Kinetic theory derivation of exchange-correlation in quantum plasma hydrodynamics

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Abstract. A quantum kinetic equation containing exchange-correlation described by an effective potential is derived, in a non-relativistic electrostatic quantum plasma. The velocity moments of the kinetic equation produce quantum fluid equations modified by the exchange-correlation potential. Closure of the hydrodynamic equations is achieved expressing the pressure dyad in terms of the number density, using a quantum corrected local velocity-displaced Wigner function equilibrium. The propagation of ion-acoustic waves in a quantum electron-ion plasma is analyzed, in the case of a completely degenerate electron gas. The fluid and kinetic approaches are compared and shown to agree in the long wavelength limit. A discussion on the equation of state and the role of the exchange-correlation and quantum diffraction effects is provided. Possible experimental parameters for the verification of the predictions are identified.

1. Introduction

In most works on quantum hydrodynamic models for charged particle systems [1, 2, 3, 4, 5], the Pauli Principle is not fully taken into account. Although the fermionic statistics can be included to some extent in terms of a Fermi-Dirac equilibrium and associated equations of state, in such references a Hartree approximation is assumed. Namely, the $N-$body electrons state is expressed as a product of one-particle wavefunctions, without taking into account the fundamental anti-symmetry of the quantum state or correlations. Therefore, the $N-$body Wigner function or equivalently the $N-$body density operator become a product of one-particle quantities. The result is a mean field theory where neither exchange effects (due to the Pauli Principle) nor correlation effects are fully incorporated. Classically, the Hartree approximation follows after neglecting the correlation between two or more particles in the BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) hierarchy of kinetic equations, directly leading to the Vlasov equation [6]. In the quantum case, the result is the quantum Vlasov (or Wigner-Moyal) equation satisfied by the Wigner function in the presence of the average collective field due to all charged particles [7, 8, 9]. From the quantum Vlasov equation, suitable macroscopic equations can be derived e.g. from the velocity moments of the Wigner function [10, 11], in the same way as the classical fluid plasma equations can be derived from the velocity moments of the particle distribution function satisfying Vlasov's equation, which is the usual route for classical plasma hydrodynamics [12, 13, 14, 15, 16].

In this context, it is indicated to improve quantum fluid models considering the anti-symmetry of the $N-$body fermion wavefunctions right from the start. In the Hartree-Fock approximation, the corresponding exchange effects are included assuming that the electrons state is given in terms of a single Slater determinant. The associated Hartree-Fock equations are integro-differential [17], analytically and computationally not very accessible for many body systems. This motivates the adoption of phenomenological effective potentials for the exchange and also for the correlation effects, which in the Adiabatic Local Density Approximation (ALDA) are functions of the particle density only [18]. In the case of quantum plasma hydrodynamics, effective exchange-correlation potential potentials were introduced in [19], by direct plugging into the fluid equations without a derivation from quantum kinetic theory. The modified physically appealing hydrodynamics provides an efficient model for linear and (specially) nonlinear problems such as quantum ion-acoustic waves [20], beam instabilities in ultra-small semiconductor devices [21] and nano-cylindrical waveguides [22]. However, the ad hoc character of the procedure from [19] is still questionable [23]. Here we show a first principles derivation of the exchange-correlation modified hydrodynamics starting from quantum kinetic theory. We follow as close as possible the well known moments method, adapted to a Fermi-Dirac local equilibrium which is suited for dense plasmas.

This work is organized as follows. In Section II, a modified quantum Vlasov equation is derived, taking into account exchange-correlation effects. In Section III, starting from a local velocity-shifted Fermi-Dirac equilibrium, the expression of the

pressure dyad is obtained, from which the appropriate equation of state and quantum diffraction effects are found. Section IV considers the case of quantum-ion acoustic waves as well as a discussion about the model's applicability. Section V is reserved to the conclusions.

