On the contribution of exchange interactions to the Vlasov equation

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Abstract

Exchange effects play an important role in determining the equilibrium properties of dense matter systems, as well as for magnetic phenomena. There exists an extensive literature concerning, e.g., the effects of exchange interactions on the equation of state of dense matter. Here, a generalization of the Vlasov equation to include exchange effects is presented allowing for electromagnetic mean fields, thus incorporating some of the dynamic effects due to the exchange interactions. Treating the exchange term perturbatively, the correction to classical Langmuir waves in plasmas is found, and the results are compared with previous work. It is noted that the relative importance of exchange effects scales similarly with density and temperature as particle dispersive effects, but that the overall magnitude is sensitive to the details of the specific problem. The implications of our results are discussed.

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I. INTRODUCTION

Recently there has been an increased interest in the properties of quantum plasmas [1–3]. The interest has been stimulated by applications to for example quantum wells [4], spintronics [5], plasmonics [6], and laser plasma interaction on solid density targets [7]. Historically, there is a vast literature concerning effects from the quantum regime on the statistical equilibrium properties of matter systems (see e.g. [8] and references therein for a discussion) Concerning dynamical problems, much of the work within the framework of kinetic theory has been based on the celebrated Wigner-Moyal approach [1–3]. While the corresponding Wigner-Moyal equation takes particle dispersive effects from first principles into account, as well as being compatible with Fermi-Dirac statistic, there are still several types of quantum effects that are not included in this model. This includes e.g. spin dynamics [9], various types of relaxation processes [10] and exchange effects [11–13].

In this work we will ignore magnetization dynamics associated with the electron spin [9], relaxation processes associated with particle correlations [10], and concentrate on the dynamical effects due to exchange interactions. This will of course limit the model in terms of applicability, but it will serve to highlight the particular nature of the exchange interactions. For long scale lengths the Wigner-Moyal reduces to the Vlasov equation. However, the relative importance of exchange effects does not generally diminish with increasing scale lengths [11], and for dense plasmas exchange terms may provide important corrections to the Vlasov equation. Generalizing the treatment of Ref. [11] to include electromagnetic mean fields, summing over the spin states, we derive an evolution equation for the distribution function in the Hartree-Fock approximation, applicable in the regime of long scale lengths. Dropping the exchange term the Vlasov equation is recovered. The theory is illustrated by considering Langmuir waves in a plasma with the temperature much larger than the Fermi temperature. The exchange term is treated as a small perturbation and the correction to the linear Langmuir dispersion relation is calculated. By comparing with similar results for low-frequency ion-acoustic waves we note that the relative importance of exchange effects scales in the same way with temperature and density for the two cases. However, while the scaling is the same for high- and low-frequency waves, the overall magnitude in the exchange effects differs quite strongly. The implications of our results are pointed out, and the relation to other theories of quantum plasmas, in particular density functional theory [14, 15], is discussed.
II. EXCHANGE EFFECTS IN PLASMAS: THE ELECTROMAGNETIC CASE

In a previous paper, Ref. [11], we considered the long scale length limit of quantum exchange effects in electrostatic plasmas of fermions. This was done by first deriving the evolution equation for the Wigner distribution in the Hartree-Fock approximation where the anti-symmetric part to the mean field electric potential was included. The equation was then simplified using the assumption that the thermal de Broglie wavelength of the particles is much smaller than the typical scale length. In this approximation the part of the evolution equation which is independent of exchange effects simplifies from an integro-differential equation, i.e. the Wigner-Moyal equation, to a Vlasov type of equation. For the exchange terms some of the involving integrals are then solvable. We further considered the case of a completely spin unpolarized plasma which further simplified the exchange terms.

In Ref. [11] only the electric field interaction was considered. Here we make the extension to also include a magnetic field in the formalism, although the particle motion is still assumed to be non-relativistic. We focus on the long scale length limit, i.e. consider a characteristic scale length $L \gg \hbar/mv_T$, where $v_T$ is the thermal velocity, $\hbar = h/2\pi$ where $h$ is Planck’s constant and $m$ is the mass. In this regime, after lengthy algebra, the evolution equation of the Wigner distribution $f(x,p,t)$ [16] is found to be

$$\partial_t f(x,p,t) + \frac{p}{m} \nabla_x f(x,p,t) + q \left[ E(x,t) + \frac{p}{m} \times B(x,t) \right] \cdot \nabla_p f(x,p,t)$$

$$= \frac{1}{2} \partial_i^j \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{r} \cdot \mathbf{p}' / \hbar} \left[ \partial_i^j V(\mathbf{r}) \right] f \left( x - \frac{\mathbf{r}}{2}, p + \frac{\mathbf{p}'}{2}, t \right) f \left( x - \frac{\mathbf{r}}{2}, p - \frac{\mathbf{p}'}{2}, t \right)$$

$$- \frac{i\hbar}{8} \partial_i^j \partial_p^j \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{r} \cdot \mathbf{p}' / \hbar} \left[ \partial_i^j V(\mathbf{r}) \right]$$

$$\times \left[ f \left( x - \frac{\mathbf{r}}{2}, p - \frac{\mathbf{p}'}{2}, t \right) \left( \partial_x^i - \partial_p^i q \left[ \partial_j A_k(x) \right] - \partial_x^i + q \left[ \partial_x^j A_k(x) \right] \partial_p^i \right) f \left( x - \frac{\mathbf{r}}{2}, p + \frac{\mathbf{p}'}{2}, t \right) \right]$$

