Exchange corrections in a low-temperature plasma

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(Received 21 April 2015; published 14 July 2015)

We have studied the exchange corrections to linear electrostatic wave propagation in a plasma using a quantum kinetic formalism. Specifically, we have considered the zero-temperature limit. In order to simplify the calculations we have focused on the long-wavelength limit, i.e., wavelengths much longer than the de Broglie wavelength. For the case of ion-acoustic waves we have calculated the exchange correction both to the damping rate and the real part of the frequency. For Langmuir waves the frequency shift due to exchange effects is found. Our results are compared with the frequency shifts deduced from commonly used exchange potentials which are computed from density-functional theory.

DOI: 10.1103/PhysRevE.92.013104 PACS number(s): 52.25.Dg, 52.35.Fp

I. INTRODUCTION

Recently much work has been devoted to quantum plasmas, see, e.g., the books and review articles [1–4]. The research is motivated by an interest in, e.g., quantum wells [5], spintronics [6], plasmonics [7], laser plasma interaction [8], astrophysical applications [9], or general theory development [10]. The theoretical descriptions range from hydrodynamical equations (e.g., Refs. [1,4,11]) to quantum kinetic models (e.g., Refs. [3,10,12,13]) and field-theoretical approaches (e.g., Ref. [14]). Most models include the physical effects of particle dispersion and Fermi pressure and, in some cases, the magnetic dipole force and magnetization due to the electron spin [10,12,15,16]. An important effect that is sometimes accounted for (e.g., Refs. [11,17–23]) but often overlooked is the exchange effects resulting from the total antisymmetry of the electron wave function. A popular approach to include the effects of exchange interaction has been to apply density-dependent potentials deduced from density-functional theory (DFT) [11,19–22]. An advantage with this is that the resulting fluid models becomes comparatively simple once the exchange potentials are established. As a consequence, problems involving both high-frequency dynamics [11,19] as well as low-frequency (ion-acoustic) dynamics [19,20] can be addressed in a straightforward way also for nonlinear problems [19]. A drawback is that the calculation of DFT potentials typically involve approximations [e.g., the local density approximation (LDA)] whose accuracy can be hard to estimate beforehand. Thus there is a general need to validate results derived from DFT by independent methods.

In the present paper we calculate the exchange contribution to the ion-acoustic dispersion relation using quantum kinetic theory derived from first principles. Previous works along this line [17,18] have assumed the ordering $T \gg T_F$ (where T is the temperature and T_F is the Fermi temperature), which has prevented a direct comparison with results based on DFT potentials that have considered the opposite ordering. In this paper we focus on the low-temperature limit $T \ll T_F$ and evaluate the exchange contribution to the ion-acoustic dispersion relation in the Hartree-Fock approximation to first order in perturbation theory. We deduce that the effects of the exchange term is to increase the phase-velocity of the ion-acoustic mode and to increase the linear damping rate (which is due to wave-particle interaction). Moreover, as a confirmation of the correctness of the quantum kinetic formalism, we compare results from our quantum kinetic formalism with previous results for the exchange contribution of high-frequency Langmuir waves. In this latter case we recover the results of Refs. [24–26] exactly within the outlined approximation scheme.

Finally, we compare our findings with results based on commonly used DFT potentials [11,19,20,22]. As the DFT potentials are incorporated in a fluid formalism, no comparison can be made for the damping due to wave-particle interaction. In general, we find a qualitative agreement. In particular, the frequency shift in the different formalisms has the same scaling with the parameters (density and wave number) for both ion-acoustic and Langmuir waves. However, there is a discrepancy concerning a numerical factor. This is discussed in more detail in the final section of the manuscript.

