

Onsager relations and hydrodynamic balance equations

M. W. Wu, H. L. Cui, and N. J. M. Horing

Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030

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In this paper we clarify the role of heat flux in the hydrodynamic balance equations, facilitating the formulation of an Onsager relation within the framework of this theory. Previously thought to be unobtainable from the present form of the theory [X.L. Lei, J. Cai, and L.M. Xie, *Phys. Rev. B* **38**, 1529 (1988)], our verification of the Onsager relation for linear particle and heat flux currents driven by electric fields and temperature gradients resolves a puzzling issue of long standing. Our results show that, for any temperature, when electron density is sufficiently high, the linear predictions of balance equation theory exactly satisfy the Onsager relation. The condition of high density is consonant with the requirement of strong electron-electron interactions for the validity of the Lei-Ting balance equations. Our results support the validity of this theory for a weakly nonuniform system. We also discuss a possible method of extending this theory to a system further removed from thermal equilibrium. [S0163-1829(96)02027-9]

I. INTRODUCTION

The balance equation transport theory of Lei and Ting^{1,2} was originally developed to treat high-field electrical condition in homogeneous semiconductors and has achieved much success in hot-electron semiconductor transport problems. This theory is based on a separation of the center of mass of the system from the relative motion of electrons in the presence of a uniform electric field. The center of mass is treated as a classical particle, whereas the relative electron system, which is composed of a large number of interacting particles, is treated fully quantum mechanically. The theory has been successfully applied to a variety of transport problems and the results obtained have exhibited good agreement with experiments.³ This theory was subsequently generalized to deal with weakly nonuniform, inhomogeneous systems by Lei *et al.*⁴ The resulting hydrodynamic balance equations obtained by them consist of the following three equations: (a) the continuity equation, (b) the momentum balance equation, and (c) the energy balance equation.

The form of these hydrodynamic balance equations appears very similar to their classical counterparts, generally called hydrodynamic models.⁵⁻¹⁶ However, in fact, they are quite different. The latter is derived from the Boltzmann transport equation, as the first three moments of that equation. Very recently, the fourth moment was discussed by Anile *et al.*¹⁷⁻¹⁹ in an attempt to include the equation describing heat flux. Although, in principle, a complete determination of Boltzmann equation is equivalent to the determination of all the moments, it is not practical to solve the infinite hierarchy of coupled equations governing the various moments. The hydrodynamic approach is based on truncation of this hierarchy after the second-order moment and simplification of the remaining equations. However, these three moment equations by themselves do not form a closed system, requiring input of information about scattering, generally supplied in the form of momentum and energy relaxation times. Nevertheless, to accurately evaluate the relaxation times requires a predetermination of the distribution function, which is precisely the task that the hydrodynamic

models strive to avoid. This difficulty is circumvented by one of the following ways. One approach is to calculate the relaxation times by Monte Carlo simulations. Another employs empirical forms of relaxation times. The third is to postulate a distribution function with unknown parameters and use the hydrodynamic equations to solve for these parameters. One of the most popular parametrized distribution functions is the drifted Maxwell distribution, which depends on two unknown parameters: the electron drift velocity and the electron temperature. The hydrodynamic balance equation approach employs a drifted local equilibrium description similar to the latter. In this it employs unknown parameters including the local electron temperature $T_e(\mathbf{R})$, local electron drift velocity $\mathbf{v}(\mathbf{R})$, and local chemical potential $\mu(\mathbf{R})$. The distinctive features of the balance equation theory rest with the ansatz of such local equilibrium parameters in an appropriately chosen initial density matrix, which is treated quantum mechanically, describing the dynamics of the many-body system of electrons, impurities, and phonons. Of course, these unknown parameters are also to be determined from the resulting balance equations. It is now believed that the specific quasiequilibrium form of the initial density matrix chosen in balance equation theory is specifically suited to the condition of strong electron-electron interactions, since it requires rapid thermalization about the drifted transport state.^{20,21} A salient feature of this hydrodynamic approach is that it includes a microscopic description of scattering in the form of a frictional force function due to electron-impurity and electron-phonon scattering, as well as an electron energy loss rate function due to electron-phonon interaction. These functions are calculated within the model itself, as functions of carrier drift velocity and carrier temperature, along with the carrier density, which are themselves determined self-consistently within the same model. These hydrodynamic balance equations have recently been applied to device simulations by Cai *et al.*²²⁻²⁴

A hitherto unresolved question, unanswered since the development of hydrodynamic balance equations, concerns the capability of this theory to lead to the correct form of Onsager relations^{25,26} and/or how to determine Onsager rela-

tions within the framework of this theory. There is even some misunderstanding that the energy flux predicted by this theory is zero. The purpose of this paper is to clarify the role of heat flux in this theory and also to show how to generate Onsager relations within the framework of this theory. We have closely checked the Onsager relation predicted by this theory and find that for any temperature, when electron density is sufficiently high, the balance equation theory satisfies Onsager relations exactly. The condition of high density is consonant with the requirement that Lei-Ting balance equations hold only for strong electron-electron interactions. Furthermore, our results support the validity of this theory in weakly nonuniform systems. To our knowledge, this is the first set of hydrodynamic equations that obeys Onsager relation exactly. Anile and Muscato showed very recently,¹⁹ by Monte Carlo simulation, that the Onsager relation fails in the traditional hydrodynamic models.

This paper is organized as follows. In Sec. II we briefly review the hydrodynamic balance equations by Lei *et al.*⁴ This is not insignificant because this is the starting point of our further discussion. Moreover, we further explicitly exhibit the role of the energy flux in this theory and rewrite the hydrodynamic force and energy balance equations in forms somewhat different from those of Lei *et al.*,⁴ which clarifies the meaning of every term. Then, in Sec. III we derive the Onsager relation for linear particle and heat flux currents driven by electric field and temperature gradient and check it closely. We present our conclusions and discussions in Sec. IV.

