Quantum kinetic theories in degenerate plasmas

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Abstract

In this review we give an overview of the recent work on quantum kinetic theories of plasmas. We focus, in particular, on the case where the electrons are fully degenerate. For such systems, perturbation methods using the distribution function can be problematic. Instead we present a model that considers the dynamics of the Fermi surface. The advantage of this model is that, even though the value of the distribution function can be greatly perturbed outside the equilibrium Fermi surface, deformation of the Fermi surface is small up to very large amplitudes. Next, we investigate the short-scale dynamics for which the Wigner–Moyal equation replaces the Vlasov equation. In particular, we study wave–particle interaction, and deduce that new types of wave damping can occur due to the simultaneous absorption (or emission) of multiple wave quanta. Finally, we consider exchange effects within a quantum kinetic formalism to find a model that is more accurate than those using exchange potentials from density functional theory. We deduce the exchange corrections to the dispersion relations for Langmuir and ion-acoustic waves. In comparison to results based on exchange potentials deduced from density functional theory we find that the latter models are reasonably accurate for Langmuir waves, but rather inaccurate for ion acoustic waves.

Keywords: kinetic theory, wave–particle interaction, Fermi surface dynamics, Wigner–Moyal equation, exchange effects

1. Introduction

There has been increasing interest in plasmas of low-temperature and high densities, where quantum properties tend to be important. A review of the recent evolution is given in e.g. [1–4]. Promising applications include quantum wells [5], spintronics [6] and plasmonics [7]. Quantum plasma effects can also be of interest in experiments with solid density targets [8]. Important classifications of dense plasmas include whether they are strongly or weakly coupled, and whether they are degenerate or non-degenerate [9]. While several works (see e.g. [1, 10–12]) have applied quantum hydrodynamics, our focus here will be on the more accurate quantum kinetic theories [13–16]. Many familiar phenomena in plasma physics depend crucially on a kinetic description; these include wave–particle interaction, instabilities due to temperature anisotropy and finite Larmor radius effects. It can thus be expected that studying quantum kinetics will reveal new physics.

The cited theories generalize classical kinetic dynamics to include effects such as the spin, the Heisenberg uncertainty principle, particle-dispersive effects, degeneracy, and particle exchange effects. New phenomena present in these theories include new wave modes [17], a modification to the ponderomotive force due to spin–orbit interaction [18], and a new wave-damping process [19] which we describe in section 3 of this paper. These theories can describe both long- and short-scale physics accurately in the non-relativistic regime. In the semi-relativistic regime, a long-scale model exists [20], and work on its fully relativistic generalization is ongoing [21].

In the treatment here we will concentrate on the physics of fully degenerate electrons [22–26], reviewing some recent findings. However, it should be noted that many of the basic equations and methods (like e.g. the Wigner–Moyal equation [4]) apply equally well to non-degenerate systems. The organization of the paper is as follows. In section 2 we put forward a quantum kinetic evolution equation that results from degeneracy alone [27]. For a degenerate plasma, perturbations
of the distribution function are never small compared to the background distribution outside of the Fermi sphere. It is thus difficult to apply standard perturbation theory. To circumvent this problem we instead study the dynamics of the Fermi surface, which is only weakly perturbed. A particular advantage with the approach outlined here is that it is straightforward to generalize in order to cover spin dynamics, see [27].

In section 3 we add the particle dispersive properties to the picture. Based on the Schrödinger equation we can then deduce the Wigner–Moyal equation. This equation reduces to the classical Vlasov equation in the limit of long scalelengths. The Wigner–Moyal equation is used to deduce a generalized condition for wave–particle resonances. This resonance condition leads to a new type of wave–particle damping [19], corresponding to the simultaneous absorption (or emission) of multiple wave quanta. This mechanism may be the dominant one for plasmas of low temperature and high densities.

In section 4 we investigate exchange dynamics. In particular we make a comparison of expressions for exchange potentials based on density functional theory (DFT) with results based on quantum kinetic theories [28]. A tentative conclusion is that the DFT potentials are reasonably accurate for high-frequency dynamics when ions are immobile, but less so when low-frequency phenomena is considered and the ion dynamics comes into play. Finally, in section 5 our results are discussed and summarized.