II. THE EXCHANGE CORRECTION AT $T = 0$ K

In a previous paper, Ref. [17], the exchange contribution to the evolution equation of the Wigner function was derived (see Eq. (7) of Ref. [17]). The correction was obtained by writing down the first equation in the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy and writing the two-particle density matrix as an antisymmetric product of one-particle density matrices. The treatment was here limited to electrostatic fields. For a generalization allowing for electromagnetic fields, see Ref. [18]. Equation (7) of Ref. [17] was further simplified by considering a plasma without spin polarization and summing over all spin states, and also by taking the long scale limit (where the macroscopic scale length is assumed to be much longer than the de Broglie wavelength). The long scale assumption implies that the Wigner function reduces to the Vlasov limit, in which case the Wigner function becomes similar to a classical distribution function. This means that the evolution equation reduces to the Vlasov equation with a correction term due to the exchange effects. The resulting expression (Eq. (12) of Ref. [17]) with the exchange correction written

in the right-hand side reads

$$\partial_t f(\mathbf{x},\mathbf{p},t)+\frac{\mathbf{p}}{m}\cdot\nabla_x f(\mathbf{x},\mathbf{p},t)+e\mathbf{E}(\mathbf{x},t)\cdot\nabla_p f(\mathbf{x},\mathbf{p},t)=\frac{1}{2}\partial_p^i\int d^3r\,d^3q\;e^{-i\mathbf{r}\cdot\mathbf{q}/\hbar}\left[\partial_r^i V(\mathbf{r})\right]f\left(\mathbf{x}-\frac{\mathbf{r}}{2},\mathbf{p}+\frac{\mathbf{q}}{2},t\right)f\left(\mathbf{x}-\frac{\mathbf{r}}{2},\mathbf{p}-\frac{\mathbf{q}}{2},t\right)$$
$$-\frac{i\hbar}{8}\partial_p^i\partial_p^j\cdot\int d^3r\,d^3q\;e^{-i\mathbf{r}\cdot\mathbf{q}/\hbar}\left[\partial_r^i V(\mathbf{r})\right]\left[f\left(\mathbf{x}-\frac{\mathbf{r}}{2},\mathbf{p}-\frac{\mathbf{q}}{2},t\right)(\overleftarrow{\partial}_x^j-\overrightarrow{\partial}_x^j)f\left(\mathbf{x}-\frac{\mathbf{r}}{2},\mathbf{p}+\frac{\mathbf{q}}{2},t\right)\right]. \tag{1}$$

Here f denotes the electron distribution function; $\mathbf{E}$ is the electrical field; $-e$ and m_e are the electron charge and mass, respectively, and $h=2\pi\hbar$ is Planck's constant and we use $\mathbf{x}$ and $\mathbf{r}$ for position vectors and $\mathbf{p}$ and $\mathbf{q}$ for momentum vectors. Furthermore, $\partial_x^i\equiv\partial/\partial x_i$ and analogously for ∂_p^i and ∂_r^i. An arrow above an operator indicates in which direction it acts. We have also used the summation convention so a sum over indices occurring twice in a term is understood. Finally, $V(\mathbf{r})=e^2/4\pi\varepsilon_0|\mathbf{r}|$ is the Coulomb potential. Here we will use Eq. (1) to consider linear wave propagation treating the exchange term on the right-hand side perturbatively. Thus we linearize Eq. (1) and make a plane-wave ansatz $E_z=E\exp(-i\omega t+ikz)$, $f(\mathbf{x},\mathbf{p},t)=f_0(p)+f_1\exp(-i\omega t+ikz)$.

To first order in a long-wavelength expansion, the linearized version of Eq. (1) then reduces to

$$-i\left(\omega-\frac{kp_z}{m_e}\right)f_1(\mathbf{p})=-qE\partial_{p_z}f_0(p)+\frac{2i\hbar^2kq^2}{\epsilon_0}\nabla_p\cdot\int d^3q\,\frac{\mathbf{q}}{|\mathbf{q}|^2}\left[\partial_{p_z}f_0(|\mathbf{p}+\mathbf{q}|)f_1(\mathbf{p}-\mathbf{q})\right]. \tag{2}$$

Previously the correction to the dispersion relations for ion acoustic waves (see Ref. [17]) and for Langmuir waves (see Ref. [18]) has been found considering a Maxwellian background by making the approximation $f_1\approx\tilde{f}_1$ in the exchange term. The symbol $\tilde{f}_1=qE/[i(\omega-kp_z/m_e)]\partial f_0/\partial p_z$ denotes the solution when exchange effects are neglected.

