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HAL Id: jpa-00210798
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Submitted on 1 Jan 1988

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On the transport properties of a dense fully-ionized hydrogen plasma. II. Quantum analysis

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(Reçu le 23 décembre 1987, accepté le 24 mars 1988)

Résumé. — La conductibilité thermique d’un gaz d’électrons faiblement couplé est obtenue dans le cadre du formalisme des fonctions de Wigner. Les corrélations quantiques sont prises en considération exactement. La comparaison des résultats avec ceux obtenus à partir d’une approche semi-classique montre que, hors d’équilibre, les effets dus à la symétrie quantique ne peuvent pas être modélisés par un potentiel effectif.

Abstract. — The thermal conductivity of a weakly coupled electron gas is obtained within the Wigner function formalism, taking quantum correlations into account exactly. Comparison of the results with those obtained from a semi-classical approach shows that, away from equilibrium, quantum symmetry effects cannot be modelized by an effective potential.

1. Introduction.

In a preceding paper [1] (hereafter denoted as I), we have analysed the transport properties of a fully ionized hydrogen plasma within the context of the classical kinetic theory. Quantum effects were taken into account by effective potentials derived from the equilibrium pair correlation function [2]. Our results indicated that the quantum symmetry reduces drastically the electronic part of the thermal conductivity in the weak coupling domain.

As it was felt that these semi-classical results might be spurious, we have computed the thermal conductivity of a weakly coupled electron gas within the framework of quantum kinetic theory. Our main conclusion already announced in reference [3], is that the quantum symmetry effects cannot be properly recovered by an effective potential as far as dynamical properties are concerned.

Many papers have been devoted to the derivation of the transport coefficients of a weakly coupled plasma from a quantum kinetic equation [4-6]. However, the quantum correlations of the electron subsystem are generally neglected even when electron-electron collisions are considered.

To our knowledge only Lampe has studied the effect of degeneracy on the electron-electron collisions [5], but his results are obtained within the weak moment transfer approximation. We do not want to use this kind of approximation since the aim of the present paper is to compare quantum and semi-classical kinetic theory with the same degree of rigour.

We have focused our attention on the effects of quantum correlations on the value of the electronic thermal conductivity, using the Wigner function formalism which is sketched in section 2. In section 3 we indicate the main steps which lead to the quantum Landau equation valid for weakly coupled systems. In order to simplify our calculation, we have not considered the dynamical shielding since its contribution cannot change the order of magnitude of our results (even if it is not negligible) [6]; instead, the divergent integrals are cut through an appropriate screening.

In section 4, we give the expression of the thermal conductivity which is deduced from the microscopic hydrodynamical modes based on the linearized kinetic equation. This result is used in section 5 to evaluate the thermal conductivity of the degenerate electron gas. Finally in section 6 we compare our quantum calculation with our semi-classical one. We
also comment briefly on the thermal conductivity of the hydrogen plasma for the relevant domain of parameters.

2. The Wigner function formalism.

The Wigner function formalism [7, 8, 9] has the advantage of providing a tool for quantum kinetic theory which has many similarities with classical theory. In particular, the quantum statistical average of an observable can be expressed with the help of a phase space quasiprobability distribution function:

\[
\langle b \rangle = \int dq_1 \, dp_1 \, \cdots \, dq_s \, dp_s \, b_s(q_1, p_1, \ldots, q_s, p_s) \times f^n_s(q_1, p_1, \sigma_1, \ldots, q_s, p_s, \sigma_s).
\]  
(2.1)

Here \( b_s(q_1, p_1, \ldots, q_s, p_s) \) is the classical observable which depends on \( s \) phase space variables while \( f^n_s(q_1, p_1, \sigma_1, \ldots, q_s, p_s, \sigma_s) \) is the \( s \)-particle Wigner function whose we conveniently define the Fourier transform:

\[
f^n_s(k_1, p_1, \sigma_1; \ldots; k_s, p_s, \sigma_s) = (8 \pi^3)^{-s} \int dq_1 \ldots dq_s \, e^{i(k_1 \cdot q_1 + \cdots + k_s \cdot q_s)} \, f^n_s(q_1, p_1, \sigma_1; \ldots; q_s, p_s, \sigma_s) = \hbar^{-3s} \text{Tr} \rho \left\{ a_{\sigma_1}^+ (p_1 - \hbar k_1) \ldots a_{\sigma_s}^+ (p_s - \hbar k_s) \right\} \left\{ a_{\sigma_1} (p_1 + \hbar k_1) \ldots a_{\sigma_s} (p_s + \hbar k_s) \right\} = f^n_s(1 \ldots s)
\]  
(2.2)

\( \rho \) is the von Neumann density operator and \( a^+ \), \( a \) are respectively the creation and annihilation operators in second quantization formalism. Note that we consider only Wigner functions which are diagonal in the spin indices \( \sigma_i \) since we shall treat only spin-independent quantities [8].

The evolution of the Wigner functions is easily deduced from the von Neumann equation:

\[
\frac{\partial}{\partial t} f^n_s(1 \ldots s) = \sum_{j=1}^{s} L_{j}^0 f^n_s(1 \ldots s) + \sum_{1 \leq j < n \leq s} L_{jn} f^n_s(1 \ldots s) + \sum_{j=1}^{s} \sum_{s_j+1} \int dp_{s+1} \int dk_{s+1} \delta(k_{s+1}) L_{j}^{n+s+1} f^n_s(1 \ldots s+1) \quad (s = 1, 2, \ldots)
\]  
(2.3)

which is the analogue of the BBGKY hierarchy. The quantum Liouvillian takes the form [9]:

\[
L_{j}^0 = - \left( i/m \right) k_j \cdot p_j,
\]  
(2.4)

\[
L_{jn} = (i\hbar)^{-1} \int dl V_l \left[ e^{-\frac{hi}{2} \delta p_n} - e^{\frac{hi}{2} \delta p_n} \right] e^{-1 \cdot \delta m},
\]  
(2.5)

with

\[
\delta m = \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_n}, \quad \delta n = \frac{\partial}{\partial k_j} - \frac{\partial}{\partial k_n},
\]  
(2.6)