2. Fermi surface dynamics

As we will see in the next section, the Wigner–Moyal equation can be derived without further approximations from the (single-particle) Schrödinger equation. Using the single-particle Schrödinger equation naturally exchange effects are neglected, which instead are covered in section 4. For macroscopic scale lengths longer than the characteristic de Broglie length, the Wigner–Moyal reduces to the well-known Vlasov equation. Nevertheless, to a certain extent, important quantum effects are observable. When the (single-particle) Schrödinger equation can be derived without further approximations from the classical Vlasov equation in the limit of long scalelengths, the Wigner–Moyal reduces to the well-known Vlasov equation. This equation reduces to

\[ \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\perp} \right) = \frac{qE_{r}}{m}, \]  

(3)

where \( \mathbf{v} = \hat{r}v_{r}, \) and \( \hat{r} \) is a unit vector in the direction of the velocity, i.e., \( \hat{r} = (\sin \theta_{\phi} \cos \phi_{\theta}, \sin \theta_{\phi} \sin \phi_{\theta}, \cos \phi_{\theta}) \). \( \nabla_{\perp} \) is a velocity gradient perpendicular to \( \mathbf{r} \), and \( E_{r} = \hat{r} \cdot \mathbf{E} \). To have a closed system we need the source terms in Maxwell’s equation in terms of \( \mathbf{v} \). Using that \( f = f_{\text{max}} \) inside the Fermi surface, we immediately find the charge density \( \rho_{c} \) as

\[ \rho_{c} = qf_{\text{max}} \int \frac{\mathbf{v}^{3}}{3} d\Omega, \]  

(4)

and the current density \( \mathbf{j} \) as

\[ \mathbf{j} = qf_{\text{max}} \int \frac{\mathbf{v}^{4} \hat{r}}{4} d\Omega, \]  

(5)

where \( d\Omega = \sin \theta_{\phi} d\phi_{\theta} d\theta_{\phi} \).

The theory outlined here cannot be generalized to cover short scale physics, as the Wigner function that generalizes the classical distribution function is not conserved along particle orbits. However, to a certain degree it is possible to cover dynamics involving the spin degrees of freedom using a generalized version of equation (3). This is explored in some detail in [27]. Furthermore, in that paper a solution of equation (3) is computed for the case of nonlinear Landau damping, that demonstrates the advantage of working with the dynamics of the Fermi surface, rather than solving the full Vlasov equation. Specifically it is shown that the Fermi surface is only weakly perturbed in the regime of strongly nonlinear bounce oscillations (see figure 2 of [27]).

3. Short-scale dynamics

For very short macroscopic scale lengths, wave function dispersion enters the picture. In this case the classical Vlasov equation is replaced by the Wigner–Moyal equation [1–4]. A simple derivation of the Wigner–Moyal equation for electrostatic fields can be made by defining the Wigner function as
\[ f(\mathbf{r}, v, t) = \frac{m^2}{(2\pi \hbar)^3} \int \psi^*(\mathbf{r} + \mathbf{r}'/2, t) \psi(\mathbf{r} - \mathbf{r}'/2, t) \times \exp(i\mathbf{v} \cdot \mathbf{r}'/\hbar) d\mathbf{r}' , \]

and computing the time evolution of \( f \) based on the single-particle Schrödinger equation

\[ i\hbar \frac{\partial \psi}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \psi + q \Phi \psi = 0, \]

where \( \Phi \) is the electrostatic potential. It is then straightforward to deduce the Wigner–Moyal equation

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{q m^2}{\hbar} \int d^{3}v' d^{3}r'/\hbar \exp[i(\mathbf{v} - \mathbf{v}') \cdot \mathbf{r}'/\hbar] \times [\Phi(\mathbf{r} + \mathbf{r}'/2, t) - \Phi(\mathbf{r} - \mathbf{r}'/2, t)]f(\mathbf{r}, \mathbf{v}', t) = 0. \]

The connection of the Wigner–Weyl formalism to the algebra of pseudo-differential operators is explored in [29]. Furthermore, the phase space analysis of wave equations presented in [30] is also highly relevant for the Wigner–Weyl formalism. As is well-known, unlike the classical Vlasov equation, \( f \) cannot be considered as a probability density. In fact, \( f \) can be negative in small regions of phase space. Nevertheless, the charge and current density can be calculated in the same manner as for a classical distribution function, i.e.

\[ \rho_c = q \int f d^3v \]

and

\[ j = q \int v f d^3v. \]

For electrostatic fields only the charge density is needed and Poisson’s equation

\[ \nabla^2 \Phi = \frac{q}{\epsilon_0} \int d^3v - \frac{q \rho_0}{\epsilon_0}, \]

together with (8) form a closed system. Here we have assumed a constant neutralizing ion charge density \( q \rho_0 \), but if needed, it is easy to relax this condition by including a dynamic model for the ions.