Here we will study the same problems but for the case when $T=0$ K. As we will demonstrate the problem is analytically tractable due to the simple form of the background distribution function f_0 which is now given by

$$f_0(\mathbf{p})=\begin{cases}2/(2\pi\hbar)^3, & |\mathbf{p}|\leqslant p_F\\ 0, & |\mathbf{p}|>p_F,\end{cases} \tag{3}$$

where $p_F=\hbar(3\pi^2n_0)^{1/3}$ is the Fermi momentum (we will also use the notation $v_F=p_F/m_e$ for the electron Fermi velocity below) and n_0 is the equilibrium electron number density. In particular, taking $f_1=\tilde{f}_1$ in the exchange term, combining Eqs. (2) and (3) with Poisson's equation, and computing the ion charge density classically we obtain

$$1=\chi_0+\chi_1, \tag{4}$$

where

$$\chi_0=\frac{\omega_i^2}{\omega^2}+\frac{3\omega_e^2}{2k^2v_F^2}\int_{-1}^{1}dz\frac{z}{\omega/(kv_F)-z} \tag{5}$$

is the combined ion and electron susceptibility in the absence of exchange effects. Here we have neglected a contribution from a small but finite ion Fermi velocity (i.e., we have used that $v_{\mathrm{Fi}}\ll\omega/k$). In the expression above ω_e and ω_i denote the electron and ion plasma frequency, respectively. The exchange correction is given by

$$\chi_1=-\frac{q^4k}{8\pi^6\epsilon_0^2\hbar^4m_e}\int d^3\mathbf{p}\,d^3\mathbf{q}\,\delta(|\mathbf{p}-\mathbf{q}|-p_F)\delta(|\mathbf{p}+\mathbf{q}|-p_F)F \tag{6}$$

with

$$F=\frac{1}{(\omega-kp_z/m_e)^2}\frac{1}{\omega-k(p_z-q_z)/m_e}\frac{p_z}{|\mathbf{p}|^2}. \tag{7}$$

By changing integration variables to $\mathbf{u}_1=\mathbf{p}+\mathbf{q}$, $\mathbf{u}_2=\mathbf{p}-\mathbf{q}$, with the Jacobian equal to $1/8$, we can use the properties of the Dirac δ functions to reduce the problem to an integral over two spheres. Introducing spherical coordinates $\mathbf{u}_i=u_i(\cos\varphi_i\sin\theta_i,\sin\varphi_i\sin\theta_i,\cos\theta_i)$, we explicitly get $\chi_1=m_e^2q^4I'/8\pi^6\epsilon_0^2k^2\hbar^4$ with I' given by

$$I'=\frac{1}{4}\int\frac{\cos\theta_1\cos\theta_2}{(2-2\cos\psi)}\frac{\cos\theta_1-\cos\theta_2}{\alpha-\cos\theta_2}\frac{d(\cos\theta_1)d(\cos\theta_2)d\varphi_1d\varphi_2}{[\alpha-(\cos\theta_1+\cos\theta_2)/2]^2}, \tag{8}$$

where ψ is the angle between $\mathbf{u}_1$ and $\mathbf{u}_2$ and $\alpha=\omega/(kv_{\mathrm{F}})$ is the dimensionless phase velocity. By the spherical law of cosines $\cos\psi=\cos\theta_1\cos\theta_2+\sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)$. By changing variables to $\varphi_1,\tilde{\varphi}=\varphi_1-\varphi_2$, the φ_1 integral is trivial. The $\tilde{\varphi}$ integral then can be performed, giving a factor $\pi/(a^2-b^2)^{1/2}$, where $a=1-\cos\theta_1\cos\theta_2$ and $b=\sin\theta_1\sin\theta_2$. Since $a^2-b^2=(\cos\theta_1-\cos\theta_2)^2$, we have that $I'=-2^{-1}\pi^2I$, where I is the double integral

$$I=\int_{-1}^{1}dx\int_{-1}^{1}dy\,\frac{xy}{\alpha-y}\frac{\mathrm{sgn}(x-y)}{[\alpha-(x+y)/2]^2}. \tag{9}$$