\( m \) is the particle mass and \( V_l \) the Fourier transform of the interaction potential which, for an electron gas, is the Coulomb potential:

\[
V_l = \frac{1}{8 \pi^3} \int dr e^{i \mathbf{r} \cdot \mathbf{r}} \, V(r) = \frac{e^2}{2 \pi^2 l^2}.
\]  
(2.7)

The quantum symmetry which is reflected in second quantization by the (anti) commutation rules of the creation and annihilation operators is included in the present formalism in symmetry properties of the Wigner functions [9]. For instance:

\[
f^n_s(k_1, p_1, \sigma_1; k_2, p_2, \sigma_2) = \theta f^n_s(k_1 + k_2, p_1 - p_2, \sigma_1 + \sigma_2) = \left[ \frac{1}{2} (k_1 + k_2) + h^{-1} (p_2 - p_1), \frac{1}{2} (p_1 + p_2) + \frac{1}{4} h (k_2 - k_1), \sigma_1 \right],
\]  
(2.8)

as can easily be checked by a permutation of two creation operators in (2.2). These symmetry properties can be used to separate pure quantum correlations from those which have classical analogues; e.g.:

\[
f^n_s(k_1, p_1, \sigma_1; k_2, p_2, \sigma_2) = f^n_s(k_1, p_1, \sigma_1) \times f^n_s(k_2, p_2, \sigma_2) + \theta \delta_{\sigma_1, \sigma_2} f^n_s \left[ \frac{1}{2} (k_1 + k_2) + h^{-1} (p_2 - p_1), \frac{1}{2} (p_1 + p_2) + \frac{1}{4} h (k_2 - k_1), \sigma_1 \right] \times f^n_s \left[ \frac{1}{2} (k_1 + k_2) + h^{-1} (p_1 - p_2), \frac{1}{2} (p_1 + p_2) + \frac{1}{4} h (k_1 - k_2), \sigma_2 \right] + \theta f^n_s(k_1, p_1, \sigma_1; k_2, p_2, \sigma_2).
\]  
(2.9)
The second term of the r.h.s of (2.9) represents pure quantum correlations while $g_{ij}$, which possesses the same symmetries as $f_{ij}$, contains the correlations due to the interactions. This distinction between these two types of correlations is useful in order to cut the hierarchy (2.3). At this stage, it is useful to introduce a symmetrisation operator as follows

\[
S(k_1, p_1, \sigma_1; k_2, p_2, \sigma_2) f_{ij}(k_1, p_1, \sigma_1) f_{ij}(k_2, p_2, \sigma_2) = S(12) f_{ij}(1) f_{ij}(2) =
\]

\[
= \delta_{\sigma_1 \sigma_2} f_{ij} \left[ \frac{1}{2} (k_1 + k_2) + i (p_2 - p_1), \frac{1}{2} (p_1 + p_2), \frac{1}{4} h(k_2 - k_1), \sigma_1 \right] \times
\]

\[
\times f_{ij} \left[ \frac{1}{2} (k_1 + k_2) + i (p_1 - p_2), \frac{1}{2} (p_1 + p_2), \frac{1}{4} h(k_2 - k_1), \sigma_2 \right]. \quad (2.10)
\]

**3. The quantum Landau equation.**

The aim of kinetic theory is to provide approximate closed equations of evolution for reduced distribution functions. This is achieved very easily in the case of weakly coupled systems even in the quantum case by an appropriate cut of the hierarchy (2.3); this has been done in the literature for spinless particles [9] (see Ref. [20] for a different approach of the problem also based on the Wigner function formalism). We shall thus indicate only the main steps which lead to the kinetic equation writing down the small changes necessary to account explicitly for the spin of the electrons.

The first member of the hierarchy (2.3) reads explicitly:

\[
\partial_\tau f_{ij}(1) = \mathcal{L}_i^0 f_{ij}(1) + \sum_{\varepsilon_2} \int dp_2 \int dk_2 \delta(k_2) \mathcal{L}_{12} \times
\]

\[
\times \left\{ [1 + \theta S(12)] f_{ij}(1) f_{ij}(2) + g_{ij} \right\} \quad (3.1)
\]

A formal solution for $g_{ij}^{(2)}(12)$ can be obtained from the first two equations (2.3). In the weak coupling limit one retains only terms which are of order 0 or order 1 in the interaction Liouvillian $\mathcal{L}_{jn}$ (2.5) and one neglects terms containing $g_{ij}^{(2)}(12)$ or $g_{ij}^{(3)}(12)$; pair or triple quantum correlations however are considered exactly:

\[
\mathcal{L}_{ij}^{(12)}(12) = e^{(L_{ij}^{(1)} + L_{ij}^{(2)})} g_{ij}^{(2)}(12, t = 0) + \int_0^t d\tau e^{(L_{ij}^{(1)} + L_{ij}^{(2)})} \left\{ \mathcal{L}_{12}^{(1)} [1 + \theta S(12)] f_{ij}(1, t - \tau) f_{ij}(2, t - \tau) +
\right.
\]

\[
+ \sum_{\varepsilon_2} \int dp_2 \int dk_2 \delta(k_2) \left[ \mathcal{L}_{12}^{(1)} [\alpha S(23) + S(13) S(12) + S(12) S(13)]
\right.
\]

\[
+ \left[ V_i \mathcal{L}_{ij}^{(1)} \right] \left[ e^{-\frac{\mathcal{L}_{ij}^{(1)}}{\hbar}} e^{-\frac{i S(23)}{\hbar}} - e^{-\frac{i S(13)}{\hbar}} e^{\frac{i S(12)}{\hbar}} \right] S(12) S(13) +
\]

\[
+ \left[ e^{-\frac{i S(12)}{\hbar}} e^{-\frac{i S(23)}{\hbar}} - e^{-\frac{i S(13)}{\hbar}} e^{\frac{i S(12)}{\hbar}} \right] S(12) S(23) \right\} f_{ij}(1, t - \tau) f_{ij}(2, t - \tau) f_{ij}(3, t - \tau) \right\} \quad (3.2)
\]