Before we discuss solutions to equations (8) and (11) let us rewrite equation (8) in an alternative way. Taylor expanding the arguments of the potentials, doing multiple partial integrations, and using a standard delta function relation, we obtain

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{2q}{\hbar} \Phi \sin \left( \frac{\hbar}{2m} \mathbf{v} \cdot \nabla \Phi \right) f(\mathbf{r}, \mathbf{v}, t) = 0. \]

Here the arrows indicate the direction the operators are acting, i.e. the spatial gradient act on \( \Phi \) and the velocity gradient act on \( f \). The sinus-operator is defined by its Taylor-expansion. By keeping just the first order term in the expansion, we recover the classical Vlasov equation. In this process the validity condition for dropping higher order terms is found to be that the macroscopic scale lengths for variations in the potential are much longer than the characteristic de Broglie length of the particles.

To illustrate a basic effect of the Wigner–Poisson system, let us study small amplitude waves. Dividing the Wigner function as \( f = F_0 + f_1(\mathbf{v}) \exp[i(kz - \omega t)] \) and linearizing, the solution for the Wigner function is

\[ f_1 = \frac{q F_0 \Phi(v + v_q) - F_0(v - v_q)}{\hbar(\omega - k v_k)} \]

where \( v_q = (\hbar k/2m) \mathbf{k} \). Inserting this expression into Poisson’s equation, the linear dispersion relation becomes

\[ 1 = -\frac{q^2 k^2}{\hbar^2} \int \frac{F_0(v + v_q) - F_0(v - v_q)}{(\omega - k v_k)} d^3v. \]

Changing integration variables the dispersion relation can be written as

\[ 1 = -\frac{q^2 k^2}{\hbar^2} \int \frac{F_0(v) - F_0(v + v_q) - F_0(v - v_q)}{(\omega - k v_k - k v_k v_q)} d^3v. \]

This result has been studied in detail in e.g. [31, 32]. The main effect we are interested in here is the modification of the resonant velocity in the Landau poles. As is apparent from equation (15), the resonant velocities are modified from the classical case according to

\[ v_{res} = \frac{\omega}{k} \rightarrow v_{res} = \frac{\omega}{k} \pm \frac{\hbar k}{2m}. \]

Let us study the physical meaning of this modification. When a particle absorbs or emits a wave quantum it can increase or decrease the momentum according to

\[ \hbar k_1 \pm \hbar k = \hbar k_2, \]

and at the same time the energy changes according to

\[ \hbar \omega_1 \pm \hbar \omega = \hbar \omega_2. \]

Next we identify \( \hbar k_1/m \) (or equally well \( \hbar k_2/m \)) with the resonant velocity \( v_{res} \) and note that for small amplitude waves the particle frequencies and wavenumbers \( (\omega_{1,2}, k_{1,2}) \) obey the free particle dispersion relation \( \omega_{1,2} = \hbar k_{1,2}^2/2m \). Using these relations we see that the energy momentum relations, equations (17) and (18), imply the modification of the resonant velocity seen in equation (16). An interesting possibility, which was studied in [19], is the simultaneous absorption (or emission) of multiple wave quanta, rather than a single wave quantum at a time. In that case equations (17) and (18) are replaced by

\[ \hbar k_1 \pm n \hbar k = \hbar k_2, \]

and

\[ \hbar \omega_1 \pm n \hbar \omega = \hbar \omega_2, \]

where \( n = 1, 2, 3, \ldots \) is an integer. Accordingly, the resonant velocities now become

\[ v_{res} = \frac{\omega}{k} \pm \frac{n \hbar k}{2m}. \]

When we pick the minus sign in equation (21), the resonant velocity for absorbing multiple wave quanta can be considerably smaller, provided the wavelengths are short. As a
consequence, in the case of Langmuir waves, the damping rate due to absorption of multiple wave quanta can be larger than the standard linear damping rate. Basically this is due to a larger number of resonant particles in the former case. These issues have been explored in some detail in [19], where the damping rates for two-plasmon damping and three-plasmon damping have been computed.

