Do hydrodynamic models underestimate exchange effects? Comparison with kinetic theory for electrostatic waves

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We have extended previous kinetic results to compute the exchange correction to the electrostatic electron susceptibility for arbitrary frequencies and wavenumbers in the low temperature limit. This has allowed us to make a general comparison with a much used hydrodynamic expression for exchange effects. It is found that the hydrodynamic expression gives a useful approximation when the phase velocity is roughly a factor 2.5 larger than the Fermi velocity. For low phase velocities, as for ion-acoustic waves, wave-particle interaction leads to a strong enhancement of the exchange correction and the hydrodynamic results is smaller by an order of magnitude.

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I. INTRODUCTION

A majority of plasmas have low densities and/or high temperatures which assures that they can be accurately described using classical theories. Recently, however, there has been an increasing interest in plasmas of low-temperature and high densities, which make quantum properties significant. A review of recent developments are given in, e.g., Refs. [1–3]. Much of the research is motivated by applications such as, e.g., quantum wells [4], spintronics [5] and plasmonics [6]. Experiments with solid density targets [7] are also relevant in this context. Dense plasmas are usually divided into strongly and weakly coupled, and into degenerate and non-degenerate electrons [8]. Here we will concentrate on the fully degenerate but weakly coupled case.

Two prominent quantum effects are exchange and particle dispersion, that both scale as the quantum parameter \( H^2 = \hbar^2 \omega^2/m_e^2 v_F^2 \) relative to classical terms. Here \( \hbar \) is the reduced Planck constant, \( \omega_p \) is the electron plasma frequency, \( m_e \) is the electron mass and \( v_F \) is the Fermi velocity. Many works studying this regime have focused on particle dispersive effects, e.g. using the kinetic Wigner-Moyal equation [9, 10] or by introducing the Bohm-de Broglie term to a fluid model [11]. Since the scaling is the same, including the former effect but not the latter can be questioned. A possible justification for dropping exchange effects is that the overall \( H^2 \)-dependence comes with a dimensionless factor that depends on the detailed field configuration, and that this factor can be smaller than unity.

From a pragmatic point of view, exchange effects are often neglected because they are complicated to model. Still there exists a popular quantum hydrodynamic model that includes not only exchange effects, but also the effect of electron correlations. It was introduced in [10] and has been much used since then [11–14]. While this model is straightforward to apply, it should be stressed that the exchange potential is derived using standard density function theory (DFT), rather than its time dependent counterpart (TDDFT). Thus it is far from clear that the model has a reasonable applicability for dynamic problems, and the omission of kinetic effects means that there are further question marks regarding the accuracy of the model.

The purpose of the present work is to use a quantum kinetic model derived from first principles [15] to evaluate the accuracy of the above mentioned hydrodynamic model of exchange effects. Previous attempts in this direction [16] have been limited to the long wavelength regime (with the phase velocity much larger than the Fermi velocity) for high wave frequencies, or to the quasi-neutral case for low wave frequencies. Here we remove these restrictions, and make a general comparison of the quantum kinetic and hydrodynamic models, for linearized electrostatic waves. Due to the complexity of the kinetic theory, the evaluation must be done under the assumption that the exchange term can be treated as a small correction. The main conclusion is that the hydrodynamic model gives a decent approximation of the exchange effects for phase velocities \( \omega/k > 2.5 v_F \), but become inaccurate for shorter wavelengths. In the low-frequency regime there is a rather pronounced enhancement of the exchange effects due to wave-particle interaction, which has no counterpart in hydrodynamic theory. As a result, the hydrodynamic theory underestimates the exchange effects by an order of magnitude, and also the hydrodynamic theory does not capture the variation with phase velocity. The enhanced exchange effects in the low-frequency regime has profound implications for the modeling of ion-acoustic waves, which is discussed in some detail in the concluding parts of the paper.