II. HYDRODYNAMIC BALANCE EQUATIONS

The starting point of hydrodynamic balance equation theory developed by Lei *et al.*⁴ consists of the fluid-element-composed electron Hamiltonian

$$H = \int d\mathbf{R} [H_e(\mathbf{R}) + H_I(\mathbf{R})]. \quad (1)$$

Here

$$H_e(\mathbf{R}) = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \delta(\mathbf{r}_i - \mathbf{R}) \quad (2)$$

denotes the kinetic energy and Coulomb interaction energy of electrons within a fluid cell around \mathbf{R} . Macroscopically this cell is small, over which all the expectations of physical quantities change little, whereas microscopically it is large enough that a great number of particles are within it. \mathbf{p}_i and \mathbf{r}_i are the momentum and coordinate of the i th electron,

$$H_I(\mathbf{R}) = \sum_i [e\phi(\mathbf{r}_i) + \Phi(\mathbf{r}_i)] \delta(\mathbf{r}_i - \mathbf{R}) \quad (3)$$

is the interaction Hamiltonian in which $\phi(\mathbf{r})$ denotes the potential of the external electric field \mathbf{E} , hence $\mathbf{E} = -\nabla\phi(\mathbf{r})$, and $\Phi(\mathbf{r}) = \sum_a u(\mathbf{r} - \mathbf{R}_a) + \sum_{\mathcal{L}} \mathbf{u}_{\mathcal{L}} \cdot \nabla v_{\mathcal{L}}(\mathbf{r} - \mathbf{R}_{\mathcal{L}})$ represents the scattering potential due to randomly distributed (\mathbf{R}_a) impurities and lattice vibrations ($\mathbf{R}_{\mathcal{L}}$ stands for the lattice sites). The number density of electrons in the cell around \mathbf{R} may be written as

$$N(\mathbf{R}) = \sum_i \delta(\mathbf{r}_i - \mathbf{R}). \quad (4)$$

Similarly the \mathbf{R} -dependent momentum density is given by

$$\mathbf{P}(\mathbf{R}) = \sum_i \mathbf{p}_i \delta(\mathbf{r}_i - \mathbf{R}). \quad (5)$$

Letting $\mathbf{v}(\mathbf{R})$ be the average electron velocity in the fluid cell about \mathbf{R} , which is a parameter to be determined self-consistently from the resulting balance equations, one can write the statistical average of the momentum density as

$$\langle \mathbf{P}(\mathbf{R}) \rangle = mn(\mathbf{R})\mathbf{v}(\mathbf{R}), \quad (6)$$

with $n(\mathbf{r}) = \langle N(\mathbf{R}) \rangle$, the statistical average of the electron number density. Introducing relative electron variables

$$\mathbf{p}'_i = \mathbf{p}_i - m\mathbf{v}(\mathbf{R}), \quad \mathbf{r}'_i = \mathbf{r}_i - \mathbf{R}, \quad (7)$$

which represent the momentum and coordinate of the i th electron relative to the center of mass of the fluid cell around \mathbf{R} , we can write the statistical average of $H_e(\mathbf{R})$ as

$$\langle H_e(\mathbf{R}) \rangle = u(\mathbf{R}) + \frac{1}{2} mn(\mathbf{R})v^2(\mathbf{R}), \quad (8)$$

with

$$u(\mathbf{R}) = \left\langle \sum_i \frac{\mathbf{p}'_i{}^2}{2m} \delta(\mathbf{r}'_i) \right\rangle \quad (9)$$

denoting the average kinetic energy of the relative electron in cell \mathbf{R} . It is noted that in deriving Eq. (8) we have treated electron-electron Coulomb interaction effect in the spirit of Landau fermi-liquid theory, which is appropriate for electrons in semiconductors and metals, i.e., it leads to a self-energy correction in the single electron energy, and also renormalizes the bare phonon frequency, jointly with the bare electron-phonon interaction vertex, and also the electron-impurity interaction vertex.^{27,26,28} We assume that these renormalized corrections are already included in the corresponding quantities. The use of the Hamiltonian above is well established and similar to those discussed in the book of Zubarev.²⁹

Lei *et al.*⁴ derived hydrodynamic balance equations by considering the statistical rates of change given by Heisenberg equations of motion for particle number density $\dot{N}(\mathbf{R}) = -i[N(\mathbf{R}), H]$, momentum density $\dot{\mathbf{P}}(\mathbf{R}) = -i[\mathbf{P}(\mathbf{R}), H]$, and electron kinetic energy density $\dot{H}_e(\mathbf{R}) = -i[H_e(\mathbf{R}), H]$. The resulting hydrodynamic balance equations describe continuity, momentum balance, and energy balance as (respectively)

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0, \quad (10)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{2}{3} \frac{\nabla u}{mn} + \frac{e}{m} \mathbf{E} + \frac{\mathbf{f}}{mn}, \quad (11)$$

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = -\frac{5}{3} u(\nabla \cdot \mathbf{v}) - w - \mathbf{v} \cdot \mathbf{f}. \quad (12)$$

In these equations, \mathbf{f} represents the resistive force experienced by the field element due to impurity and phonon scatterings and w is the electron energy loss rate. They are given by

$$\mathbf{f}(\mathbf{R}) = - \left\langle \sum_i \nabla \Phi(\mathbf{r}'_i + \mathbf{R}) \delta(\mathbf{r}'_i) \right\rangle, \quad (13)$$

$$w(\mathbf{R}) = \frac{1}{2} \left\langle \sum_i \frac{\mathbf{p}'_i}{m} \cdot \nabla \Phi(\mathbf{r}'_i + \mathbf{R}) \delta(\mathbf{r}'_i) \right\rangle + \frac{1}{2} \left\langle \sum_i \nabla \Phi(\mathbf{r}'_i + \mathbf{R}) \cdot \frac{\mathbf{p}'_i}{m} \delta(\mathbf{r}'_i) \right\rangle - \mathbf{v}(\mathbf{R}) \cdot \mathbf{f}(\mathbf{R}). \quad (14)$$

Introducing the particle flux density operator $\mathbf{J}(\mathbf{R})$, which can be derived from the momentum density operator Eq. (5) as

$$\mathbf{J}(\mathbf{R}) = \frac{1}{m} \mathbf{P}(\mathbf{R}) = \sum_i \frac{\mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}), \quad (15)$$

we can rewrite the momentum balance equation (11) as

$$\frac{\partial}{\partial t} \langle \mathbf{J}(\mathbf{R}) \rangle + \nabla \cdot [\langle \mathbf{J}(\mathbf{R}) \rangle \mathbf{v}] = - \frac{2}{3m} \nabla u(\mathbf{R}) + \frac{en(\mathbf{R})\mathbf{E}}{m} + \frac{\mathbf{f}(\mathbf{R})}{m}. \quad (16)$$