For times larger than the correlation time (i.e. the mean time while two particles interact), one neglects in (3.2) the initial correlation $g_{ij}^{(2)}(12, t = 0)$ and one extend the upper limit of the $\tau$-integration to infinity. This approximate solution for $g_{ij}^{(2)}$ is then introduced into equation (3.1). In the case of a spatially homogeneous system for which

\[
f_{ij}(k_1, p_1, \sigma_1) = 8 \pi^3 n \delta(k_1) \varphi_{\sigma_1}(p_1)
\]

one obtains a closed kinetic equation for $\varphi_{\sigma_1}(p_1)$:

\[
\partial_\tau \varphi_{\sigma_1}(p_1) = -\frac{8 \pi^3 n}{\hbar^2} \int_{-\infty}^{+\infty} d\tau \sum_{\varepsilon_2} \int dp_2 \int dl \mathcal{L}_{ij}^{(1)} \left[ V_i \mathcal{L}_{ij}^{(1)} \right] \left[ \varphi_{\sigma_1}(p_1) \varphi_{\sigma_1}(p_2) \right] [1 + \theta n h^3 \varphi_{\sigma_1}(p_1 + \hbar l) + \theta n h^3 \varphi_{\sigma_1}(p_2)]
\]

\[
\times \left\{ \varphi_{\sigma_1}(p_1 + \hbar l) \varphi_{\sigma_1}(p_2 - \hbar l) [1 + \theta n h^3 \varphi_{\sigma_1}(p_1) + \theta n h^3 \varphi_{\sigma_1}(p_2)] \right\} \quad (3.4)
\]
Finally, the integration is performed to give:
\[
\delta_i \varphi_{\sigma_i}(p_1) = -\frac{16\pi^4 nm}{h^2} \sum_{\sigma_2} \int dp_2 \int d\mathbf{r} \frac{\delta (1 \cdot p_{12} + \hbar l^2)}{V_l^2 + \theta \delta_{\sigma_1 \sigma_2}} V_l V \left| 1 + \frac{p_1}{\hbar} \frac{p_2}{\hbar} \right| \times
\]
\[
\left\{ \varphi_{\sigma_1}(p_1) \varphi_{\sigma_2}(p_2) \Psi_{\sigma_1}(p_1 + \hbar l) \Psi_{\sigma_2}(p_2 - \hbar l) - \varphi_{\sigma_1}(p_1 + \hbar l) \varphi_{\sigma_2}(p_2 - \hbar l) \Psi_{\sigma_1}(p_1) \Psi_{\sigma_2}(p_2) \right\}
\]

where
\[
p_{12} = p_1 - p_2
\]
and
\[
\Psi_{\sigma}(p) = 1 + \theta nh^2 \varphi_0(p).
\]

The quantum kinetic equation (3.5) is reminiscent of the Uehling-Uhlenbeck equation [10] with the cross section appropriate to Coulomb interaction in the first Born approximation. It is thus the quantum analogue of the classical Landau equation [9, 11]. However, it differs from the latter in three respects:
(i) as a consequence of the Heisenberg uncertainty principle, it takes into account finite momentum transfer \( \hbar l \) (this is also apparent by the fact that the interaction Liouvillian (2.5) is a finite difference operator); (ii) exchange effects are included in the cross section and (iii) there appear cubic terms in the distribution functions as a consequence of the pure quantum correlations. It is an easy matter to show [9] that equation (3.5) possesses all the required properties of a kinetic equation: conservation of mass, momentum and kinetic energy, H-theorem. Moreover, it admits one equilibrium state described by Bose-Einstein or Fermi-Dirac distribution functions:
\[
\varphi_0^\sigma(p) = \frac{1}{\sqrt{2\pi m \hbar^2 \beta}} \int \frac{d\mathbf{p}}{e^{-\beta \mu + \theta}}
\]

where \( \beta = 1/k_B T \) is the reciprocal temperature and \( \mu \) is the chemical potential. So far, all the results are quite general and are valid for any kind of weakly coupled charged particles. In the next section we shall specialize to a system of electrons slightly displaced from equilibrium.

4. Microscopic definition of the thermal conductivity.

In order to study the transport properties of the degenerate electron gas (jellium), we shall start from a kinetic equation linearized around the equilibrium state:

\[
\delta_i \varphi_{\sigma_i}(p_1) = \frac{16\pi^4 n m}{h^2} \sum_{\sigma_2} \int dp_2 \int d\mathbf{r} \frac{\delta (1 \cdot p_{12} + \hbar l^2)}{V_l^2 + \theta \delta_{\sigma_1 \sigma_2}} V_l V \left| 1 + \frac{p_1}{\hbar} \frac{p_2}{\hbar} \right| \times
\]
\[
\left\{ \varphi_{\sigma_1}(p_1) \varphi_{\sigma_2}(p_2) \Psi_{\sigma_1}(p_1 + \hbar l) \Psi_{\sigma_2}(p_2 - \hbar l) - \varphi_{\sigma_1}(p_1 + \hbar l) \varphi_{\sigma_2}(p_2 - \hbar l) \Psi_{\sigma_1}(p_1) \Psi_{\sigma_2}(p_2) \right\}
\]