(1)

where $V(\mathbf{r}) = q^2/(4\pi \epsilon_0 r)$, $q$ is the charge, $\epsilon_0$ is the vacuum permittivity, $p$ and $p'$ denote kinetical momentum which is related to the canonical momentum $p_c$ according to $p = p_c - qA$ where $A$ is the vector potential. Furthermore, $x$ and $r$ denotes position vectors, and we have also defined $\partial_r^i = \partial/\partial r_i$ and an arrow above a differential operator indicates in which direction it acts. In the terms of the right hand side sums over repeated indices are understood, with $i,j,k = 1,2,3$. Note that the equation still explicitly contains the vector potential and is not gauge invariant in its current form. However, the Wigner function still gives gauge independent results for observables.
such as the charge and current densities, which are given by \( \rho_c = q \int d^3 p f \) and \( j = (q/m) \int d^3 p f p \) respectively, see Ref. [9] for further discussion.

III. EXCHANGE EFFECTS ON LANGMUIR WAVES

The equation above is quite complicated and in general some further approximations are needed. In Ref. [11] we studied the exchange effects on the damping of ion acoustic waves. This was done by linearizing the equation and using an iterative approach where the lowest order (i.e. exchange independent) solution was inserted in the terms on the right hand side. Here we study another example of electrostatic oscillations, namely Langmuir waves [17]. To find the dispersion relation, we linearize the evolution equation (1) together with the Poisson equation

\[
\nabla \cdot E = \frac{1}{\varepsilon_0} \sum s q_s f_s,
\]

where the sum is over the species in the plasma. To be specific we will here consider the the particles to be electrons, drop the species index on the distribution function, and let \( q_e = -e \). The positively charged ions constitute a neutralizing background.

We start with Eq. (1) and make the ansatz

\[
f = f_0 + f_1 \exp[i(kz - \omega t)] \quad \text{and} \quad E = \hat{z} E_1 \exp[i(kz - \omega t)],
\]

where \( \hat{z} \) is a unit vector in the z-direction. Inserting this into the linearized evolution equation (1) we obtain

\[
i \left( -\omega + \frac{k p_z}{m} \right) f_1(p) = qE \cdot \nabla_p f_0(p)
\]

\[
+ \frac{i}{2} \frac{\partial}{\partial p^I} \int d p' - i (p' + \hbar k \hat{z} / 2) \cdot r / \hbar \left[ \partial^I V(r) \right] \left[ f_1 \left( p + \frac{p'}{2} \right) f_0 \left( p - \frac{p'}{2} \right) + f_0 \left( p + \frac{p'}{2} \right) f_1 \left( p - \frac{p'}{2} \right) \right]
\]

\[
- \frac{\hbar k}{8} \frac{\partial}{\partial p^I} \frac{\partial}{\partial p^J} \int d p' - i (p' + \hbar k \hat{z} / 2) \cdot r / \hbar \left[ \partial^I V(r) \right] \left[ f_0 \left( p - \frac{p'}{2} \right) f_1 \left( p + \frac{p'}{2} \right) - f_0 \left( p + \frac{p'}{2} \right) f_1 \left( p - \frac{p'}{2} \right) \right].
\]

At this stage it is possible to solve the integrals over \( r \) as this can be recognized as the Fourier transform of the derivative of the Coulomb potential. Since we are aiming for the lowest order quantum mechanical correction, the result is expanded to leading order in \( \hbar k / (m v_T) \). Since we focus on the regime where the exchange terms will only give a small correction we may insert the lowest order solution (where exchange effects are neglected) in the integrals of the right hand side, that is we let

\[
f_1 \rightarrow f_1^{(0)} = \frac{q E_z}{i (\omega - k p_z / m)} \frac{\partial f_0}{\partial p_z}.
\]
Assuming that the thermodynamic temperature is much higher than the Fermi temperature the appropriate distribution function is given by the Maxwell-Boltzmann distribution

\[
    f_0(p) = \frac{n_0}{(2\pi mk_BT)^{3/2}} \exp\left(-\frac{p_y^2 + p_z^2}{2mk_BT}\right),
\]

where \( n_0 \) is the equilibrium density and \( T \) is the temperature of the electrons and \( k_B \) is the Boltzmann constant. Note that this assumption is not necessarily at odds with the assumption of a sufficiently dense plasma for exchange effect to be of importance. For further refinement of the current calculation one may add semiclassical corrections to the Maxwell-Boltzmann distribution function. After solving for \( f_1 \) to first order in the exchange term and inserting this into the linearized version of the Poisson equation (2) we get