2. Kinetic equation

We start from the Schrödinger equation for the one-electron wavefunction $\psi_\alpha = \psi_\alpha(\mathbf{r}, t)$ in a statistical ensemble $\{p_\alpha, \psi_\alpha; \alpha = 1, 2, ...\mathcal{N}\}$,

$$i\hbar\frac{\partial\psi_\alpha}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_\alpha - (e\phi + V_X)\psi_\alpha\,. \tag{1}$$

Here, $p_\alpha \geq 0$ is the statistical weight of the state ψ_α, such that $\sum_{\alpha=1}^{\mathcal{N}} p_\alpha = 1$. Moreover, $\hbar$ is the reduced Planck constant, m is the electron mass, $-e$ is the electron charge, ϕ is the electrostatic potential and V_X is the exchange potential. Correlation effects will be introduced soon. Notice the sign convention for V_X.

For the sake of definiteness, at first we suppose the Dirac expression for the exchange potential [25], which is based on the average Hartree-Fock potential for the homogeneous electron gas,

$$V_X = g_D\left(\frac{n}{n_0}\right)^{1/3}, \quad g_D = 0.985\,\frac{(3\pi^2)^{2/3}}{4\pi}\,\frac{\hbar^2\omega_e^2}{mv_F^2}\,. \tag{2}$$

Here, the number density is

$$n = \sum_\alpha p_\alpha|\psi_\alpha|^2\,, \tag{3}$$

with an equilibrium number density n_0, while $\omega_e = [n_0e^2/(m\varepsilon_0)]^{1/2}$ is the electrons plasma frequency, ε_0 is the vacuum permittivity and $v_F = (\hbar/m)(3\pi^2n_0)^{1/3}$ is the Fermi velocity. Each quantum state is normalized according to $<\psi_\alpha|\psi_\alpha>= N$, where N is the total number of particles. Notice that the evolution of each ψ_α is influenced by the quantum ensemble as a whole, due to Eq. (3).

The Wigner function $f = f(\mathbf{v}, \mathbf{r}, t)$ is defined [24] by

$$f = \left(\frac{m}{2\pi\hbar}\right)^3\sum_\alpha p_\alpha\int d\mathbf{s}\exp\left(\frac{im\mathbf{v}\cdot\mathbf{s}}{\hbar}\right)\psi_\alpha^*\left(\mathbf{r}+\frac{\mathbf{s}}{2},t\right)\psi_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},t\right), \tag{4}$$

in terms of phase-space coordinates $(\mathbf{v}, \mathbf{r})$ and time. As is well known, the velocity moments of the Wigner function determine the relevant macroscopic quantities such as particle, current and energy densities. In particular,

$$n = \int d\mathbf{v}f \quad , \tag{5}$$

which is equivalent to Eq. (3) with normalization $\int d\mathbf{v}d\mathbf{r}f = N$. Besides, we have

$$n\mathbf{u} = \int d\mathbf{v}f\mathbf{v}\,, \tag{6}$$

$$\mathbf{P} = m\left(\int d\mathbf{v}f\mathbf{v}\otimes\mathbf{v} - n\mathbf{u}\otimes\mathbf{u}\right). \tag{7}$$

where $\mathbf{u}$ and $\mathbf{P}$ are interpreted as the quantum fluid velocity field and pressure dyad, respectively.

The time-evolution of the Wigner function can be obtained from standard methods [7, 9], using the Schrödinger equation and its complex conjugate, as well as suitable identities such as

$$\int d\mathbf{v} \exp\left(-\frac{im\mathbf{v}\cdot\mathbf{s}}{\hbar}\right) f(\mathbf{v},\mathbf{r},t) = \sum_\alpha p_\alpha \psi_\alpha^*\left(\mathbf{r}+\frac{\mathbf{s}}{2},t\right)\psi_\alpha\left(\mathbf{r}-\frac{\mathbf{s}}{2},t\right) . \quad (8)$$