II. THE KINETIC AND HYDRODYNAMIC DISPERSION RELATIONS

A. The quantum kinetic case

Our calculations here are based on the evolution equation for the Wigner-function first derived in Refs. [15, 17]. In that paper the first level in the BBGKY-hierarchy was applied, and the two-particle density matrix was writ-
ten as an anti-symmetric product of one-particle density matrices. Neglecting two-particle correlations a correction due to exchange effects was obtained. In the absence of spin polarization (summing over all spin states) and making long-scale approximations (assuming spatial scale lengths longer than the characteristic de Broglie wavelength), the following evolution equation was derived

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

\[ \frac{1}{2} \frac{\partial}{\partial p} \int d^3q d^3 q^* e^{-i r \cdot [\partial_r, V(r)]f} \left( x - \frac{r}{2} + \frac{q}{2} \right) \left( x - \frac{r}{2} - \frac{q}{2} \right) \]

\[ - \frac{i}{8} \frac{\partial}{\partial p} \cdot \int d^3q d^3 q' e^{-i q' / \hbar} [\partial_{q'}, V(r)] \left( f \left( x - \frac{r}{2}, p + \frac{q}{2}, t \right) \right. \]

\[ \left. \left( \frac{\alpha}{\delta} \right) \left( \partial_{q'} - \partial_q \right) \right) f \left( x - \frac{r}{2}, p + \frac{q}{2}, t \right) \right]. \]

The system is closed with Poisson’s equation which takes its classical form,

\[ \nabla \cdot E = \frac{q}{\epsilon_0} \int d^3 p f. \]  

As is evident, the left hand side in eq. (1) is the classical Vlasov operator for electrostatic fields, and it should be noted that the expression would be slightly more complicated in the presence of electromagnetic fields [17]. The right hand side corresponds to the exchange contribution to linear electrostatic waves in a homogeneous electron-ion plasma with degenerate electrons. (The hydrogen) ions were assumed to be cold and treated classically. The exchange effect was treated as a small correction, such that first order perturbation theory was applicable. Based on eqs. (1) and (2) and the conditions given above, Ref. [16] derived a dispersion relation

\[ 1 + \chi^{(i)} + \chi^{(e)} + \chi^{(x)} = 0 \]  

for the poles should be used (i.e., we add a small imaginary part \( i \delta \) to \( \omega \) and take the limit \( \delta \to 0 \)). When deriving eq. (7), no assumption regarding the value of \( \omega/kv_F \) was made, i.e., the given dispersion relation applies to both ion-acoustic waves (\( \omega/kv_F \ll 1 \)) and Langmuir waves (\( \omega/kv_F > 1 \)).

Due to the relative complexity of the integral \( I(\alpha) \), only two cases was computed in Ref. [16]. The long wavelength regime of Langmuir waves when \( \alpha \gg 1 \), and the quasi-neutral limit of ion-acoustic waves when \( \alpha = c_s/v_F = \sqrt{m_e/3m_i} \), where \( c_s = v_F \sqrt{m_e/3m_i} \) is the ion-acoustic velocity in the limit of fully degenerate electrons. Below we will generalize this treatment and compute the exchange-integral \( I(\alpha) \) for the general ranges \( 0 < \alpha \leq \sqrt{m_e/3m_i} \) (ion-acoustic waves) and \( 1 < \alpha < \infty \) (Langmuir waves). Note that for completely degenerate electrons, \( \alpha > 1 \) for Langmuir waves, which means that we will have no Landau damping for this wave mode [23].

### B. The quantum hydrodynamic case

Exchange effects can be incorporated in a quantum hydrodynamic framework based on density functional theory Refs. [2] [18]. Using dimensionless variables (\( t \to \omega_p t, \ r \to \omega_p r/v_F, \ n \to n/n_0, \ v \to v/v_F, \ \phi \to e\phi/mv_F^2 \)), where \( n_0 \) is the unperturbed background density and \( \phi \) the electrostatic potential, the model consists of the continuity and momentum equations for electrons,

\[ \partial_t n + \nabla \cdot (nv_e) = 0 \]  

\[ (\partial_t + v_e \cdot \nabla) v_e = \]

\[ \nabla \left( \phi + 0.985 \frac{3\pi^2}{4\pi m_e^2 v_F^4} n_0^{1/3} \right) - \frac{1}{5n} \nabla n, \]