$\langle \mathbf{J}(\mathbf{R}) \rangle$ denotes the statical average of $\mathbf{J}(\mathbf{R})$ and it follows that

$$\langle \mathbf{J}(\mathbf{R}) \rangle = n(\mathbf{R}) \mathbf{v}(\mathbf{R}). \quad (17)$$

The energy flux operator, which is central to identifying system response to a temperature gradient, is given by

$$\mathbf{J}_H(\mathbf{R}) = \sum_i \frac{\mathbf{p}'_i}{2m} \frac{\mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}) \quad (18)$$

and its statistical average is

$$\langle \mathbf{J}_H(\mathbf{R}) \rangle = \frac{5}{3} u(\mathbf{R}) \mathbf{v}(\mathbf{R}) + \frac{1}{2} mn(\mathbf{R}) v^2(\mathbf{R}) \mathbf{v}(\mathbf{R}). \quad (19)$$

This is just the energy flux predicted by hydrodynamic balance equation theory. Using $\langle \mathbf{J}_H(\mathbf{R}) \rangle$, the energy balance equation can be rewritten as

$$\frac{\partial u}{\partial t} + \nabla \cdot \langle \mathbf{J}_H \rangle = \frac{2}{3} \mathbf{v} \cdot \nabla u + \frac{1}{2} m v^2 \nabla \cdot (n \mathbf{v}) + \frac{1}{2} mn \mathbf{v} \cdot \nabla v^2 - w - \mathbf{v} \cdot \mathbf{f}. \quad (20)$$

Equations (10) and (16) are now structurally in the same form as those of hydrodynamic model, which are derived from first and second moments of the Boltzmann equation as in Refs. 17–19.

The resistive force \mathbf{f} and the energy transfer rate w , together with the local kinetic energy u and the local density n , are calculated within the framework of balance equation theory,¹ which requires knowledge of the density matrix $\hat{\rho}$. This density matrix can be determined by solving the Liou-

ville equation $i \partial \hat{\rho} / \partial t = [H, \hat{\rho}]$ with an appropriate initial condition. In the balance equation theory, the electron-impurity and electron-phonon couplings are turned on from $t=0$, together with the electric field \mathbf{E} . Meanwhile, in the present model the interactions between different fluid cells are included approximately in the local potential with a mean-field treatment. Therefore different cells are dynamically independent and thus evolve separately from their own initial state. Thus the \mathbf{R} -dependent initial density matrix is chosen such that the relative electron system in the fluid cell is in a local quasi-thermal equilibrium state at electron temperature $T_e(\mathbf{R})$ and chemical potential $\mu(\mathbf{R})$, which are parameters to be determined self-consistently from the resulting hydrodynamic balance equations, whereas the phonon system is assumed in thermal equilibrium

$$\hat{\rho}_0 = \frac{1}{Z} \exp \left\{ - \sum_{\mathbf{R}} [H_e(\mathbf{R}) - \mathbf{v}(\mathbf{R}) \cdot \mathbf{P}(\mathbf{R}) - \mu N(\mathbf{R})] / T_e(\mathbf{R}) \right\} \times \exp(-H_{\text{ph}}/T), \quad (21)$$

with H_{ph} and T being the phonon Hamiltonian and temperature, respectively. It follows that the resistive force and the energy transfer rate are given by

$$\begin{aligned} \mathbf{f}(\mathbf{R}) &= \mathbf{f}(n(\mathbf{R}), T_e(\mathbf{R}), \mathbf{v}(\mathbf{R})) = n_i \sum_{\mathbf{q}} \mathbf{q} |u(\mathbf{q})|^2 \Pi_2(\mathbf{q}, \mathbf{q} \cdot \mathbf{v}(\mathbf{R})) \\ &\quad - 2 \sum_{\mathbf{q}, \lambda} \mathbf{q} |M(\mathbf{q}, \lambda)|^2 \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}_d) \\ &\quad \times \left[n \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) - n \left(\frac{\Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}(\mathbf{R})}{T_e(\mathbf{R})} \right) \right], \\ w(\mathbf{R}) &= w(n(\mathbf{R}), T_e(\mathbf{R}), \mathbf{v}(\mathbf{R})) \\ &= 2 \sum_{\mathbf{q}, \lambda} \Omega_{\mathbf{q}\lambda} |M(\mathbf{q}, \lambda)|^2 \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}_d) \\ &\quad \times \left[n \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) - n \left(\frac{\Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}(\mathbf{R})}{T_e(\mathbf{R})} \right) \right], \end{aligned} \quad (23)$$

with $n(x) = (e^x - 1)^{-1}$ being Bose distribution function, n_i the impurity density, $\Omega_{\mathbf{q}\lambda}$ the phonon frequency of wave \mathbf{q} and mode λ , $u(\mathbf{q})$ the electron-impurity interaction potential, and $M(\mathbf{q}, \lambda)$, the electron-phonon correction matrix element. $\Pi_2(\mathbf{q}, \lambda)$ denotes the imaginary part of electron density-density correction function. Note that \mathbf{f} and w depend on \mathbf{R} through the quantities $n(\mathbf{R})$, $T_e(\mathbf{R})$, and $\mathbf{v}(\mathbf{R})$. The average local kinetic energy density of the relative electrons is

$$u = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} f[(\varepsilon_{\mathbf{k}} - \mu)/T_e] \quad (24)$$

and the local chemical potential $\mu(\mathbf{R})$ is related to the local density $n(\mathbf{R})$ of electrons through the relation

$$n = 2 \sum_{\mathbf{k}} f[(\varepsilon_{\mathbf{k}} - \mu)/T_e], \quad (25)$$

with $\varepsilon_{\mathbf{k}} = k^2/2m$ and $f(x) = 1/(e^x + 1)$ representing the energy dispersion of electrons and fermi distribution function, respectively.