The result is

$$\begin{aligned}\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f = \left(\frac{m}{2\pi\hbar}\right)^3 \frac{g_D}{i\hbar}\int d\mathbf{s}\, d\mathbf{v}' \exp\left[\frac{im(\mathbf{v}-\mathbf{v}')\cdot\mathbf{s}}{\hbar}\right] f(\mathbf{v}',\mathbf{r},t)\times \\ \times\left[\left(n_0^{-1}\int d\mathbf{v}'' f(\mathbf{v}'',\mathbf{r}+\frac{\mathbf{s}}{2},t)\right)^{1/3} - \left(n_0^{-1}\int d\mathbf{v}'' f(\mathbf{v}'',\mathbf{r}-\frac{\mathbf{s}}{2},t)\right)^{1/3}\right] , \\ + \frac{e}{i\hbar}\left(\frac{m}{2\pi\hbar}\right)^3 \int d\mathbf{s}\, d\mathbf{v}' \exp\left[\frac{im(\mathbf{v}-\mathbf{v}')\cdot\mathbf{s}}{\hbar}\right] f(\mathbf{v}',\mathbf{r},t)\times \\ \times\left(\phi(\mathbf{r}+\frac{\mathbf{s}}{2},t)-\phi(\mathbf{r}-\frac{\mathbf{s}}{2},t)\right) , \end{aligned} \quad (9)$$

which generalizes the Wigner-Moyal equation by the inclusion of the exchange effects.

It is instructive to obtain the kinetic equation starting from the simple Dirac form of the exchange potential. However, a quick examination shows that all steps in the procedure remain unchanged if $V_X(n)$ given by Eq. (2) is replaced by an exchange-correlation potential $V_{\rm XC}$ depending (in the ALDA spirit) on the particle density only,

$$V_{\rm XC} = V_{\rm XC}(n) = V_{\rm XC}\left(\int d\mathbf{v}\, f\right) . \quad (10)$$

The generalized Wigner-Moyal equation reads

$$\begin{aligned}\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f + \frac{1}{i\hbar}\left(\frac{m}{2\pi\hbar}\right)^3 \int d\mathbf{s}\, d\mathbf{v}' \exp\left(\frac{im(\mathbf{v}-\mathbf{v}')\cdot\mathbf{s}}{\hbar}\right) f(\mathbf{v}',\mathbf{r},t)\times \\ \times\left(V(\mathbf{r}+\frac{\mathbf{s}}{2},t)-V(\mathbf{r}-\frac{\mathbf{s}}{2},t)\right) = 0 , \end{aligned} \quad (11)$$

where

$$V(\mathbf{r},t) = -e\phi(\mathbf{r},t) - V_{\rm XC}\left(\int d\mathbf{v} f(\mathbf{v},\mathbf{r},t)\right) + V_{\rm XC}(n_0) . \quad (12)$$

The constant $V_{\rm XC}(n_0)$ was added for later convenience. Obviously, besides the exchange-correlation and scalar potentials one could also include an external potential as an additive term.

For instance, a popular parametrization [26, 27] is given by the Hedin-Lundqvist (HL) potential

$$V_{\rm XC}(n) = g_D\left(\frac{n}{n_0}\right)^{1/3}\left(1+\frac{0.034}{a_B n^{1/3}}\ln\left(1+18.37 a_B n^{1/3}\right)\right) , \quad (13)$$

where $a_B = 4\pi\varepsilon_0\hbar^2/(me^2)$ is the Bohr radius. Without the logarithmic term, which is associated to correlations, the Dirac exchange potential is recovered. Notice that the HL

choice optimizes the description of stationary states of atomic and molecular systems, so that it is not necessarily adapted to plasma and general non-equilibrium problems.

The quantum statistical ensemble approach allows to derive a kinetic equation for the one body Wigner function taking into account exchange-correlation in terms of an effective potential. An alternative to include exchange effects is to start from an anti-symmetric $N-$body density matrix and then deriving a quantum BBGKY hierarchy [28, 29, 30]. The later method, however, does not includes correlation corrections. In the next Section, we derive hydrodynamic equations taking suitable moments of the kinetic equation (11).

3. Quantum hydrodynamic model

It is straightforward to derive macroscopic equations using the moments (5), (6) and (7) and the kinetic equation (11), yielding

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) \qquad = 0\,, \tag{14}$$

$$m\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) \;=\; -\frac{\nabla\cdot\mathbf{P}}{n} + e\nabla\phi + \nabla V_{\mathrm{XC}}(n)\,, \tag{15}$$

It is remarkable that exchange-correlation effects appear precisely in the form proposed in [19], as a simple gradient of the effective potential. The scalar potential is self-consistently determined by Poisson's equation (Section IV).