and Poisson’s equation, again taking its classical form,

\[ \nabla \cdot E = \frac{q}{\epsilon_0 n}. \]
When deducing the dimensionless form of the momentum equation we have assumed that the Fermi pressure can be written $P = P_0(n/n_0)^\gamma$, with the unperturbed Fermi pressure $P_0 = mv_F^2/5$. For the case of collision-free electrons, it is natural to determine the exponent $\gamma$ from a comparison with kinetic theory. We note that we get agreement with the Langmuir dispersion relation in the long wavelength limit if we let $\gamma = 3$, and hence we will use this value in what follows. The numerical coefficient 0.985 in the exchange contribution is determined from time-independent DFT [18].

When writing down eq. (9) it should be noted that we have omitted two terms often kept in quantum hydrodynamic theories. First, we have dropped the Bohm-de-Broglie term, which is justified if we consider spatial scale lengths longer than the characteristic de Broglie wavelength. Second, we have omitted a contribution to the effective potential from electron-electron correlations. While this term scales slightly differently with the electron number density, as compared to exchange effects, in practice these two terms can often be comparable in magnitude [10].

The motivation for still dropping correlation effects is two-fold. Firstly, our aim is to compare with quantum kinetic theories that have only included exchange effects, and thus we do not want to complicate the picture by keeping physical effects that are irrelevant to the comparison. Secondly, our basic assumption is that exchange and correlation effects are both small, such that they can be treated perturbatively. To first order, perturbations can thus be treated independently and their respective contributions to the dispersion relation summed at the end.

Considering electrostatic wave propagation around a homogeneous equilibrium, linearizing eqs. (8) to (10), and including also the classical ion contribution to the charge density (in the zero temperature limit), we can write the hydrodynamic version of the dispersion relation in the same form as (7). Naturally the ion susceptibility is the same as in the previous case, eq. (4), but now the classical part of the electron susceptibility is

$$\chi^{(e)} = -\frac{\omega^2}{\omega^2 - (3/5)k^2v_F^2} \left[ \frac{\alpha^2}{\alpha^2 - (3/5)} \right]$$

and the electron exchange contribution is

$$\chi^{(x, h)} = \frac{1}{16}\frac{9\hbar^2\alpha_0^4}{m^2k_F^2v_F^3} \left[ \frac{\omega^2}{\omega^2 - (3/5)k^2v_F^2} \right]$$

where

$$P^h(\alpha) = \frac{0.445}{(\alpha^2 - (3/5))^{1/2}}$$

Here we have denoted the hydrodynamic quantities with an index "h" to distinguish them from their quantum kinetic counterparts. When deriving the hydrodynamic expression, the exchange correction appears as a modification of the classical electron susceptibility. Since the exchange contribution is taken to be small, however, we can Taylor-expand the modified susceptibility such that the exchange effect end up as a separate term, in agreement with eq. (8).

As is well-known, the classical electron susceptibility differs somewhat in the hydrodynamic and kinetic descriptions. However, we note that with our choice of $\gamma = 3$ in the equation of state both the hydrodynamic and kinetic electron susceptibility can be written as $\simeq -(\omega^2 + (3/5)k^2v_F^2)/\omega^2$ in the long wavelength limit $k^2v_F^2 \ll \omega^2$. Moreover, when taking out the common factor $9\hbar^2\alpha_0^4/16m^2k^2v_F^6$ from the exchange susceptibility, both the kinetic and hydrodynamic expressions depend on a single function of the (normalized) phase velocity, denoted by $I(\alpha)$ and $P^h(\alpha)$ respectively.