At this point, no approximations have been made beyond those leading to the evolution equation (2), taking $f_1 = \tilde{f}_1$, and $T = 0$ K. For these approximations the exchange correction is therefore proportional to (9) for all frequency regimes. Thus Poisson's equation, with exchange corrections, is

$$1 = \chi_0 - \frac{9\omega_e^4\hbar^2}{16k^2m_e^2v_F^6}I. \tag{10}$$

where χ_0 is given by Eq. (5). From now on we must treat the low-frequency ion-acoustic case separately from the high-frequency Langmuir case in order to simplify the expression for I.

A. Ion-acoustic waves

The integral I can be evaluated analytically in terms of α with computer algebra software. We will consider the quasineutral limit ($\omega \ll \omega_i$) where the left-hand side of Eq. (10) is negligible. For ion-acoustic waves we can then make the approximation that $\alpha = \sqrt{m_e/(3m_i)}$ when solving the integral (9). It is also possible to plug in the value of α and evaluate the integral numerically. The dispersion relation for ion-acoustic waves with exchange corrections is then

$$\omega^2 = \alpha^2k^2v_F^2\left[1 - \frac{\hbar^2\omega_e^2}{3m_e^2v_F^4}(14.9 + 7.11i)\right]. \tag{11}$$

To the best of our knowledge this result has not been derived before.

B. Langmuir waves

In the high-frequency regime $\omega/k \gg v_F$, an expansion of I in powers of $v_F\ k/\omega$ can be made. With the lowest order nonvanishing correction, the dispersion relation in this regime is

$$\omega^2 = \omega_e^2 + \frac{3}{5}v_F^2k^2 - \frac{3\hbar^2\omega_e^2k^2}{20m_e^2v_F^2}. \tag{12}$$

This is in exact agreement with previous calculations using several different methods, see Refs. [24–26].

III. DFT COMPARISON

Equation (9) together with the specific results (11) and (12) are the main results of the present paper. The exact agreement of (12) with previous results also confirms the validity of (9). A strength of the quantum kinetic formalism is that it follows from first principles and that it can address wave particle interaction, such as the enhanced Landau damping rate found in Eq. (11). However, a drawback is that the formalism is difficult to use for more complicated problems. Thus there is a need to develop theories that are easier to apply in a more general context. One such possibility is offered by DFT. A commonly used exchange potential (see, e.g., Refs. [11,19,20,22]) computed from DFT is

$$V_x = \frac{0.985(3\pi^2)^{2/3}}{4\pi}\frac{\hbar^2\omega_e^2}{m_ev_F^2}\left(\frac{n}{n_0}\right)^{1/3}, \tag{13}$$

which has been used for low-frequency ion-acoustic phenomena (e.g., Refs. [19,20]) as well as high-frequency Langmuir waves (e.g., Refs. [11,19]). Including the contribution from Eq. (13) in the electron momentum equation (see, e.g., Ref. [11]) and treating the term as a small perturbation when calculating the ion-acoustic dispersion relation, we get a qualitative agreement with Eq. (11). In particular the ion-acoustic frequency is decreased and this change scale as $\hbar^2\omega_e^2/m_e^2v_F^4$, in accordance with (11). The numerical value of the frequency shift deviates rather significantly from our result, however. We note that if we make the adjustment $0.985 \to 6.52$ of the numerical prefactor in (13) we would get agreement with the real part of the frequency in Eq. (11). Here we stress that the wave damping cannot be compared with the DFT formalism, as this requires a quantum kinetic framework.