The moment transport equation (15) depends on the higher-order moment, namely the pressure dyad. One could proceed for the time-evolution equation for $\mathbf{P}$, which contains the next order moment. Pursuing this approach one gets an infinite hierarchy of equations, to be made finite by means of a choice of closure. The closure problem can be attacked in a variety of ways [31]. Here we follow [1], supposing a local quantum corrected velocity displaced thermodynamic equilibrium [32, 33]. This approach allows to determine both the pertinent equation of state and the role of quantum diffraction, which is still hidden since there is no sign of $\hbar$ in the fluid equations. In this context, the generalized quantum Vlasov equation is solved to the leading order in the quantum diffraction effects. Namely, one consider the semiclassic form of Eq. (11),

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f - \frac{1}{m}\nabla V\cdot\frac{\partial f}{\partial \mathbf{v}} + \frac{\hbar^2}{24m^3}\,\frac{\partial^3 V}{\partial x_i\partial x_j\partial x_k}\,\frac{\partial^3 f}{\partial v_i\partial v_j\partial v_k} = \mathcal{O}(\hbar^4)\,, \tag{16}$$

where the summation convention is implied. Actually [1], the expansion parameter is $\hbar^2/(8m<K>L^2)$, where $<K>$ is the average kinetic energy and L is a characteristic length. However, it is more expedite to use the shorthand $\mathcal{O}(\hbar^2)$. In addition, we assume that quantum diffraction is a higher order effect compared to exchange-correlation, so that $V = -V_{\mathrm{XC}} - e\phi$ is left untouched in the expansion (16). This assumption should be quantified in specific applications.

Since electrons in quantum plasmas can be at any degeneracy degree, it is useful to consider the $\mathcal{O}(\hbar^2)$ stationary solution of the Eq. (16) starting from an unperturbed Thomas-Fermi equilibrium where all quantities are assumed to be time-independent,

obtained in [34] without exchange-correlation. Actually, the presence of $V_{\rm XC}$ into the potential V does not change anything in the semiclassical solution, which reads

$$f = f_0 + \frac{\hbar^2}{8m}\Big(-\nabla^2 V \frac{\partial^2 f_0}{\partial \mu^2} + \frac{1}{3}\left[(\nabla V)^2 + m(\mathbf{v}\cdot\nabla)^2 V)\right]\frac{\partial^3 f_0}{\partial \mu^3}\Big)\,, \tag{17}$$

where

$$f_0 = f_0(E) = \frac{\alpha}{\exp\left[\beta(E-\mu)\right]+1}\,, \tag{18}$$

with $v = |\mathbf{v}|$ and

$$\alpha = 2\left(\frac{m}{2\pi\hbar}\right)^3\,, \quad \beta = \frac{1}{\kappa_B T}\,, \quad E = \frac{mv^2}{2} + V\,, \quad V = V(\mathbf{r})\,. \tag{19}$$

Here, κ_B is the Boltzmann constant, T is the temperature, μ is the chemical potential and E is the particle's energy. The chemical potential μ is determined [35] from

$$n_0 = -\alpha\left(\frac{2\pi}{\beta m}\right)^{3/2}{\rm Li}_{3/2}\left(-e^{\beta\mu}\right)\,, \tag{20}$$

where ${\rm Li}_{3/2}$ is a polylogarithm function. Polylogarithms can be defined in terms of Fermi-Dirac integrals,

$${\rm Li}_\nu(-z) = -\frac{1}{\Gamma(\nu)}\int_0^\infty \frac{s^{\nu-1}ds}{z^{-1}e^s+1}\,, \quad \nu > 0\,, \tag{21}$$

where $\Gamma(\nu)$ is the Gamma function. When $\nu < 0$ one applies

$${\rm Li}_\nu(-z) = \left(z\frac{\partial}{\partial z}\right){\rm Li}_{\nu+1}(-z) \tag{22}$$

as many times as necessary.