C. Comparison of $I(\alpha)$ and $P^h(\alpha)$

From the definitions of two functions $I(\alpha)$ and $P^h(\alpha)$, we see that they coincide if and only if the kinetic and fluid-DFT contributions to the exchange effects are the same. However, the well-known phenomena of wave-particle interaction (leading to imaginary pole contributions in $I(\alpha)$ when $\alpha < 1$) means that a perfect agreement is ruled out from the start. Nevertheless it is possible that the fluid DFT expression for the exchange effects can serve as a useful approximation under suitable conditions. For an electron-proton plasma we do not need to investigate the full range of $\alpha$. Either $1 < \alpha < \infty$ (the Langmuir mode) or $0 < \alpha < \sqrt{m_e/3m_i} \approx 0.013$ (the ion acoustic mode). While in principle we may also have a damped electron-acoustic mode [19] with $\alpha \lesssim 1$, it is not meaningful to compare $P^h(\alpha)$ and $I(\alpha)$ in this case, as the electron-acoustic mode depends critically on a ki-
the real parts.

dence in the fluid description, but we can still compare
Landau damping rate. Naturally this has no correspon-
part can be viewed as an exchange modification of the

Thus when comparing
previous works using several different methods [20–22].

analytically, the kinetic expression agrees exactly with

α ≪ 1, and we will therefore have pole contributions
to \( I(\alpha) \), giving a complex susceptibility. The imaginary
part can be viewed as an exchange modification of the
Landau damping rate. Naturally this has no correspond-
dence in the fluid description, but we can still compare
the real parts.

In fig. 2 we show the real and imaginary parts of \( I(\alpha) \),
and \( I^b(\alpha) \) in the ion-acoustic range where \( 0 < \alpha < 0.013 \).
While the real parts of \( I(\alpha) \) and \( I^b(\alpha) \) are both positive,
we see that we are now very far from agreement. Impor-
tantly \( I(\alpha) \) is an order of magnitude larger, and shows a
significant dependence on \( \alpha \), whereas \( I^b(\alpha) \) is approxi-
mately constant in the ion-acoustic regime.

We note that the integral \( I(\alpha) \) has large contributions
from the regions where the denominators are small, cor-
responding to exchange-mediated wave-particle interac-
tion. Since wave-particle interaction is important when-
ever \( \alpha < 1 \), it is not entirely surprising that the fluid
model becomes inaccurate in this regime. This is fur-
ther emphasized by the rather large imaginary part of
\( I(\alpha) \). The imaginary part shows very little variation with
\( \alpha \), but the large magnitude means that the exchange-
modification of the Landau damping rate can be signif-
ificant even for a modest value of the quantum parameter
\( \hbar^2 \) that determines the importance of exchange effects,
see eq. 6. Note also the magnified kinetic exchange con-
tribution in fig. 4 in the short wave limit, where \( \alpha \to 1 \).

III. DISCUSSION

The main goal of the present investigation has been to
examine the validity of a much used (see, e.g., Refs. 11–
14) quantum hydrodynamic expression for exchange ef-
fects. The conclusion is that for linear theory, the hy-
drodynamic expression provides a useful approximation
for phase velocities \( \omega/kv_F \gtrsim 2.5 \). While the investiga-
tion is based on linear theory alone, presumably this
may generalize also to nonlinear scenarios. However,
for low-frequency dynamics with small phase velocities
\( \omega/kv_F \ll 1 \), wave-particle interaction is important, and
the hydrodynamic theory underestimates the importance
of exchange effects by at least an order of magnitude.
This failure is in addition to the obvious neglect of wave-
particle damping mechanisms.

The unexpectedly large magnitude of exchange ef-
fects for low-frequency phenomena has a broader signifi-
cance. Many theoretical papers study quantum effects
in plasmas concentrating on the effect of particle dis-
persion. This can be done quantum kinetically through
the use of the Wigner equation, or quantum hydrody-
namically by including the Bohm-de Broglie term.
In any case the quantum effects of this type are important
for short scale lengths, with wavenumbers of the order
\( \hbar k \sim mv_F \). However, if the particle density is low (with
\( \omega_F^2 \ll k^2v^2_F \)) collective plasma behavior will be more or
less negligible, and essentially the particles will be free-
streaming (or possibly governed by an external field) Thus
for plasma effects to be important we also need a suffi-
cient density \( \omega_F^2 \sim k^2v^2_F \). For scales short enough
to make the particle dispersive effects important (i.e.,
\( k \sim mv_F/\hbar \)) we therefore must have \( \hbar^2\omega^2_{pc}/m^2v^4_F \sim 1 \).
With \( H^2 = \hbar^2\omega^2_{pc}/m^2v^4_F \sim 1 \) the exchange contribution
to susceptibility is still rather small for \( \alpha > 1 \), except
very close to unity. Although the exchange susceptibil-
ity tends to increase somewhat when $\alpha \to 1$, it is still a decent approximation to ignore exchange effects even for $H^2 \sim 1$. Hence it makes sense to describe high-frequency Langmuir waves including particle dispersive effects but dropping exchange effects. Naturally high accuracy still requires the inclusion of the exchange contribution, but if only modest precision is required, such an approximation can be justified.