Within the framework of hydrodynamic balance equation theory, the velocity field $\mathbf{v}(\mathbf{R})$, the electron temperature field $T_e(\mathbf{R})$, as well as the chemical potential field $\mu(\mathbf{R})$ are fundamental parametric variables. The other pertinent variables to be determined are particle flux $\langle \mathbf{J} \rangle$, energy flux $\langle \mathbf{J}_H \rangle$, average local kinetic energy density $u(\mathbf{R})$, local number density of electrons $n(\mathbf{R})$, as well as local electrical potential $\phi(\mathbf{R})$ or field $\mathbf{E}(\mathbf{R})$. Moreover, there are three balance equations (10), (16), and (20), supplemented by four relations (17), (19), (24), and (25), as well as the Poisson equation relating the electron density with the potential

$$\nabla^2 \phi = -4\pi e[n(\mathbf{R}) - n^+], \quad (26)$$

with n^+ as the density of the ionized donor background. These eight equations form a close set of equations for the hydrodynamic device modeling.

III. ONSAGER RELATION IN THE HYDRODYNAMIC BALANCE EQUATION APPROACH

In this section, we demonstrate the Onsager relation;^{25,26} more accurately, we verify the validity of hydrodynamic balance equations in regard to the Onsager relation. It is well known that the Onsager relation is a manifestation of microscopic irreversibility for any statistical system near thermal equilibrium. Therefore any properly formulated statistical physics model should satisfy this relation. It is very easy to verify this relation in the framework of Kubo linear-response theory. Moreover, if one can determine the distribution function from the Boltzmann equation, it is also straightforward to verify the Onsager relation by calculating the pertinent moments of the distribution function. However, for the traditional hydrodynamic model,⁵⁻¹⁶ verification has been elusive. In fact, in a very recent article, Anile and Muscato¹⁹ showed that the Onsager relation breaks down in this model. Although they tried to circumvent this difficulty, they did not establish the existence of the relation they employed within the model itself by Monte Carlo simulation. Here we will examine the Onsager relation within the framework of the hydrodynamic balance equations.

The Onsager relation²⁶ is concerned with the linear response of the particle current $\langle \mathbf{J} \rangle$ and the heat flux $\langle \mathbf{J}_Q \rangle$ near thermal equilibrium, which flow as a result of forces \mathbf{X}_i on the system:

$$\langle \mathbf{J} \rangle = L^{11} \mathbf{X}_1 + L^{12} \mathbf{X}_2, \quad (27)$$

$$\langle \mathbf{J}_Q \rangle = L^{21} \mathbf{X}_1 + L^{22} \mathbf{X}_2, \quad (28)$$

with $\mathbf{X}_1 = -(1/T) \nabla(\mu + e\phi)$ and $\mathbf{X}_2 = \nabla(1/T)$. The Onsager relation states that

$$L^{12} = L^{21}. \quad (29)$$

The heat flux $\langle \mathbf{J}_Q \rangle$ relates to the energy flux in Eq. (19) through

$$\langle \mathbf{J}_Q \rangle = \langle \mathbf{J}_H \rangle - \mu \langle \mathbf{J} \rangle. \quad (30)$$

The fluxes $\langle \mathbf{J} \rangle$ and $\langle \mathbf{J}_H \rangle$ have already been defined in the previous section by Eqs. (17) and (19). Our first task is to express them in terms of linear response in the form of Eqs. (27) and (28).

The first relation can be acquired directly by linearization of force balance equation (16) near thermal equilibrium, so that we only need to consider a steady state with the external electric field \mathbf{E} and the spatial gradient being very small.³⁰ Then $T_e = T$ and \mathbf{v} is also very small. We take \mathbf{E} , ∇T , and \mathbf{v} to be in the x direction and treat Eq. (16) to first order in the small quantities. This means, for instance, that the gradient operator $\nabla_x \equiv \partial/\partial x$ is a first-order small quantity and v_x is also a first-order small quantity; thus $\nabla_x v_x$ is a higher-order small quantity and can be neglected. These facts should be kept in mind in all of our following calculations. Therefore the force balance equation (2) can be written as

$$0 = -\frac{2}{3nm} \nabla_x u + \frac{eE_x}{m} + \frac{f_x}{nm}. \quad (31)$$

All the quantities in the other two directions are zero. For small v_x , f_x is proportional to v_x ,² thus proportional to $\langle J_x \rangle$, and

$$\rho = -\frac{f_x}{n^2 e^2 v_x} = -\frac{f_x}{n e^2 \langle J_x \rangle} \quad (32)$$

is the resistivity and independent of v_x ($\langle J_x \rangle$), which is given by

$$\begin{aligned} \rho = & -\frac{4\pi}{n^2 e^2} \sum_{\mathbf{q}, \lambda} q_x^2 |M(\mathbf{q}, \lambda)|^2 \left[-\frac{1}{T} n' \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) \right] \left[f \left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T} \right) \right. \\ & \left. - f \left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T} \right) \right] \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \Omega_{\mathbf{q}\lambda}) \\ & - \frac{n_i}{n^2 e^2} \sum_{\mathbf{q}} q_x^2 |u(\mathbf{q})|^2 \frac{\partial}{\partial \omega} \Pi_2(\mathbf{q}, \omega) \Big|_{\omega=0}. \end{aligned} \quad (33)$$

We then have

$$\langle J_x \rangle = \frac{E_x}{e\rho} - \frac{2}{3} \frac{\nabla_x u}{n e^2 \rho}. \quad (34)$$

Employing Eqs. (24) and (25), we can express Eq. (34) in the form of Eq. (27), with

$$L^{11} = \frac{T}{\rho e^2}, \quad (35)$$

$$L^{12} = \frac{T^2}{\rho e^2} \left[\frac{5}{3} \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} - \zeta \right]. \quad (36)$$