4. Exchange dynamics

The Wigner–Moyal equation studied in section 3 was derived from the single-particle rather than the many-body version of the Schrödinger equation. As a result, it does not include exchange effects. Before we turn to the quantum kinetic theories, let us consider an expression for exchange effects that has been used rather extensively in a fluid formalism, see e.g. [10, 34–37]. Here exchange potentials derived from density functional theory (DFT) [33] have been incorporated in a fluid formalism [10]. For one-dimensional spatial variations along $z$ the momentum equation reads

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial z} - \frac{q}{m} E + \frac{1}{m} \frac{\partial V}{\partial z} + \frac{k^2}{2m^2} \frac{\partial}{\partial z} \left( \frac{\partial (\sqrt{n})}{\partial z^2} \right) = -\frac{1}{m} \frac{\partial P}{\partial z},$$

(22)

Here $u$ is the fluid velocity, $P$ is the fluid pressure, $n$ is the number density and the third term of the right-hand side is the Bohm–de Broglie potential that accounts for particle dispersive effects. The DFT exchange potential is given by

$$V_x = 0.985 \kappa \frac{\hbar^2 \omega_p^2}{4 \pi} \left( \frac{n}{n_0} \right)^{1/3},$$

(23)

where $\kappa = (3\pi^2)^{2/3}$ and $n_0$ is the unperturbed number density. Equations (22) and (23) are complemented by the continuity equation (same as in the classical case) and Poisson’s equation. A few things should be noted. Firstly, the exchange effects are often presented along with a contribution from particle correlations (collisions). The correlation contribution has been dropped here, as we would like to make a comparison with the quantum kinetic exchange effects only. Secondly, the derivation of the exchange potential has been made assuming a fully degenerate plasma, i.e. the pressure $P$ in equation (22) is the Fermi pressure. Thirdly, we will be concerned with the long-scale limit (i.e. characteristic wave-numbers $k$ that fulfill $\hbar k \ll m v_F$), in which case the Bohm–de Broglie term can be neglected. Finally we note that the sign of the exchange term is such as to counteract the pressure. It is worth noting that there has been some confusion over the sign of the term in the literature, but the original papers [10, 33] have the same (correct) sign as in equation (22).

While the DFT formalism can be derived from first principles, the use of trial functions and approximations such as the adiabatic local density approximation (ALDA) makes it important to verify the DFT potentials by independent means. This can be made using a quantum kinetic formalism. By writing down the first equation in the BBGKY-hierarchy and writing the two-particle density matrix as a anti-symmetric product of one-particle density matrices, a correction due to exchange effects can be obtained. Assuming a plasma without spin polarization and summing over all spin states, the following expression

$$\partial_t f(x,p,t) + \frac{p}{m} \cdot \nabla_x f(x,p,t) + eE(x,t) \cdot \nabla_p f(x,p,t)$$

$$= \frac{1}{2} \partial_p \int d^3r \int d^3q \ e^{-irq} \ h \ [\partial \tilde{\rho}(V(r))]$$

$$\times f\left( x - \frac{r}{2}, p + \frac{q}{2}, t \right) f\left( x - \frac{r}{2}, p - \frac{q}{2}, t \right)$$

$$- \frac{i\hbar}{8} \partial_p \partial_p \int d^3r \int d^3q \ e^{-irq} \ h \ [\partial \tilde{\rho}(V(r))]$$

$$\times \left[ f\left( x - \frac{r}{2}, p - \frac{q}{2}, t \right) \left( \partial_{\tilde{\rho}} - \partial_{\rho} \right) f\left( x - \frac{r}{2}, p + \frac{q}{2}, t \right) \right]$$

(24)

was derived in the long scale limit in [38]. It should be noted that equation (24) is limited to electrostatic fields (for a treatment allowing for electromagnetic fields, see [39]). The long scale limit means that the macroscopic scale lengths are longer than the characteristic de Broglie length, such that the left-hand side of equation (24) corresponds to the Vlasov limit. In the right-hand side of equation (24) we use $x$ and $r$ for position vectors and $p$ and $q$ for momentum vectors. Furthermore, $\partial_{\tilde{\rho}} \equiv \partial / \partial \rho_k$ and analogously for $\partial_p$ and $\partial_{\rho_k}$. An arrow above an operator indicates in which direction it acts. We have also used the summation convention so that a sum over indices occurring twice in a term is understood. Finally $V(r) = e^2/4\pi \varepsilon_0 |r|$ is the Coulomb potential.