However, for low-frequency ion-acoustic phenomena the situation is different due to the large value of $I(\alpha)$, see fig. [2]. Since the exchange effects scales as $I(\alpha)H^2$, see eqs. (5) and (6), for low-frequency phenomena these quantum effects dominates over particle dispersive effects, whose contribution is limited by $H^2$. Thus for ion-acoustic waves it does not make sense to use the Wigner equation for electrons, or quantum hydrodynamical equations with the Bohm term, without an exchange contribution.

In the above context it is a fundamental problem that the quantum kinetic theory is so complicated that it can be only solved perturbatively, and for relatively simple cases (like linear theory for homogeneous media). By contrast the fluid theory is fairly straightforward to use even for complicated nonlinear problems, but as shown here it underestimates the importance of exchange effects rather severely. A conceivable solution when describing low-frequency phenomena would be to use the DFT-expression but with a numerical coefficient increased according to $0.985 \to 20$, compare fig. [2] [24].

Still this is not entirely satisfactory, as there is no guarantee such an approach gives a decent approximation beyond this specific case (perturbative treatment of linear ion-acoustic wave). Moreover this would not capture the rather large contribution from the imaginary term of $I(\alpha)$. The general conclusion from this discussion is that it is a major challenge to make an accurate quantitative description of quantum ion-acoustic waves, even for the simple case of linear homogeneous wave propagation. The descriptions most commonly used (Wigner equation and various quantum hydrodynamical models) either ignore or underestimate the large contribution from exchange effects, and the quantum kinetic theory we have based this work on can only be applied in a perturbative setting. Thus for the case when $H^2 \sim 1$, all treatments of ion-acoustic waves have serious shortcomings. A possible way forward could be based on time-dependent density functional theory but finding accurate functionals in the presence of strong wave-particle interaction is likely not straightforward.

IV. CONCLUDING REMARKS

Some of the above arguments may suggest that the hydrodynamical model based on standard DFT should be avoided for all time-dependent phenomena. However, that conclusion is likely too strong. As far as we know it is considerably better for high-frequency phenomena. Intuitively one may think that time independent DFT should work better for slowly varying phenomena, but the lack of wave particle interaction (as is usually the case for high frequencies) tends to make the hydrodynamic theories more accurate for rapid processes. Moreover it should be stressed that the quantum kinetic models we have used here have several practical limitations. Most importantly these theories are very hard to apply for nonlinear and/or inhomogeneous problems. With that said, the general conclusion is that the hydrodynamical DFT based model for exchange effects must be applied with a lot of caution. Still much more work needs to be done – experimental or theoretical – in order to get a clear picture of the applicability of the current DFT theories. On the theoretical side, there is a need for the quantum kinetic formalism presented here to be complemented by works using, e.g., time-dependent density functional theory.

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[24] In Ref. [16] a substitution with a somewhat smaller factor was mentioned in a similar context. It should be noted that the figure is depending on the polytropic factor $\gamma$ in the equation of state: $(P/P_0) = (n/n_0)^\gamma$. If we replace our value $\gamma = 3$ with $\gamma = 5/3$ which is sometimes used [2, Section 5.2], the discrepancy between the fluid model and the kinetic model shown in fig. 2 would be reduced by a factor $9/5$ — i.e., the mismatch would roughly be a factor 10 instead of a factor 20.