\[
    k - \omega_p^2 k \left\{ \frac{1}{\omega^2} + \frac{3k^2v_T^2}{\omega^4} \right\} - I = 0,
\]

where

\[
    I = \frac{\omega_p^4h^2k^2}{4\pi^2m^2v_T^4} \int du dv \frac{1}{(\omega kv_Tu)^2} \int d\bar{u} d\bar{v} \frac{\bar{u}\bar{v}}{\bar{u}^2 + \bar{v}^2} \left[ \frac{\omega}{\omega - kv_T(u - \bar{u})} - \frac{2(u - \bar{u})^2}{\omega - kv_T(u - \bar{u})} \right] e^{-\left(u^2 + \bar{u}^2 + v^2 + \bar{v}^2\right)},
\]

where \( v_T^2 = k_BT/m \) and \( \omega_p = (4\pi n_0 e^2/m)^{1/2} \) is the plasma frequency. Since we are interested in corrections to Langmuir waves where \( \omega \approx \omega_p \gg kv_T \) and since we neglect Landau damping, we may expand the denominator in Eq. (8) to the lowest non-vanishing order in \( k \). After this the integrals can be straightforwardly solved and the resulting dispersion relation reads

\[
    \omega^2 = \omega_p^2 + 3k^2v_T^2 \left(1 + \frac{17}{720} \frac{\hbar^2\omega_p^2}{m^2v_T^4}\right).
\]

The exchange correction is of the same form as that by Ref. [18], although there is a difference of the numerical factor of order unity, due to the different background distribution \( f_0 \). We note that the relative magnitude of exchange effects scales with temperature and density as \( H^2 = h^2\omega_p^2/m^2v_T^4 \), with the same quantum parameter \( H^2 \) that appears in many other types of problems [1–3].

IV. SUMMARY AND DISCUSSION

The main result of the present paper is the inclusion of exchange effects in the Vlasov equation (see Eq. (4)), where the derivation of [11] is generalized to include electromagnetic mean fields. In our treatment we have neglected collisional effects (correlations), whose relative importance roughly scale as \( N^{-1} \), where \( N = n\lambda_D^3 \) is the number of particles in a Debye cube. This should be compared to the relative importance of exchange effects, that tend to scale as \( uH^2 \), where \( u \)
is a dimensionless factor that is dependent on the details of the specific problem at hand and $H^2 = \hbar^2 \nu_p^2 / m^2 v_F^4$. Clearly $H^2$ and $N$ increase with density and decrease with thermal energy, although the two scalings are not identical, and the opposing regimes $H^2 > N$ and $H^2 < N$ are both possible. As long as both exchange effects and collisions are small enough to be treated perturbatively, however, their respective contributions can be computed separately and added afterwards. Naturally a qualitative difference between collisions and exchange effects is that the former increase entropy and drives the system towards the equilibrium distribution.

A difficulty when trying to estimate the importance of exchange effect is that the value of the factor $u$ is hard to predict. In the present problem it turned out that $u \approx 0.024$, as can be seen from Eq. (9). Following the details of the calculation leading up to (9) we see that this modest value does not come from a small parameter of any sort, but is just due to successive multiplications of a few numbers each slightly smaller than unity. However, if the problem of Langmuir waves is replaced by ion-acoustic waves, the situation happens to be different [11]. The relative importance of exchange effects still has the overall scaling of $H^2$, but the value of $u$ is much larger. In Ref. [11] both the correction to the real and the imaginary value to the ion-acoustic dispersion relation was calculated, and the corresponding values of $u$ came out as $\text{Re} \, u \approx 0.80$ and $\text{Im} \, u \approx 3.0$. This seem to have important theoretical consequences. A common approach when modelling quantum plasma kinetically is to use the Wigner-Moyal equation [1–3] which includes particle dispersive effects but ignores exchange effects. When applying the Wigner-Moyal equation to collective phenomena (where the self-consistent field is important), the relative importance of the particle dispersive effects also scales as $H^2$ (provided the scale lengths are sufficiently short, of the order of the thermal de Broglie wavelength). Thus for Langmuir waves it may be safe to keep particle dispersive effects and drop exchange effects, as $u \ll 1$ assures the validity of this approach. For ion-acoustic waves, on the other hand, the same approach is questionable. The relative magnitude of particle dispersive effects still scales as $H^2$ (for short enough scalelengths), but as the magnitude of $u$ is no longer smaller than unity exchange effects is equally important. A reservation that must be made here is that the results above for applies for $T_F \ll T$, whereas many works have studied the opposite ordering. Qualitatively one would expect that much of the results described above remains the same, but with $H^2 \to \hbar^2 \nu_p^2 / m_k^2 v_F^2$ when $T \ll T_F$. To some degree this assertion is supported by comparison with the results presented in Ref. [15]. Here DFT-calculate equations lead to fluid equations with corrections due to the exchange effect of the order $\hbar^2 \nu_p^2 / m_k^2 v_F^2$. An interesting prospect for future work is to make more detailed comparisons of the
theories presented here with calculation based on time-dependent density functional theory [14].