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Linear response treatment of the Hall effect within the Zubarev formalism

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Abstract
A model for the Hall coefficient is developed within the framework of the Zubarev formalism and linear response theory. Comparison is made with the relaxation time approximation. Further results are given including electron–electron interactions within linear response theory.

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1. Introduction

Properties of noble gas plasmas in magnetic fields have recently been investigated by Shilkin *et al* [1–3] using shock wave generated plasmas. Data were obtained for both the DC electrical conductivity and the Hall coefficient. In the case of no magnetic field, results for the conductivity and other thermoelectric properties are well understood from linear response theory (LRT) within the Zubarev formalism [4–6]. Previous attempts at describing the Hall effect within the Zubarev approach have yielded overly complex results [7], which thus far remain uncalculated. On the other hand, the widely used relaxation time approximation (RTA) to transport based on the Boltzmann kinetic equation, see for example [8], provides a simple approach and has been successful in describing magnetic field effects in metallic systems as well as in Lorentz plasmas. In this paper, we derive an expression for the Hall coefficient using the Zubarev approach, which leads to identical results as the RTA in the low density limit when considering small magnetic fields. We then go beyond the RTA description by including the electron–electron (e–e) interactions within LRT in addition to the electron–ion (e–i) interactions considered in the RTA.

2. Linear response theory

For a non-equilibrium system, we consider a specific set of so-called relevant observables which characterize the non-equilibrium properties of the system, see [9]. The choice of observables must reflect the system in question and is crucial to finding a convenient and effective description of that system. When considering a plasma in an electric field $\vec{E}$, particle motion is clearly important. In the additional presence of a magnetic field $\vec{B}$, we find that it is most suitable to use a set of generalized velocities $\{\dot{\vec{R}}_n\}$ as the relevant observables and not the generalized momenta $\{\vec{P}_n\}$ as used in previous works describing the conductivity [4, 5]. Generalized velocities are defined via a generalized centre of mass $\vec{R}_n$ and the generalized momenta are given by a summation over wave vectors:

$$\begin{aligned}\hat{\vec{R}}_n &= \mathrm{i}\sum_{kk'}(\beta\epsilon_k)^n \frac{\partial}{\partial\vec{k}'}\delta(\vec{k}-\vec{k}')\hat{a}^\dagger_{k'}\hat{a}_k,\\ \hat{\vec{P}}_n &= \sum_k \hbar\vec{k}(\beta\epsilon_k)^n\hat{a}^\dagger_k\hat{a}_k,\end{aligned} \tag{1}$$

where ϵ_k is the electron kinetic energy and $\beta = (k_BT)^{-1}$. Note that the subscript n in $\vec{R}_n$ and $\vec{P}_n$ refers to the power of energy in these relevant observables. We take time derivatives using $\dot{X} = (\mathrm{i}\hbar)^{-1}[X, \hat{\mathcal{H}}]$, where the Hamiltonian $\hat{\mathcal{H}}$ contains the equilibrium Hamiltonian $\hat{\mathcal{H}}_0$ as well as contributions due to all external perturbations:

$$\begin{aligned}\hat{\mathcal{H}} &= \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\mathrm{ext}},\\ \hat{\mathcal{H}}_0 &= \sum_k \epsilon_k\hat{a}^\dagger_k\hat{a}_k + \sum_c V^{ec},\\ \hat{\mathcal{H}}_{\mathrm{ext}} &= e\vec{E}\cdot\hat{\vec{R}}_0 + \frac{e}{2m_e}\vec{B}\cdot(\hat{\vec{R}}_0\times\hat{\vec{P}}_0),\end{aligned} \tag{2}$$

where V^{ec} is the interaction potential between an electron and species c of the plasma. Taking then the time derivatives of the generalized centres of mass we find the generalized velocities and forces:

$$\begin{aligned}m_e\dot{\vec{R}}_n &= \vec{P}_n + \frac{e}{2}(\vec{B}\times\vec{R}_n),\\ m_e\ddot{\vec{R}}_n &= \vec{F}_n - e[\vec{E} + (\dot{\vec{R}}_n\times\vec{B})],\end{aligned} \tag{3}$$

where we define a generalized force due to internal interactions by $\vec{F}_n = \frac{\mathrm{i}}{\hbar}\sum_c[V^{ec}, \vec{P}_n]$. We use these observables under a maximum entropy condition to create a relevant non-equilibrium statistical operator (NESO):

$$\begin{aligned}\hat{\varrho}_{\mathrm{rel}} &= \frac{1}{Z_{\mathrm{rel}}}\exp\left(-\beta\left(\hat{\mathcal{H}}_0 - \mu_e\hat{N}_e + \sum_n \phi_n\hat{\dot{\vec{R}}}_n\right)\right),\\ Z_{\mathrm{rel}} &= \mathrm{Tr}\left\{\exp\left(-\beta\left(\hat{\mathcal{H}}_0 - \mu_e\hat{N}_e + \sum_n \phi_n\hat{\dot{\vec{R}}}_n\right)\right)\right\},\end{aligned} \tag{4}$$

where $\hat{N}_e$ is the electron number operator and μ_e is the electron chemical potential. The generalized velocities $\dot{\vec{R}}_n$ are accompanied by Lagrange multipliers ϕ_n. For the formation of the averages of relevant observables, we then require that

$$\langle\dot{\vec{R}}_n\rangle = \mathrm{Tr}\{\hat{\varrho}_{\mathrm{rel}}\hat{\dot{\vec{R}}}_n\}. \tag{5}$$

We create the complete NESO $\hat{\varrho}$ and remove time reversibility by solving a modified quantum Liouville equation containing an infinitesimally small source term:

$$\frac{\partial\hat{\varrho}}{\partial t} + \frac{\mathrm{i}}{\hbar}[\hat{\mathcal{H}}, \hat{\varrho}] = -\lim_{\varepsilon\to 0}\varepsilon(\hat{\varrho} - \hat{\varrho}_{\mathrm{rel}}). \tag{6}$$

We then linearize $\hat{\varrho}$ with respect to the set $\{\dot{\vec{R}}_n\}$ and external perturbations and use the self-consistency condition (5) to determine the Lagrange multipliers. We compare the statistical and phenomenological descriptions of the electric current density $\vec{j}$ to find the conductivity σ and the Hall coefficient R_H:

$$\langle\vec{j}\rangle = -\frac{e}{\Omega_0}\langle\dot{\vec{R}}_0\rangle = \sigma\vec{E} + \sigma R_H(\vec{j}\times\vec{B}). \tag{7}$$

The average of the current density can be given in terms of the equilibrium correlation functions:

$$N_{nm} = \frac{1}{m_e}(\vec{P}_n;\vec{P}_m), \qquad A_{nm} = \frac{1}{m_e}\langle\vec{P}_n;\dot{\vec{P}}_m\rangle, \qquad d_{nm} = \langle\vec{F}_n;\vec{F}_m\rangle, \tag{8}$$

where we define the equilibrium correlation functions of operators X and Y by

$$\begin{aligned}(X;Y) &= \frac{1}{\beta}\mathrm{Tr}\left\{\hat{\varrho}_0\int_0^\beta \mathrm{d}\tau\, X(-\mathrm{i}\hbar\tau)Y\right\},\\ \langle X;Y\rangle &= \lim_{\varepsilon\to 0}\int_{-\infty}^0 \mathrm{d}t\,\mathrm{e}^{(\varepsilon-\mathrm{i}\omega)t}(X(t);Y),\end{aligned} \tag{9}$$

with ω being the frequency of the external field, which we set to zero in this work, and $\hat{\varrho}_0$ being the equilibrium statistical operator:

$$\hat{\varrho}_0 = \frac{1}{Z_0}\mathrm{e}^{-\beta(\hat{\mathcal{H}}_0-\mu_e\hat{N}_e)}, \qquad Z_0 = \mathrm{Tr}\{\mathrm{e}^{-\beta(\hat{\mathcal{H}}_0-\mu_e\hat{N}_e)}\}. \tag{10}$$

