methods used for the real problem.

II. SUMMARY OF FORMAL RESULTS OF I

In this section we briefly summarize the formal results of I. We write the Boltzmann equation in the abstract operator form

$$\frac{\partial}{\partial t} f = (D_0 + D_1)f = Df \,, \tag{2.1}$$

where D_0 is an operator representing all the convective terms of the Boltzmann equation, which in the $(\vec{k}\vec{r})$ representation is

$$D_0 = \vec{F}(\vec{r}) \cdot \vec{\nabla}_k + \vec{v}(\vec{k}) \cdot \vec{\nabla}_r \,. \tag{2.2}$$

D_1 is the difference between the in-scattering and out-scattering operators,

$$D_1 = W - w \,. \tag{2.3}$$

For translationally invariant systems, where $\vec{r}$ can be ignored, W in the $\vec{k}$ representation is just the integral operator $\int d^3k' W(\vec{k}, \vec{k}')$ acting on any function of $\vec{k}'$ and w is just the diagonal operator $\int d^3k' w(\vec{k}) \delta(\vec{k} - \vec{k}')$, where

$$w(\vec{k}) = \int d^3k'' W(\vec{k}'', \vec{k}) \,. \tag{2.4}$$

The time development of $f(t)$ is formally given by

$$f(t) = e^{Dt} f(0) \,. \tag{2.5}$$

Various methods of evaluating e^{Dt} were suggested, including straightforward stepwise integration,

$$f((n+1)\Delta t) = e^{D_0 t}(1 + D_1 \Delta t) f(n\Delta t) \quad \text{as} \quad \Delta t \to 0 \,, \tag{2.6}$$

and use of higher-order integration methods on the equation in the "interaction picture,"

$$\frac{\partial}{\partial t} f^I(t) = D_1^I(t) f^I(t) \,, \tag{2.7}$$

where

$$f^I(t) = e^{-D_0 t} f(t) \tag{2.8a}$$

and

$$D_1^I(t) = e^{-D_0 t} D_1 e^{D_0 t} \,. \tag{2.8b}$$

In all such approaches, use is made of the fact that $e^{D_0 t}$ translates all particles along their classical trajectories for a time t without scattering.

A stepwise integration method by Rees[2] appears in this formalism as

$$f(t + 1/\Gamma) = \Gamma \int_0^\infty dt' e^{-\Gamma t'} e^{D_0 t'} (1 + D_1/\Gamma) f(t) \quad \text{as} \quad \Gamma \to \infty \,, \tag{2.9}$$

which is similar to but more complicated than (2.6).

The time-independent problem for the steady-state solution f^s is to be solved by iterating the equation

$$f^s_{n+1} = (U - D_0)^{-1}(D_1 + U) f^s_n \,, \tag{2.10}$$