Here $\zeta = \mu/T$ and the function $F_\nu(y)$ is defined by

$$F_\nu(y) = \int_0^\infty \frac{x^\nu dx}{\exp(x-y) + 1}. \quad (37)$$

The procedure for identifying the linearized heat flux is, of course, similar to that of particle flux. Therefore we consider the rate of change of the energy flux operator \mathbf{J}_H defined by Eq. (18):

$$\begin{aligned}
\dot{\mathbf{J}}_H(\mathbf{R}) &= -i[\mathbf{J}_H(\mathbf{R}), H] \\
&= -\nabla \cdot \mathcal{A} + \frac{1}{2} \sum_i \frac{(e\mathbf{E} + \mathbf{F}_i) \cdot \mathbf{p}_i}{2m} \frac{\mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}) \\
&\quad + \frac{1}{2} \sum_i \frac{\mathbf{p}_i \cdot (e\mathbf{E} + \mathbf{F}_i)}{2m} \frac{\mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}) \\
&\quad + \frac{1}{2} \sum_i \frac{\mathbf{p}_i^2}{2m} \frac{e\mathbf{E} + \mathbf{F}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}) \\
&\quad + \frac{1}{2} \sum_i \frac{e\mathbf{E} + \mathbf{F}_i}{m} \frac{\mathbf{p}_i^2}{2m} \delta(\mathbf{r}_i - \mathbf{R}) \\
&\quad + \frac{1}{2} \sum_i \frac{\mathbf{p}_i}{m} \frac{(e\mathbf{E} + \mathbf{F}_i) \cdot \mathbf{p}_i}{2m} \delta(\mathbf{r}_i - \mathbf{R}) \\
&\quad + \frac{1}{2} \sum_i \frac{\mathbf{p}_i}{m} \frac{\mathbf{p}_i \cdot (e\mathbf{E} + \mathbf{F}_i)}{2m} \delta(\mathbf{r}_i - \mathbf{R}), \tag{38}
\end{aligned}$$

where we have used the relations

$$\dot{\mathbf{r}}_i = -i[\mathbf{r}_i, H] = \mathbf{p}_i/m, \tag{39}$$

$$\dot{\mathbf{p}}_i = -i[\mathbf{p}_i, H] = [e\mathbf{E} - \nabla\Phi(\mathbf{r}_i)]/m \equiv (e\mathbf{E} + \mathbf{F}_i)/m. \tag{40}$$

The tensor \mathcal{A} is defined as

$$\mathcal{A} = \sum_i \frac{\mathbf{p}_i^2}{2m} \frac{\mathbf{p}_i}{m} \frac{\mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}). \tag{41}$$

Performing the statistical average of Eq. (38), we have

$$\begin{aligned}
\langle \dot{\mathbf{J}}_H \rangle + \nabla \cdot \langle \mathcal{A} \rangle &= \langle \mathbf{B} \rangle + \frac{5}{3m} eu\mathbf{E} + en\mathbf{E} \cdot \mathbf{v}\mathbf{v} \\
&\quad + \frac{1}{2} env^2\mathbf{E} + \frac{1}{2} v^2\mathbf{f} - w\mathbf{v}. \tag{42}
\end{aligned}$$

It is understood that the right-hand side of Eq. (42) is derived by transforming the coordinate and moment operators to the relative variables of Eq. (7), before performing the statistical averages. The expression of $\langle \mathbf{B} \rangle$ is given in the Appendix and $\langle \mathcal{A} \rangle$ can be expressed as

$$\langle \mathcal{A} \rangle = \frac{1}{3} [S(\mathbf{R}) + uv^2] \mathcal{I} + \langle \mathbf{J}_H \rangle \mathbf{v} + \mathbf{v} \langle \mathbf{J}_H \rangle - u\mathbf{v}\mathbf{v} - \frac{1}{2} mnv^2\mathbf{v}\mathbf{v}, \tag{43}$$

with

$$S(\mathbf{R}) = \left\langle \sum_i \frac{\mathbf{p}_i^4}{2m^3} \delta(\mathbf{r}'_i) \right\rangle. \tag{44}$$

This average can be calculated in the balance equation theory mentioned using the density matrix $\hat{\rho}$ discussed in Sec. II, with the result

$$S(\mathbf{R}) = 2 \sum_{\mathbf{k}} \frac{k^4}{2m^3} f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right). \tag{45}$$

It should be emphasized here that if the density matrix employed in the balance equation is exactly the real physical

one, then Eq. (42) should be consistent with Eqs. (10)–(20). This is to say that if we calculate every unknown parameter from the hydrodynamic balance equations presented in Sec. II and substitute them in Eq. (42), then Eq. (42) should merely be an identity. Unfortunately, in fact, this is not the case, especially when the system is a bit far away from weakly nonuniform system. However, here we do not care about it because we only need this equation holds near thermal equilibrium. In this circumstance, the density matrix, chosen in balance equation theory, has already been shown to be reasonable, in particular for a system with strong electron-electron interactions.^{20,21} Therefore Eq. (42) should yield agreement with the balance equations near thermal equilibrium and we may use it to determine the linear response relation of $\langle \mathbf{J}_H \rangle$ with the external forces \mathbf{X}_i and examine whether the result obtained satisfies Onsager relation.

Thus, to the first order in the small quantities, Eq. (42) can be written in the form

$$\frac{5}{3m} eu(\mathbf{R})E_x - \frac{1}{3} \nabla_x S(\mathbf{R}) + \langle B_x \rangle = 0. \tag{46}$$

In deriving this equation, we have used the linearized force and energy balance equations (11) and (12) and $\langle B_x \rangle$ has also been linearized and is proportional to $\langle \mathbf{J}_H \rangle$, which is $\frac{5}{3} uv_x$ to first order. Thus we may define

$$\frac{1}{\tau} = \frac{\langle \mathbf{B} \rangle}{n(\mathbf{R}) \langle \mathbf{J}_H \rangle}, \tag{47}$$

which is also independent of v_x ($\langle \mathbf{J}_H \rangle$). Substituting this relation into Eq. (46) and calculating the gradient of $S(\mathbf{R})$ in Eq. (45), we find that the average energy flux is given by

$$\begin{aligned}
\langle \mathbf{J}_H \rangle &= -\frac{5}{3} \frac{T^2}{m} \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} \tau \mathbf{X}_1 - \frac{T^3}{m} \left[\frac{7}{3} \frac{F_{5/2}(\zeta)}{F_{1/2}(\zeta)} F_{1/2}(\zeta) \right. \\
&\quad \left. - \frac{5}{3} \zeta \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} \right] \tau \mathbf{X}_2. \tag{48}
\end{aligned}$$