3. Results in the low density limit

Using the same notation as given in [8], we find for small magnetic field and arbitrary density the following expressions for the conductivity and the Hall coefficient:

$$\sigma = e^2K_{01}, \qquad R_H = -\frac{1}{em_e}\frac{K_{02}}{K_{01}^2}, \tag{11}$$

$$K_{01} = -\frac{\beta}{\Omega|D|}\begin{vmatrix}0 & N_0\\ \bar{N}_0 & D\end{vmatrix}, \qquad K_{02} = -\frac{\beta}{\Omega|D|}\begin{vmatrix}0 & N_0\\ \bar{A}_0 & D\end{vmatrix}, \tag{12}$$

where N_0, $\bar{N}_0$ and $\bar{A}_0$ are vectors defined by $N_i = (N_{i0}N_{i1},\ldots,N_{iL})$, $\bar{N}_i = (N_{0i}N_{1i},\ldots,N_{Li})^T$ and $\bar{A}_i = (A_{i0}A_{i1},\ldots,A_{iL})^T$, and D is an $(L+1)\times(L+1)$ matrix with elements d_{nm}. In the low density limit, we compare dimensionless parameters, the reduced conductivity σ^* and the Hall factor r_H:

$$\begin{aligned}\sigma^* &= \frac{\sqrt{m_e}\beta^{3/2}}{e^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\sigma \equiv \frac{f}{\ln\Lambda},\\ r_H &\equiv -en_eR_H,\end{aligned} \tag{13}$$

where $\ln\Lambda$ is the Coulomb logarithm. Low density limits of the correlation functions N_{nm} and d_{nm} are given in [4]. A_{nm} must be solved for by partial integration and can be written in a determinant expression:

$$A_{nm} = -\frac{m_e}{|D|}\begin{vmatrix}0 & N_n\\ \bar{N}_m & D\end{vmatrix}. \tag{14}$$

Taking progressively larger sets $\{\dot{\vec{R}}_n\}$, we can show that when considering only e–i interactions, we obtain convergence to the known RTA results [8]. Inclusion of e–e interactions gives convergence to the Spitzer [10] result for the conductivity and we also obtain a smaller result for the Hall coefficient, see table 1. While e–e interactions reduce the conductivity by about 42%, the Hall coefficient is lowered by about 38%.

Table 1. Convergence of the LRT approach with progressively larger sets $\{\dot{\tilde{R}}_n\}$ according to (11) compared with the RTA [8] and the Spitzer [10] results. Conductivity results as found in [4, 5].

	f		r_H	
$\{R_n\}$	ei	ei + ee	ei	ei + ee
0	0.2992	0.2992	1	1
0, 1	0.9724	0.5781	1.5325	1.2586
0, 1, 2	1.0145	0.5834	1.9786	1.2068
0, 1, 2, 3	1.0157	0.5875	1.9343	1.2077
0, 1, 2, 3, 4	1.0158	0.5892	1.9333	1.2036
0, 1, ..., 10	1.0159	–	1.9328	–
RTA	1.0159	–	1.9328	–
Spitzer	1.0159	0.5908	–	–

4. Summary

We have shown that LRT gives results consistent with other well-known approaches to electron transport. Moreover, LRT provides a very general description of transport capable of including interactions within a plasma in a consistent manner. Other transport coefficients such as the thermopower and the Lorentz number can also be described within LRT. Future work will extend this description to cover arbitrary densities and magnetic field strengths. Experimental temperature and pressure regions are known to produce partially ionized plasmas, therefore we must also consider electron–atom interactions. In principle, accurate descriptions of transport coefficients allow the determination of the charge carrier concentration, and therefore the ionization degree within a partially ionized plasma. This is of fundamental interest for plasma diagnostics and the development of plasma equations of state.

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