that the range of the inhomogeneities is much larger than the range of the collisions; one easily obtains:
\[
\sum_{\sigma_1} (C f)(q, p_1, \sigma_1) = \int dp_2 \int d\mathbf{r} W(l ; p_1, p_2) \times
\]
\[
\left\{ f_\sigma(p_1) \varphi_0^\sigma(p_2) \Psi_0^\sigma(p_1 + \hbar l) - f_\sigma(p_2) \varphi_0^\sigma(p_1) \Psi_0^\sigma(p_2 - \hbar l) \right\}
\]

where we have defined:
\[
f_\sigma(p) = \sum_\sigma f(q, p, \sigma)
\]

\[
W(l ; p_1, p_2) = \frac{16\pi^4 n m}{h^2} \delta (1 \cdot p_{12} + \hbar l^2) \times
\]
\[
\left\{ \frac{1}{2} V_l^2 + V_l^2 \left| 1 + \frac{p_1}{\hbar} - \frac{p_2}{\hbar} \right| + \theta \delta_{\sigma_1 \sigma_2} V_l V \left| 1 + \frac{p_1}{\hbar} \frac{p_2}{\hbar} \right| \right\}
\]

Let us mention that Boercker and Dufty [12] have deduced in a different context a more general linearized collisional term whose equation (4.2) is the weak coupling limit (see Eq. (4.18) or Ref. [12]).

In equation (4.1), \( V_L \) is the linearized Vlassov term of which we retain only the singular part:
\[
V_L f_\sigma(p_1) = -8\pi^3 ni V_\sigma \left[ k \cdot \frac{\partial}{\partial p_1} \varphi_0^\sigma(p_1) \right] \int dp_2 f_\sigma(p_2).
\]

The regular part, which originates from quantum properties, does not contribute to the transport coefficients in the domain of parameters we are considering. We shall come back to this point in a next paper.

By using the following symmetry properties:
\[
W(l ; p_1, p_2) =
\]
\[
= W(-1 ; p_2, p_1) = W(-1 ; -p_1, -p_2)
\]
\[
= W(-1 + \frac{p_2}{\hbar} ; p_1, p_2)
\]
\[
= W(-1 ; p_1 + \hbar l ; p_2 - \hbar l)
\]
and
\[
\varphi^0_\sigma(p) \Psi^0_\sigma(p + p') = \\
= \varphi^0_\sigma(p + p') \Psi^0_\sigma(p) e^{-\frac{p^2}{2m}} \left( \frac{e^{p' - p} - 1}{e^{p - p'} - 1} \right)
\] (4.7)

it is easy to show that the linearized collision operator \( C \) is hermitian for the scalar product:

\[
\langle f | g \rangle = \int dp \, f^*(p) \, P^{-1}(p) \, g(p)
\] (4.8)

where the weight function is:

\[
P(p) = \bar{a} \sum_{\sigma = \pm 1/2} \varphi^0_\sigma \Psi^0_\sigma = 2 \bar{a} \varphi^0_\sigma \Psi^0_\sigma
\]

\[
\bar{a} = \left[ 2 \int dp \, \varphi^0_\sigma \Psi^0_\sigma \right]^{-1}.
\] (4.9)

From equation (4.2), one indeed deduces:

\[
\langle f | C | g \rangle = \int dp_1 \, P^{-1}(p_1) \, f^*(p_1) \, C g(p_1) = \\
= \frac{\bar{a}}{2} \int dp_1 \int dp_2 \int dl \, W(l ; p_1, p_2) \times \\
\times \varphi^0_\sigma(p_1) \varphi^0_\sigma(p_2) \Psi^0_\sigma(p_1 + h l) \Psi^0_\sigma(p_2 + h l) \\
\times \left[ \frac{f(p_1)}{P(p_1)} \frac{f(p_2)}{P(p_2)} - \frac{f(p_1 + h l)}{P(p_1 + h l)} \frac{f(p_2 - h l)}{P(p_2 - h l)} \right]^* \\
\times \left[ \frac{g(p_1)}{P(p_1)} \frac{g(p_2)}{P(p_2)} - \frac{g(p_1 + h l)}{P(p_1 + h l)} \frac{g(p_2 - h l)}{P(p_2 - h l)} \right]
\]

\[
= \langle g | C^\dagger | f \rangle.
\] (4.10)

The orthonormalized eigenfunctions of \( C \) with zero-eigenvalues which correspond to the collisional invariants are written as:

\[
\Phi^0_\sigma(p) = P(p) \\
\Phi^0_\sigma(p) = a_k p_k P(p) \quad (k = 2, 3, 4 = x, y, z) \\
\Phi^0_\sigma(p) = a_s (p^2 - b_s) P(p)
\] (4.11)

where the coefficients \( a_k \) and \( b_s \) are expressed in terms of Fermi integrals:

\[
a_k = 2 (c_{-1})^{-1} \\
a_k = \left( \frac{\beta}{2m} \right)^{1/2} (c_{-1})^{1/2} \quad (k = 2, 3, 4) \\
a_s = \frac{\beta}{2m} \frac{c_{-1}}{(5c_3 - c_{-1} - 9)^{1/2}} \\
b_s = \frac{6m}{\beta} (c_{-1})^{-1}
\] (4.12)

where

\[
c_n = \frac{I_{n/2}(\beta \mu)}{I_{1/2}(\beta \mu)}
\] (4.13)

with

\[
I_n(\beta \mu) = \int_0^\infty dx \, x^{n/2} (e^{\beta x} - 1)^{-1}.
\] (4.14)

With the properties just reviewed, it is an easy matter to define the transport coefficients by following step by step one of the known methods (developed for classical kinetic theory); for instance one can use the paper by Rozmus [13] or the Resibois method [14] revised by Mareschal [15]. We shall not reproduce any of these methods since the only difference consists in the weight function (4.9) and consequently of the explicit values of the coefficients such as (4.12).