In classical plasma theory, a frequent method [16] for the derivation of equations of state is to start from a local quasi-equilibrium velocity-shifted distribution, assuming the macroscopic quantities to be slowly varying in time and space. The same strategy was pursued in [1], taking into account the lowest order quantum diffraction effects and a local velocity-shifted perturbed Maxwellian, which is appropriate for the electron gas in non-degenerate ultra-small semiconductor devices [7, 8]. Presently, we consider the velocity-shifted version of the solution (18), obtained through the replacements

$$\mathbf{v} \to \mathbf{v}' = \mathbf{v} - \mathbf{u}(\mathbf{r},t)\,, \quad E \to E' = \frac{m}{2}(\mathbf{v}-\mathbf{u}(\mathbf{r},t))^2 + V(\mathbf{r},t)\,. \tag{23}$$

Also the temperature and the chemical potential could be allowed to be variable, but for our present purposes they will be assumed strictly constant.

Calculating the moments n and $\mathbf{P}$ from the velocity-shifted version of Eqs. (17) and (18) together with Eqs. (5) and (7) we get

$$\begin{aligned} n \;&= \frac{n_0}{{\rm Li}_{3/2}(-e^{\beta\mu})}\Big[{\rm Li}_{3/2}(-e^{\beta\bar{\mu}}) + \frac{\hbar^2\beta^2}{12m}\times \\ &\times\;\left(-\nabla^2 V\,{\rm Li}_{-1/2}(-e^{\beta\bar{\mu}}) + \frac{\beta}{2}(\nabla V)^2{\rm Li}_{-3/2}(-e^{\beta\bar{\mu}})\right)\Big]\,, \end{aligned} \tag{24}$$

$$P_{ij} = \frac{n_0}{\beta}\frac{\mathrm{Li}_{5/2}(-e^{\beta\bar{\mu}})}{\mathrm{Li}_{3/2}(-e^{\beta\mu})}\delta_{ij} + \frac{\hbar^2 n_0\beta}{12m}\frac{\mathrm{Li}_{1/2}(-e^{\beta\bar{\mu}})}{\mathrm{Li}_{3/2}(-e^{\beta\mu})}\left(-\nabla^2 V\,\delta_{ij} + \frac{\partial^2 V}{\partial x_i \partial x_j}\right) + \frac{n_0\hbar^2\beta^2(\nabla V)^2}{24m}\frac{\mathrm{Li}_{-1/2}(-e^{\beta\bar{\mu}})}{\mathrm{Li}_{3/2}(-e^{\beta\mu})}\delta_{ij}\,, \tag{25}$$

where $\bar{\mu} = \mu - V$. By construction, Eq. (6) is already satisfied. In the case $V = 0$ and without quantum diffraction, the well-known [35] pair of equations of state for the ideal non-relativistic Fermi gas is recovered. In the dilute limit with a small fugacity $z = \exp(\beta\mu) \ll 1$, the expressions from [1] are recovered, using $\mathrm{Li}_n(-z) \approx -z$.

From now on, for simplicity we restrict to the deep degenerate case $\kappa_B T \ll E_F$. In this situation, $\mu = E_F$ and

$$\mathrm{Li}_\nu(-z) \approx -\frac{(\ln z)^\nu}{\Gamma(\nu+1)}\,, \quad \beta E_F \gg 1\,, \tag{26}$$

yielding

$$n = n_0\left(1 - \frac{V}{E_F}\right)^{3/2} - \frac{n_0\hbar^2}{16mE_F^2}\left(\frac{\nabla^2 V}{\left(1 - V/E_F\right)^{1/2}} + \frac{(\nabla V)^2}{4E_F\left(1 - V/E_F\right)^{3/2}}\right)\,, \tag{27}$$

$$P_{ij} = \frac{2}{5}n_0 E_F\left(1 - \frac{V}{E_F}\right)^{5/2}\delta_{ij} + \frac{n_0\hbar^2}{8mE_F}\left(1 - \frac{V}{E_F}\right)^{1/2}\times \times\left(-\nabla^2 V\,\delta_{ij} + \frac{\partial^2 V}{\partial x_i\partial x_j}\right) + \frac{n_0\hbar^2(\nabla V)^2}{32mE_F^2}\left(1 - \frac{V}{E_F}\right)^{-1/2}\delta_{ij}\,. \tag{28}$$

It was also assumed that $\beta\bar{\mu} \gg 1$, which in the deep degenerate case is assured except if $V \approx E_F$.