Subtracting $\mu \langle \mathbf{J} \rangle$, we obtain the linearized heat flux in terms of \mathbf{X}_1 and \mathbf{X}_2 and can identify the linear coefficients of Eq. (28) as

$$L^{21} = \frac{T^2}{\rho e^2} \left[-\frac{\tau \rho e^2}{m} \frac{5}{3} \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} - \zeta \right], \tag{49}$$

$$\begin{aligned}
L^{22} &= -\frac{\tau T^3}{m} \left[\frac{7}{3} \frac{F_{5/2}(\zeta)}{F_{1/2}(\zeta)} F_{1/2}(\zeta) - \frac{5}{3} \zeta \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} \right] \\
&\quad - \frac{\zeta T^3}{\rho e^2} \left[\frac{5}{3} \frac{F_{3/2}(\zeta)}{F_{1/2}(\zeta)} - \zeta \right]. \tag{50}
\end{aligned}$$

Comparing Eq. (49) with Eq. (36), we find that the condition under which the Onsager relation holds is given by

$$I \equiv -\frac{\tau \rho e^2}{m} = 1. \tag{51}$$

We have closely examined Eq. (51) for a GaAs system to see if it is indeed satisfied in balance equation theory. Both ρ [Eq. (33)] and $\langle B_x \rangle$ (Appendix) are composed of contributions due to electron-impurity, electron-LO-phonon, and

electron–acoustic-phonon scatterings (with the electron–acoustic-phonon scatterings due to longitudinal mode acoustic phonons via deformation potential and piezoelectric interactions, and transverse mode via piezoelectric interaction). We have examined each scattering contribution in detail to check Eq. (51) separately for each interaction. It is clear that if $-(e^2\rho_i/m)/(1/\tau)_i=1$ is satisfied for each interaction, we have $-(e\sum_i\rho_i/m)/\sum_i(1/\tau)_i=1$. Moreover, this procedure effects the fact that the result should be independent of impurity concentration and parameters of the electron-phonon interaction matrixes.

The expressions for I obtained from the balance equations are given by

$$I_{ei} = \frac{\sum_{\mathbf{q}} q^2 |u(\mathbf{q})|^2 \left[\frac{\partial}{\partial \omega} \Pi_2^e(\mathbf{q}, \omega) \right] \Big|_{\omega=0}}{\left(\frac{5}{3} \right) \left(\frac{u}{n} \right) \sum_{\mathbf{q}} q^2 |u(\mathbf{q})|^2 \left[\frac{\partial}{\partial \omega} \Pi_2(\mathbf{q}, \omega) \right] \Big|_{\omega=0}}, \quad (52)$$

due to electron-impurity scattering; and

$$I_{e\text{-ph}}(\lambda) = \frac{\sum_{\mathbf{q}} |M(\mathbf{q}, \lambda)|^2 \Omega_{\mathbf{q}\lambda} (\varepsilon_{\mathbf{q}} + \Omega_{\mathbf{q}\lambda}) n' \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda})}{\left(\frac{5}{3} \right) \left(\frac{u}{n} \right) \sum_{\mathbf{q}} |M(\mathbf{q}, \lambda)|^2 \frac{\mathbf{q}^2}{m} n' \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda})} + \frac{-\sum_{\mathbf{q}} |M(\mathbf{q}, \lambda)|^2 \frac{\mathbf{q}^2}{m} n' \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) \Pi_2^e(\mathbf{q}, -\Omega_{\mathbf{q}\lambda})}{\left(\frac{5}{3} \right) \left(\frac{u}{n} \right) \sum_{\mathbf{q}} |M(\mathbf{q}, \lambda)|^2 \frac{\mathbf{q}^2}{m} n' \left(\frac{\Omega_{\mathbf{q}\lambda}}{T} \right) \Pi_2(\mathbf{q}, \Omega_{\mathbf{q}\lambda})}, \quad (53)$$

due to electron-phonon scattering, for phonons of mode λ . $I_{e\text{-ph}}(\lambda)$ is further composed of contributions due to electron–LO-phonon scattering $I_{e\text{-LO}}$, due to electron–longitudinal acoustic phonons by deformation potential coupling I_{edl} , by piezoelectric interaction I_{ept} , and due to electron–transverse acoustic phonons by piezoelectric interaction I_{ept} . Π_2^e in Eqs. (52) and (53) is defined by

$$\Pi_2^e(\mathbf{q}, \omega) = 2\pi \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \omega) \left[f \left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T} \right) - f \left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T} \right) \right]. \quad (54)$$

For the LO phonon, $\Omega_{\mathbf{q}, \text{LO}} = \Omega_0 = 35.4$ meV and the Frölich matrix element is $|M(\mathbf{q}, \text{LO})|^2 = e^2 (\kappa_{\infty}^{-1} - \kappa^{-1}) \Omega_0 / (2\varepsilon_0 q^2) \propto 1/q^2$. [Since the constants in the matrix elements cancel in Eq. (53), in the following we only specify their relation to

q .] The matrix element due to longitudinal deformation potential coupling is $|M(\mathbf{q}, dl)|^2 \propto q$, that due to longitudinal piezoelectric interaction is $|M(\mathbf{q}, pl)|^2 \propto (q_x q_y q_z)^2 / q^7$, and for the two branches of the independent transverse piezoelectric interaction $\sum_{j=1,2} |M(\mathbf{q}, pt_j)|^2 \propto [q_x^2 q_y^2 + q_y^2 q_z^2 + q_z^2 q_x^2 - (3q_x q_y q_z)^2 / q^2] / q^5$. For acoustic phonons $\Omega_{\mathbf{q}\lambda}$ can be written as $v_s q$, with the longitudinal sound speed v_s being 5.29×10^3 m/s and the transverse sound speed being 2.48×10^3 m/s. The effective mass of electron is $0.07m_e$, with m_e denoting the free-electron mass.