For the degenerate electron gas we are considering, the thermal conductivity reads:

\[
\chi_q = -\frac{n k_B^2 T}{9m} (21c_3 - 25c_3^2) \left\langle \Phi_{11} | Q \frac{1}{C^\dagger} Q | \Phi_{11} \right\rangle
\] (4.15)

where \( \Phi_{11} \) is the heat flux state:

\[
\Phi_{11} = a_{11} p_1 (p^2 - b_{11}) P(p) \\
a_{11} = 3 \left( \frac{\beta}{2m} \right)^{3/2} \left[ \frac{c_{-1}}{21c_3 - 25c_3^2} \right]^{1/2} \\
b_{11} = \frac{10m}{3} \beta c_3
\] (4.16)

and \( Q \) is an operator which projects out the collisional invariant states (4.11). In the first Sonine polynomial approximation, equation (4.15) becomes (see I):

\[
\chi_q = -\frac{n k_B^2 T}{9m} (21c_3 - 25c_3^2) \left\langle \Phi_{11} | C | \Phi_{11} \right\rangle^{-1}.
\] (4.17)

The evaluation of the thermal conductivity is thus essentially that of the matrix element \( \left\langle \Phi_{11} | C | \Phi_{11} \right\rangle \).

5. Quantitative evaluation of the thermal conductivity.

From equations (4.10) and (4.16) and the conservation of momentum (cf. Eq. (4.11)), one has:

\[
\left\langle \Phi_{11} | C | \Phi_{11} \right\rangle = \\
- \frac{8 \pi^4 n m^2 \alpha_{11}^2}{h^2} \int dl \int dp_1 \int dp_2 \delta (1 \cdot p_1 - h l)^2 \times \\
\times [V_1^2 + V_{1+}^2] - V_1 \left[ V_1 + p_{1+}/h l \right] \\
\times \varphi^0_\sigma(p_1) \varphi^0_\sigma(p_2) \Psi^0_\sigma(p_1 + h l) \Psi^0_\sigma(p_2 - h l) \\
\times (h(p_1) + h(p_2) - h(p_1 + h l) - h(p_2 - h l))^2
\] (5.1)

with

\[
h(p) = p_x p_y^2.
\] (5.2)

Here the x-direction is arbitrary. Expression (5.1) is a 9-dimensional integral which does not decouple so long as \( \varphi^0_\sigma(p) \) is the Fermi distribution; it is
analytically tractable only when the system is non degenerate as we shall see in next section.

By adopting the following dimensionless variables:

\[ u = \left( \frac{\beta}{2m} \right)^{1/2} \xi \]
\[ v = \left( \frac{\beta}{2m} \right)^{1/2} p_1 \]
\[ w = \left( \frac{\beta}{2m} \right)^{1/2} (p_2 - p_1 - \xi) \] (5.3)

it is possible to show (see appendix) that (5.1) can be written as:

\[ \langle \Phi_{11} | \Phi_{11} \rangle = \frac{16}{3} \sqrt{6} \Gamma^{3/2} \left( \frac{r}{T} \right)^3 (21c_5 - 25c_3^{-1}) J \] (5.4)

where \( J \) is a dimensionless involved integral:

\[ J = \int_0^\infty dv \frac{v^2}{\xi} \bar{\varphi}(v) \int_0^\infty du \times \]
\[ \int_0^\infty dw \frac{(u^2 - w^2)^2 + u^2 w^2}{uw} \]
\[ \int_0^\infty dy \prod_{i=1}^{\infty} \frac{d(\cos \theta)}{(1 + \delta e^{\nu \sin \theta \cos \gamma})(1 + \alpha e^{\nu \sin \theta \cos \gamma})} \] (5.5)

and

\[ \bar{\varphi}(r) = [e^{r^2 - \beta \mu} + 1]^{-1}; \quad \bar{\varphi}(r) = e^{r^2 - \beta \mu} \varphi(r) \]
\[ \cos \theta = \frac{v \cdot w}{uw}; \quad \delta = e^{-\beta \mu} e^{u^2 + v^2} \]
\[ \alpha = e^{\nu^2 + 2nu \cos \theta}; \quad \nu = 2uw. \] (5.6)

A Coulomb divergence at large distance now appears, due to the change of variables (5.3), as \( u \to 0 \) or \( w \to 0 \) (remember that the divergence at short distance is removed by the quantum diffraction). We choose to cut the integrations over \( u \) and \( w \) at \( \varepsilon \) whose precise value, related to the screening length, will be given below and write:

\[ J = \int_\varepsilon^\infty du \int_\varepsilon^\infty dw \frac{f(u, w)}{uw} \] (5.7)

where \( f(u, w) \) is a regular function which is simple to deduce from (5.5):

\[ f(u, w) = \int_0^\infty dv \bar{\varphi}(v) [u^4 + w^4 - u^2 w^2] \times \]
\[ \int_{-1}^1 d(\cos \theta) \times \int_0^\pi d\gamma \prod_{i=1}^{\infty} \frac{d(\cos \gamma)}{(1 + \delta e^{\nu \sin \theta \cos \gamma})(1 + \alpha e^{\nu \sin \theta \cos \gamma})} \] (5.8)

In order to isolate the logarithmic singularity, we decompose \( J \) into a regular \( (J_1) \) and a singular \( (J_2) \) part:

\[ J = J_1 + J_2 \]
\[ J_1 = \int_\varepsilon^\infty du \int_\varepsilon^\infty dw \frac{f(u, w) - f(u, 0) - f(0, w)}{uw} + \]
\[ + \int_\varepsilon^\infty du \int_\varepsilon^\infty dw \frac{f(u, w)}{uw} \]
\[ + \int_\varepsilon^\infty du \int_\varepsilon^\infty dw \frac{f(u, w) - f(0, w)}{uw} \]
\[ + \int_\varepsilon^\infty du \int_\varepsilon^\infty dw \frac{f(u, w) - f(0, 0)}{uw} \] (5.9)