The same comparison can be made in the high-frequency regime. Thus we again include the contribution from (13) in the electron momentum equation, calculating the frequency shift of the Langmuir dispersion relation. Also here we have qualitative agreement, i.e., the Langmuir frequency increases proportionally to k^2, and the scaling with density is in accordance with the factor $\hbar^2\omega_e^2/m_e^2v_F^4$. This time the numerical accuracy is better, although not perfect, and we need to make a less significant substitution of the numerical factor in Eq. (13), $0.985 \to 1.23$ in order to get agreement with our result (12). Thus we conclude that the DFT exchange potential Eq. (13) is in qualitative agreement with the results obtained here, but that the numerical accuracy is better for Langmuir waves than for ion-acoustic waves.

IV. SUMMARY AND CONCLUSION

In the present paper we have computed the exchange contribution to the ion-acoustic dispersion relation in a plasma using a quantum kinetic formalism. The validity of our approach was confirmed by comparison with similar results for high-frequency Langmuir waves [24,25], in which case we get exact agreement for the exchange correction. This is to be expected, as our formalism as well as that of Refs. [24,25] is based on first principles. While the quantum kinetic formalism is of fundamental importance, it has the drawback of producing complicated formulas [cf. Eq. (1)] that can be solved only perturbatively. In fact, even a perturbative treatment is far from straightforward. Thus there is a need for a formalism that can be used in more complex situations. Such a possibility is offered by DFT, where the resulting exchange potentials can be used in fluid theories and straightforwardly applied to a number of linear and nonlinear problems [11,19,20,22]. However, as the computation of DFT potentials typically involves approximations [e.g., the local density approximation (LDA)] whose accuracy is unknown, there is a need to evaluate DFT potentials against independent methods. A key motivation in the present paper has been to evaluate the DFT potentials used in Refs. [11,19,20,22] against the quantum kinetic results computed in our formalism. This comparison reveals that there is a reasonable qualitative agreement. In both cases the relative magnitude of the exchange term scales as $\hbar^2\omega_e^2/m_e^2v_F^4$, and both the Langmuir and ion-acoustic wave frequencies decrease due to the exchange interaction, in agreement with Eqs. (11) and (12). The numerical value of this frequency shift differ somewhat, however. To some extent

this can be fixed by replacing the numerical prefactor in the exchange potential. If this approach is chosen, we note that different substitutions must be used for low-frequency and high-frequency phenomena (i.e., $0.985 \rightarrow 6.52$ in the former case and $0.985 \rightarrow 1.23$ in the latter case). It is an open question to what extent this result is robust (i.e., whether the same numerical coefficient is a good approximation for different problems at a given frequency scale) or if more advanced expressions for the exchange potentials are needed to cover a broad spectrum of problems.

The fact that there is not a perfect agreement between the DFT exchange potential and the quantum kinetic theory should not be overly surprising. The DFT potentials used in Refs. [11,19,20,22] have not necessarily been optimized for the situation we have been studying. In our case the fields dynamically vary (such that time-dependent density-functional theory applies), and the system is weakly collisional such that the collision-free Vlasov equation holds to leading order. The systems of relevance for the present study generally include plasmas with a high density and a modest temperature $T \ll T_F$. In a laboratory context this applies to, e.g., solid-state plasmas and inertial confinement fusion plasmas before the heating stage, and in an astrophysical context this include, e.g., white dwarf stars. In that case the perturbed distribution function will be comparatively far from thermodynamic equilibrium, and approaches which do not include the full quantum kinetic details run the risk of losing information. Nevertheless, an approach based on density-functional theory is a valuable option, in particular for problems where the approach used here becomes too complicated.

ACKNOWLEDGMENT

This research was supported by the Swedish Research Council Grant No. 2012-3320.

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