The results of our numerical calculations are presented in Figs. 1 to 5, where contributions to I due to the various interactions discussed above are plotted against electron den-

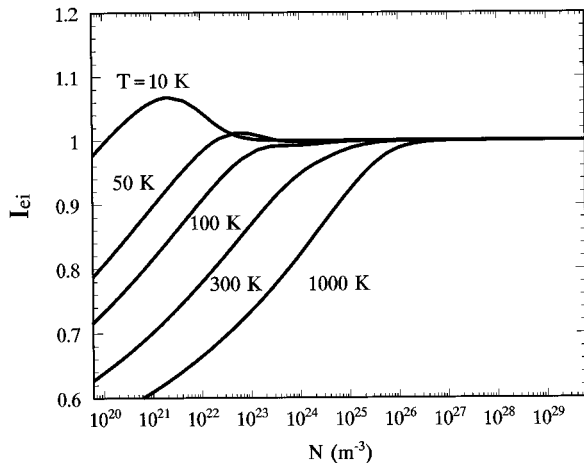


FIG. 1. I due to electron-impurity scattering is plotted as a function of electron density for several different temperatures.

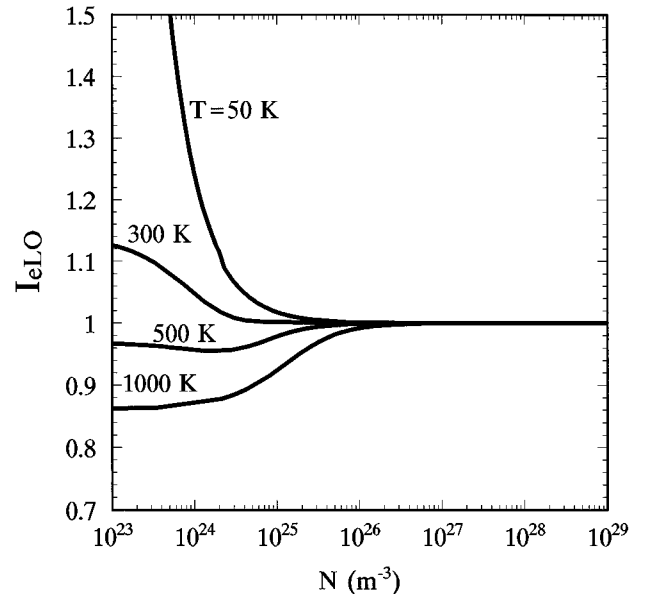


FIG. 2. I due to electron–LO-phonon scattering is plotted as a function of electron density for several different temperatures.

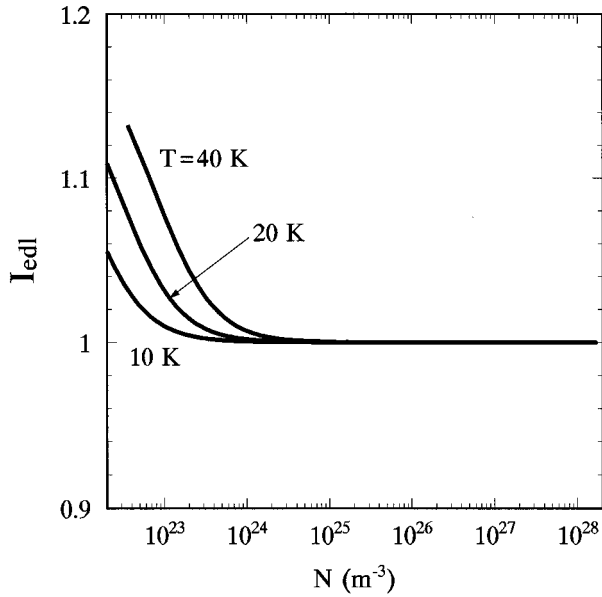


FIG. 3. I due to electron–longitudinal acoustic-phonon scattering via deformation potential coupling is plotted as a function of electron density for several different temperatures.

sity for several different temperatures. As it is generally believed that the contribution of acoustic phonons is important only at low temperature, while the contribution of LO phonons is dominant at high temperature, our temperatures are chosen as 10, 20, and 40 K for the former and 50, 300, 500, and 1000 K for the latter. Impurity scattering is present at any temperature, so we take $T=10, 50, 100, 300,$ and 1000 K in Fig. 1. From these figures it is evident that, for any temperature, when electron density is sufficiently high I is exactly unity, indicating that the Onsager relation holds.

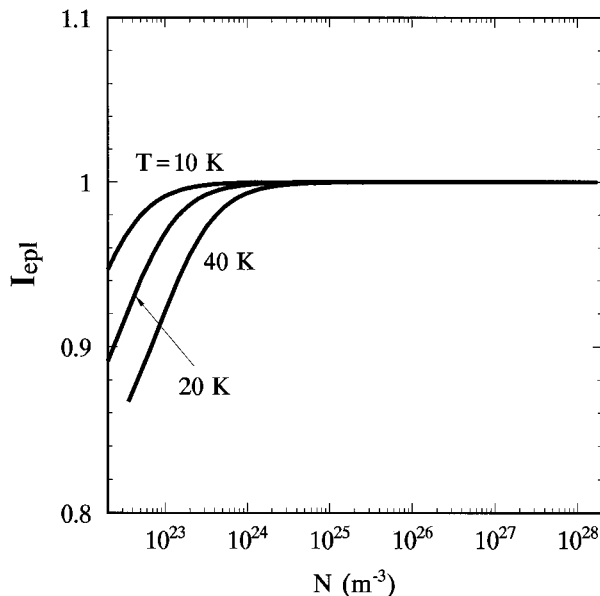


FIG. 4. I due to electron–longitudinal acoustic-phonon scattering via piezoelectric interaction is plotted as a function of electron density for several different temperatures.