One easily verifies that \( J_1 \) has no singularities as \( \varepsilon \to 0 \). Moreover, the numerical value of \( J_1 \) is not significantly modified when \( \varepsilon \) is taken equal to zero; \( J_1 \) is thus roughly independent of \( \varepsilon \). On the other hand, the singular term is reduced to a four-dimensional integral:

\[ J_2 = - (\ln \varepsilon) J_3 \]
\[ J_3 = \int_\varepsilon^\infty dw \frac{f(0, w)}{uw} + \int_\varepsilon^\infty du \frac{f(u, 0)}{u}. \] (5.10)

Once again, \( J_3 \) is roughly independent of \( \varepsilon \) since its numerical value is not significantly changed when one sets \( \varepsilon = 0 \). The evaluation of \( J_1 \) and \( J_3 \) has been performed numerically with a precision of 10% and 1% respectively.

6. Results.

From (4.15), (5.4), (5.9) and (5.10), the dimensionless thermal conductivity \( \kappa_q^* = \kappa_q/(k_B a^2 \omega_p) \) (where \( \omega_p \) is the plasma frequency and \( a \) the ionosphere radius) takes the form:

\[ \kappa_q^* = \frac{25}{24} \sqrt{3} \pi \Gamma^{-5/2} A_q^{-1} \] (6.1)

where \( A_q \) is the quantum Coulomb logarithm:

\[ A_q = (-A \ln (e + B) C \] (6.2)

and

\[ A = \left( \frac{r_s}{T} \right)^3 J_3 \]
\[ B = \left( \frac{r_s}{T} \right)^3 J_1 \]
\[ C = \frac{450 \sqrt{\pi}}{\pi^{5/2} (21c_5 - 25c_3^2)^2}. \] (6.3)

The coupling parameter \( \Gamma \) and density parameter
The quantities \( J_1, J_3, c_n \) are functions of \( \beta \mu \) alone or equivalently of \( r_s/\Gamma \), since from the normalisation of the Fermi function (3.7), one has the implicit relation:

\[
I_{1/2}(\beta \mu) = \frac{3 \pi}{4 \sqrt{2}} \left( \frac{\Gamma}{r_s} \right)^{3/2}.
\]  

This parameter \( \Gamma/\Gamma_s \) in turn is a measure of the degeneracy of the system:

\[
\frac{\Gamma}{r_s} = 2 \left( \frac{4}{\pi \sqrt{3}} \right)^3 \frac{T_F}{T} \approx 0.5 \frac{T_F}{T}.
\]  

The Coulomb logarithm \( \Lambda_q \) depends thus only on the degeneracy of the system via \( \Gamma/\Gamma_s \) and on the value of the cut \( \epsilon \). This cut, which is inherent to the Landau kinetic equation in quantum as well as in classical mechanics [9], is related to the screening length \( \lambda \), i.e. the Debye length at high temperature and the Thomas-Fermi length at 0 K. We have chosen [16]:

\[
\lambda^{-2} = 4 \pi ne^2 \beta \frac{c-1}{2}.
\]

which gives correctly the two limits. Taking into account the change of variables (5.3), one has

\[
e = \left( \frac{\beta}{2m} \right)^{1/2} \hbar \lambda^{-1} = \left( \frac{3}{2} \frac{\Gamma^2}{r_s} \frac{e-1}{2} \right)^{1/2}.
\]

The numerical results for \( \beta \mu, \epsilon^2/\Gamma, A, B, C \) are given in Table I as a function of \( \Gamma/\Gamma_s \). From (6.1) to (6.3), the value of \( \kappa_q \) is then easily obtained for any value of \( \Gamma \). Remember however that formula (6.1) is valid only for a weakly coupled electron gas \( (r_s \approx 0.1) \). Let us mention that the results of Lampe [5] agree with our as long as, in equation (6.2), \( B \) is negligible in comparison with \( C \ln \epsilon \).

When the electron system is not degenerate \((- \beta \mu \gg 1)\) the Fermi distribution (3.7) can be replaced by the Maxwellian:

\[
\phi^0_\epsilon(p) = \frac{e^{\beta \mu}}{nh^3} e^{-\left(\beta p^2/2m\right)}
\]

and

\[
\Psi^0(p) \to 1.
\]

In that condition, the thermal conductivity (4.17) can be easily evaluated analytically. Indeed, one verifies:

\[
c_3 \to \frac{3}{2}; \quad c_5 \to \frac{15}{4}
\]

and

\[
\langle \Phi_{11}|\Phi_{11} \rangle = -\frac{\omega_p}{5 \sqrt{3} \pi} \int_0^{\infty} \frac{du}{u} [4 - u^2] e^{-u^2/2}
\]

where \( u = (\beta/2m)^{1/2} \hbar \Gamma \). The logarithmic divergence appears of course for small values of \( u \) for which we use the classical limit of the cut (6.7). As a result of the quantum diffraction, the integrand of (6.11) is effectively cut for \( u \approx \sqrt{2} \), i.e. for distances less than the thermal de Broglie length. Quantum symmetry effects are still present through the non divergent exchange term but all quantum correlations have disappeared from (6.11). The result of the integration of (6.11) gives:

\[
\langle \Phi_{11}|\Phi_{11} \rangle = -\frac{\omega_p}{5 \sqrt{3} \pi} \int_0^{\infty} \frac{du}{u} [4 - u^2] e^{-u^2/2}
\]