We are now interested in comparing the DFT predictions based on equation (22) with the quantum kinetic predictions based on equation (24). For this purpose we consider the simple examples of linear Langmuir waves and linear ion acoustic waves in homogeneous plasmas. We perform the calculations perturbatively, i.e. treating the exchange contribution as a small correction. The background distribution of electrons is assumed to be fully degenerate (see equation (1)). For the case of Langmuir waves, the ions are assumed to be immobile, and for the case of ion-acoustic waves, the ions are treated classically and have a temperature $T = 0$. Full details of the calculations are presented in [28]. Here we just proceed to the results. Starting with Langmuir waves for wavenumbers $k \ll \omega_p / (\hbar v_F)$ (such that Landau damping do not occur) the result derived from equation (24) is

$$\omega^2 = \omega_p^2 + \frac{3}{5} \frac{\omega_p^2 k^2}{v_F^2} - \frac{3}{20} \frac{\omega_p^2 k^2}{v_F^2}$$

(25)

where the last term is the exchange correction. This is in exact agreement with previous calculations using several different methods, see [40–42]. However, equation (24) as well as the methods used in [40–42] are rather cumbersome to apply for more complicated problems (e.g. nonlinear and/or inhomogeneous systems). Thus it is interesting to note that the considerably simpler fluid formalism, based on equation (22) is able to give a comparatively good agreement. Replacing the numerical
coefficient in equation (23) according to 0.985 → 1.23 would give agreement with equation (25). Now we turn to the case of ion-acoustic waves. The dispersion relation derived from equation (24) is then given by

$$\omega^2 = \frac{m \kappa^2 v_p^2}{3m_i} \left[ 1 - \frac{\hbar^2 \omega^2}{3m_i v_p^2} (14.9 + 7.11i) \right]. \quad (26)$$

where the exchange correction coefficients 14.9 and 7.11 come from numerical solutions of certain integrals (see [28]). Naturally the fluid formalism cannot produce the imaginary correction corresponding to wave–particle interaction. However, comparing with the dispersion relation based on equation (22) it turns out that also the real part of the dispersion relation is somewhat inaccurate. To get agreement, we would need to modify the numerical coefficient in equation (23) according to 0.985 → 6.52. A tentative conclusion is that the DFT potential given in equation (23) is reasonably accurate for high-frequency phenomena involving only electrons, whereas it is inaccurate for low-frequency phenomena involving also the ion dynamics. Such a conclusion might be surprising, since it is usually more easy to obtain accurate DFT approximations for time-independent or slowly varying phenomena. A possible explanation is that wave–particle interaction is important for the low-frequency regime, but not for the high-frequency regime. Hence a quantum kinetic treatment is more crucial in the former case. However, more research is needed before a definitive conclusion can be reached.

5. Summary and discussion

In order to have a clear focus, we have in this brief review concentrated on fully degenerate systems, and in some cases also limited ourselves to electrostatic fields. Moreover, we have neglected all effects due to spin polarized systems (e.g. a magnetic dipole force due to the spin, spin magnetization currents, spin precession, etc) and also neglected relativistic effects. However, most of the theories presented here can be generalized to cover more general cases. Examples of works that discuss quantum kinetic theories of spin polarized plasmas are (2-spin-kin, [13, 14, 16]). Furthermore, weakly [20] and strongly [43–45] quantum relativistic effects have also been studied. Of particular interest is a strongly quantum relativistic treatment that also cover the spin dynamics [21].

The conclusions from the present paper are as follows. Firstly we note that the analysis of fully degenerate systems can be much simplified by studying the dynamics of the Fermi surface, as described by equations (3)–(5). Secondly, we note that replacing the classical Vlasov equation with the Wigner–Moyal equation modifies wave–particle interaction considerably. As is well-known, the usual Landau poles have a velocity shift ±hk/2m. Moreover, we deduce that new poles are produced when a nonlinear analysis is made. This is associated with multi-plasmon damping, as discussed in more detail in [19]. Thirdly, we have used quantum kinetic theories of exchange effects, in order to evaluate the accuracy of exchange potentials based on the DFT formalism. We have found that the DFT potentials give reasonably correct results for the dispersion relation of Langmuir waves. By contrast, the accuracy when it comes to the ion acoustic dispersion relation is very low [28]. It is suggestive to think that this implies a more general conclusion, i.e. that the DFT potentials are accurate when pure electron motion is considered, but not when the ion dynamics is involved. However, more research is needed to see if such a conclusion is justified.

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