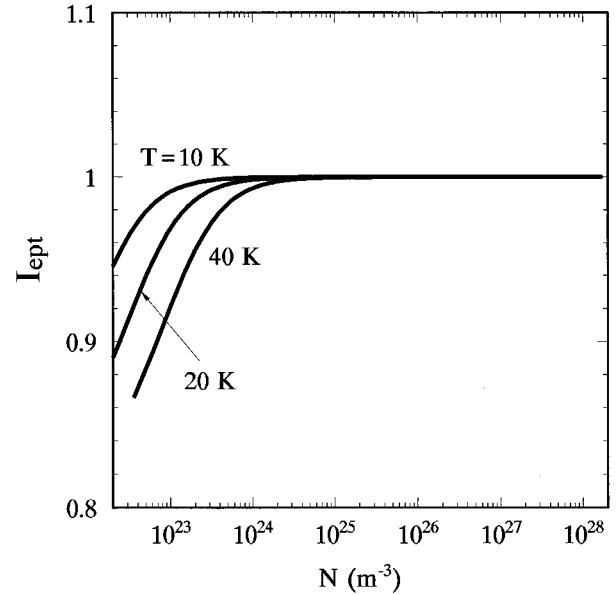


FIG. 5. I due to electron–transverse acoustic-phonon scattering via piezoelectric interaction is plotted as a function of electron density for several different temperatures.

It is also seen from the figures that as temperature becomes higher, the electron density needed to make the Onsager relation hold is also higher. An interesting exception is the LO phonon in Fig. 2, in which we can see that the needed density for $T=300$ K is lower than that for $T=50$ K, to ensure that $I_{eLO}=1$.

IV. CONCLUSIONS AND DISCUSSION

In this paper, we have clarified the role of heat flux in hydrodynamic balance equations. We have further shown that, for any temperature, when electron density is sufficiently high, the hydrodynamic balance equation theory satisfies the Onsager relation. This is consistent with the understanding that the Lei-Ting balance equation theory holds only for strong electron-electron interactions. Our result supports the validity of this theory in a weakly nonuniform system. To our knowledge, this is the first set of hydrodynamic equations that satisfies the Onsager relation self-contained and without the *ad hoc* introduction of terms that do not originate within the theory.

However, we should also point out that the hydrodynamic balance equations can only be used to describe weakly nonuniform systems. When the temperature gradient is large and/or there is a large heat flux in the system, for example, in phenomena such as impact ionization and heat generation in nonuniform systems, the energy flux equation [Eq. (42)], or heat flux equation, which is of paramount importance in describing these phenomena, is no longer consistent with the other balance equations (Eqs. (10)–(20)) and a contradiction emerges. This reflects the inadequacy of the assumed initial density matrix, Eq. (21), in the Lei-Ting balance equation theory, by failing to include the detailed information about the physics of heat flux. This can be further illustrated as follows: In our deriving the average energy flux operator Eq. (18), there should be another term

$$\langle \mathbf{j}_H \rangle = \left\langle \sum_i \frac{\mathbf{p}'_i{}^2}{2m} \frac{\mathbf{p}'_i}{m} \delta(\mathbf{r}'_i) \right\rangle \quad (55)$$

on the right-hand side of Eq. (19). Moreover, in obtaining the average of the tensor \mathcal{A} in Eq. (41), there should be another term $\mathbf{v} \cdot \langle \sum_i (\mathbf{p}'_i/m)(\mathbf{p}'_i/m)(\mathbf{p}'_i/m) \delta(\mathbf{r}'_i) \rangle$ on the right-hand side of Eq. (43). These two terms do not vanish when the system is not near thermal equilibrium and should be included in the theory if they are calculated from a *real* physical density matrix. Anile and Muscato¹⁹ have included such terms in their traditional hydrodynamic equations mentioned in the Introduction. Unfortunately, these terms are exactly zero as predicted by balance equation theory.

It is clear that for mediately nonuniform systems and/or systems far from thermal equilibrium, an accurate prediction of the behavior of heat flux requires the inclusion of one or

more additional unknown parameters in the initial density matrix (in high-order terms so that they do not violate the particle and momentum balance equations) to be followed by their determination from expanded balance equations, which now include the heat flux equation(s). This problem is currently under investigation and the results are planned to be published elsewhere.

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APPENDIX

The expression of $\langle \mathbf{B} \rangle$ is composed of two parts. One is due to collisions with impurities ($\langle \mathbf{B}_i \rangle$) and the other is due to interaction with phonons ($\langle \mathbf{B}_{ph} \rangle$). They are given by

$$\begin{aligned} \langle \mathbf{B}_i \rangle = & 2\pi n_i \sum_{\mathbf{k}, \mathbf{q}} |u(\mathbf{q})|^2 (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \frac{\mathbf{k} + \mathbf{q}/2}{m} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \mathbf{q} \cdot \mathbf{v}) \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \\ & + 2\pi n_i \sum_{\mathbf{k}, \mathbf{q}} |u(\mathbf{q})|^2 \left(\mathbf{q} \cdot \mathbf{v} \frac{\mathbf{k} + \mathbf{q}}{m} + \mathbf{k} \cdot \mathbf{v} \frac{\mathbf{q}}{m} \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \mathbf{q} \cdot \mathbf{v}) \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \\ & + \pi n_i \sum_{\mathbf{k}, \mathbf{q}} |u(\mathbf{q})|^2 (\varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}) \frac{\mathbf{q}}{m} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \mathbf{q} \cdot \mathbf{v}) \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \end{aligned} \quad (A1)$$

and

$$\begin{aligned} \langle \mathbf{B}_{ph} \rangle = & -4\pi \sum_{\mathbf{k}, \mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \frac{\mathbf{k} + \mathbf{q}/2}{m} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}) \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \\ & \times \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}}{T_e}\right) \right] - 4\pi \sum_{\mathbf{k}, \mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 \left(\mathbf{q} \cdot \mathbf{v} \frac{\mathbf{k} + \mathbf{q}}{m} + \mathbf{k} \cdot \mathbf{v} \frac{\mathbf{q}}{m} \right) \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}) \\ & \times \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}}{T_e}\right) \right] - 2\pi \sum_{\mathbf{k}, \mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 (\varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}) \\ & \times \frac{\mathbf{q}}{m} \delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}) \left[f\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{T_e}\right) - f\left(\frac{\varepsilon_{\mathbf{k}+\mathbf{q}} - \mu}{T_e}\right) \right] \left[n\left(\frac{\Omega_{\mathbf{q}\lambda}}{T}\right) - n\left(\frac{\Omega_{\mathbf{q}\lambda} - \mathbf{q} \cdot \mathbf{v}}{T_e}\right) \right]. \end{aligned} \quad (A2)$$

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