where \( E_1 \) is the exponential integral and \( \gamma = 0.577... \) is the Euler constant [17]. The second line of (6.12) is obtained by a small argument expansion of \( E_1 \) [17]. In that way, the non-degenerate limit \( \kappa_{nd}^* \) of \( \kappa_q^* \) can be put in the form:

\[
\kappa_{nd}^* = \frac{25}{24} \sqrt{3} \sqrt{\pi} \Gamma^{-5/2} \Lambda_{nd}^{-1}
\]

with

\[
C_{nd} = \frac{8 \sqrt{2}}{9 \sqrt{5} \pi} \approx 0.72
\]

\[
A_{nd} = \frac{9 \pi^{5/2}}{8 \sqrt{2}} \approx 13.9
\]

\[
B_{nd} = -\left( \gamma + \frac{1}{2} - \ln 2 \right) \frac{9 \pi^{5/2}}{16 \sqrt{2}} \approx -2.67.
\]
The values of these last quantities which are compatible with those of Braginskii [11] recover those of table I for \( \Gamma/r_\sigma \ll 10^{-1} \). This means that the system can be considered as non degenerate for temperature such that \( T/T_F \gg 5 \). We note however that \( \kappa_{q*}^* \) and \( \kappa_{\sigma d}^* \) are in agreement within 10% as far as \( \Gamma/r_\sigma \ll 0.5 \) or \( T > T_F \).

7. Comparison with the semi-classical approach.

The motivation of this work was to test the validity of the effective potentials [2] which take into account quantum effects in the context of classical mechanics. So we have compared our pure quantum results with those which can be obtained from the use of the two model potentials considered in I (cf. I, Eq. (2.7)). The thermal conductivity of an electron gas can be deduced from that of the hydrogen plasma by neglecting all electron-proton and proton-proton interactions. In the one-Sonine-polynomial approximation, this can be achieved by cancelling \( f_{\text{ep}} \) and \( f_{\text{pp}} \) in (I, Eq. (5.4)). The semi-classical evaluation of the thermal conductivity of the electron gas, then takes the form:

\[
\chi_{\text{sc}}^* = \frac{25}{24} \sqrt{\pi} \Gamma^{-5/2} A_i^{-1} \quad (i = 1, 2) .
\] (7.1)

For the model I (I, Eq. (2.7a)) which takes into account diffraction effects alone, one has (cf. I, Eq. (5.8)):

\[
A_1 = \frac{1}{2} \ln \left( 1 + \frac{\pi}{6} \frac{r_\sigma}{\Gamma^2} \right) - \frac{1}{1 + \frac{6}{\pi} \frac{\Gamma^2}{r_\sigma}}
\] (7.2)

while for the model II (I, Eq. (2.7b)) which in addition accounts for the quantum symmetry, one has (cf. I, Eq. (5.9)):

\[
A_2 = A_1 + \frac{1}{2} \left( \frac{\alpha_1}{\sqrt{\Gamma r_\sigma}} + \frac{\alpha_2}{\Gamma r_\sigma} \right)
\] \((\alpha_1 = 0.96, \alpha_2 = 0.26) . \quad (7.3)

These results are compared with those obtained from pure quantum mechanics (cf. Eqs. (6.1, 6.2) and Tab I) in figures 1 and 2.

Not many comments are necessary after inspection of these figures. They show how inadequate is the description of the symmetry effects by an effective potential, even when the system is not degenerate \( (\beta \mu \ll -1) \). In particular the reduction of the thermal conductivity by symmetry effects is spurious. On the contrary \( \chi_{\text{sc}}^* \) is in agreement with \( \kappa_q \) so long as the system is not too degenerate \( (\beta \mu \ll -1) \) (1).

These conclusions are confirmed by the fact that both \( \Lambda_q \) (6.2) and \( \Lambda_1 \) (7.2) are functions of the cut \( \varepsilon \) and \( \Gamma/r_\sigma \) while the symmetry part of \( \Lambda_2 \) (7.3) depends on \( \Gamma \times r_\sigma \) i.e. on the temperature alone. On the other hand, for a fixed value of the density \( (r_\sigma) \), in the weak coupling limit \( (\Gamma \to 0) \) while \( \kappa_{q*}^* \) behaves like \( \Gamma^{-3/2} \), \( \kappa_{q}^* \) and \( \kappa_{\sigma d}^* \) behave like \( (\Gamma^{-5/2} \ln \Gamma)^{-1} \) as does the classical result of Braginskii [11]. For these reasons, the use of effective potentials, which were believed to be valid in a physically interesting domain of the \( \Gamma - r_\sigma \) plane, should be restrained to the diffraction potential (I, Eq. (2.4)) and thus to a smaller domain as indicated in figure 3.

(1) Let us mention that a semi-classical calculation of the thermal conductivity with the Kelbg effective potential (cf. formulas (25, 26) of Ref. [19]) would give an expression similar to (6.11) (except that it does not contain any exchange contribution). The major difference is only that the integrand would be cut at large \( u \) by a factor \( \exp(-u^2) \). This could explain why the values of \( \kappa_{q*}^* \) are not bad since they are obtained when using the diffraction potential (I, Eq. (2.4)) whose properties are very similar to those of Kelbg's potential.
To our present knowledge, the study of the transport properties of degenerate systems must be made in the framework of quantum mechanics. This has generally been achieved in the case of the hydrogen plasma by considering some generalized Lorentz model, i.e. by neglecting the electron-electron collisions (see e.g. Refs. [4, 18]). However, these are not negligible as shown in figure 4 since they give a contribution to thermal conductivity of the same order of magnitude as the electron-proton collisions (Roughly, \(1/\kappa = 1/\kappa_{el} + 1/\kappa_{ep}\)). Lampe [5] has shown that this could even be true for very highly degenerate plasmas. Some more work is thus necessary to obtain precise values of the transport coefficients of the degenerate hydrogen plasma. A forthcoming paper will be devoted to this problem.

8. Conclusions.

Our main conclusion is that out of equilibrium the quantum symmetry effects cannot be modeled by an effective potential of the type (I, Eq. (2.5)) which is constructed in order to reproduce equilibrium properties. On the contrary, use of the diffraction potential (I, Eq. (2.4)) seems allowable to calculate the transport coefficients of non degenerate plasmas; since the degeneracy parameter is \(\Gamma/r_s\) and not \(\Gamma\) itself, these conclusions which were reached for weakly coupled systems (\(\Gamma \ll 1\)) should also apply to strongly coupled plasmas (\(\Gamma \geq 1\)).

Acknowledgments.

We acknowledge stimulating discussions and exchanges with Profs. R. Balescu, L. G. Suttorp and C. Lhuillier.

Appendix.

DERIVATION OF EQUATIONS (5.4, 5.5). — From (5.1) and (5.3), one has:

\[
\omega_p^{-1} \langle \Phi_{11} | C | \Phi_{11} \rangle = \frac{\sqrt{6}}{2\pi^3} \left(21c_3 - 25c_3^2\right) \frac{r_s^3}{\Gamma^{3/2}} \tilde{f}
\]  

(A.1)

where \(\omega_p = (4\pi e^2 n/m)\) is the plasma frequency and

\[
\tilde{I} = \int du \int dv \int dw \delta(u \cdot v) \left( (u^{-2} - w^{-2})^2 + u^{-2} w^{-2} \right) \varphi(v) \varphi(|u + v + w|) \times
\]

\[
\Psi(|u + v|) \Psi(|v + w|) \{w_x(u^2 + 2u \cdot v) + w_x(w^2 + 2v \cdot w)\}^2
\]

(A.2)

with \(\varphi\) and \(\Psi\) defined in (5.6). \(\tilde{I}\) is symmetric for an exchange \(u \leftrightarrow w\); it can thus be written as:

\[
\tilde{I} = 2 \int du \int dv \int dw \delta(u \cdot w) g(u, v, w) \varphi(|u + v + w|) \Psi(|u + v|) \Psi(|v + w|) \times
\]

\[
\{w_x^2(u^2 + 2u \cdot v)^2 + w_x u_x(u^2 + 2u \cdot v)(w^2 + 2v \cdot w)\}
\]

(A.3)
with $g(u, v, w) = \delta (v)[(u^{-2} - w^{-2})^2 + u^{-2} w^{-2}]$. Because of the isotropy and the $\delta$-function, this becomes:

$$\bar{I} = \frac{2}{3} \int du \int dv \int dw \delta (u \cdot w) g(u, v, w) \delta(|u + v + w|) \bar{\psi}(|u + v|) \bar{\bar{\psi}}(|v + w|) \times w^2 (u^2 + 2 u \cdot v)^2.$$  \hfill (A.4)

We begin by the integration over the angular variables of $u$ by choosing the axes in figure 5, so that

$$u \cdot w = uw (\cos \theta_u \cos \theta_w + \sin \theta_u \sin \theta_w \cos \varphi_u)$$  \hfill (A.5)

and

$$\int_0^{2\pi} d\varphi_u \delta (u \cdot w) = \frac{2}{uw \sin \theta_u \sin \theta_w} \int_0^\pi d\varphi_u \delta (\cos \varphi_u + Z) \left\{ \begin{array}{ll} 1 & \text{if } Z^2 < 1 \\
\frac{1}{2} & \text{if } Z^2 = 1 \\
0 & \text{if } Z^2 > 1 \end{array} \right.$$  \hfill (A.6)

with $Z = \cotg \theta_u \cotg \theta_w$.

Setting $y = \cos \theta_u$, the condition $Z^2 = \cotg^2 \theta_u \cotg^2 \theta_w < 1$ becomes $-\sin \theta_w < y < \sin \theta_w$ and

$$\bar{I} = \frac{4}{3} \int dv \int dw \int_0^\infty du \frac{u^2}{uw} g(u, v, w) \bar{\psi}(|v + w|) \int_{-\sin \theta_w}^{\sin \theta_w} \frac{1}{(\sin^2 \theta_w - y^2)^{1/2}} \times w^2 (u^2 + 2 uv)^2 \bar{\bar{\psi}}(\sqrt{u^2 + v^2 + 2 uv}) \varphi(\sqrt{(v + w)^2 + u^2 + 2 uv}).$$  \hfill (A.7)

By integration over the azimuthal angle of $w$, we obtain:

$$\bar{I} = \frac{8}{3} \pi \int dv \int_0^\infty du \int_0^\infty dw g(u, v, w) u^3 w^3 \int_{-1}^{+1} \frac{dx}{\sqrt{1 - x^2}} \times (u + 2 tx \sin \theta_w)^2 \bar{\psi}(|v + w|) \frac{\delta \varphi}{(1 + \delta \varphi \sin \theta_w \varphi)} (1 + \alpha \varphi \sin \theta_w \varphi)$$  \hfill (A.8)

where $x = y/\sin \theta_w$; other quantities are defined in (5.6). Finally, since the integrand is independent of the angles of $v$ (5.4) results from (A.1) and (A.8).

Fig. 5. — Choice of angular variables in integral (A.4).
References

   WALLENBORN, J., BERNU, B. and ZEHNLÉ, V., Strongly Coupled Plasma Physics, Eds. F. J.
   Rogers and H. E. Dewitt (Plenum) 1987, p. 133.
   HUBBARD, W. B., Appl. J. 146 (1966) 858;
[16] See e.g. ASHCROFT, N. W. and MERMIN, N. D., Solid State Physics, Eds. Holt, Rinehart and
   Winston (1976) chapter 17.