Solving up to $\mathcal{O}(\hbar^2)$, it is straightforward to eliminate V between Eqs. (27) and (28), yielding

$$P_{ij} = \frac{2}{5}\,n_0\,E_F\left(\frac{n}{n_0}\right)^{5/3}\delta_{ij} + \frac{\hbar^2}{18m}\nabla^2 n\,\delta_{ij} - \frac{\hbar^2}{12m}\left(\frac{\partial^2 n}{\partial x_i\partial x_j} - \frac{1}{3n}\frac{\partial n}{\partial x_i}\frac{\partial n}{\partial x_j}\right)\,. \tag{29}$$

The pressure dyad (29) agrees with [36, 37], derived from a principle of maximization of the quantum entropy and expansion on the quantum diffraction parameter.

Inserting Eq. (29) into the force equation (15) we find

$$m\frac{d\mathbf{u}}{dt} = -\frac{\nabla p}{n} + e\nabla\phi + \nabla V_{\mathrm{XC}} + \frac{\hbar^2}{18m}\nabla\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right)\,, \quad p = \frac{2}{5}\,n_0\,E_F\left(\frac{n}{n_0}\right)^{5/3}. \tag{30}$$

The continuity equation (14) and the momentum transport equation (30) constitute the fluid equations for electrons, complemented by the equation of state for the scalar pressure and the chosen effective exchange-correlation potential. The electrostatic potential obeys Poisson's equation. This is exactly the model proposed *ad hoc* in [19], now derived from quantum kinetic theory.

4. Quantum ion-acoustic waves

Low frequency electrostatic waves can be explored including the ion dynamics. Due to their larger mass, ions can be described by classical cold plasma fluid equations, namely

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{u}_i) = 0\,, \tag{31}$$

$$\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \;\; = \; - \frac{e \nabla \phi}{M}\,. \tag{32}$$

Here, n_i, $\mathbf{u}_i$, e and $M \gg m$ are respectively the ions number density, velocity field, charge and mass. In this context, Poisson's equation reads

$$\nabla^2 \phi = \frac{e}{\varepsilon_0}(n - n_i)\,. \tag{33}$$

Considering inertialess electrons, viz. neglecting the left-hand side of Eq. (30), we can linearize Eqs. (14) and (30)-(33) around the equilibrium $n = n_i = n_0, \mathbf{u} = \mathbf{u}_i = 0, \phi = 0$. Supposing plane wave perturbation proportional to $\exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]$, one gets the linear dispersion relation for quantum ion-acoustic waves,

$$\omega^2 = \frac{\left(1 + \frac{\hbar^2 k^2}{36 M m c_s^2}\right) c_s^2 k^2}{1 + \left(1 + \frac{\hbar^2 k^2}{36 M m c_s^2}\right) \frac{c_s^2 k^2}{\omega_i^2}}\,, \tag{34}$$

where $w_i = [n_0 e^2/(M\varepsilon_0)]^{1/2}$ is the ions plasma frequency and c_s given by

$$c_s^2 = \frac{(dp/dn)_0 - n_0 (dV_{\rm XC}/dn)_0}{M} \tag{35}$$

is the ion-acoustic velocity. The derivatives in Eq. (35) should be evaluated at the equilibrium $n = n_0$. In the long wavelength limit and to lowest order in quantum diffraction, one has

$$\omega^2 = c_s^2 k^2 \left(1 - \frac{c_s^2 k^2}{\omega_i^2} + \frac{\hbar^2 k^2}{36 M m c_s^2}\right) + \mathcal{O}\left((\frac{k c_s}{\omega_i})^6\right)\,. \tag{36}$$

The results (34) and (36) formally agree with those from [38, 39, 40], except that now the ion-acoustic velocity is generalized to include exchange-correlation effects.

In principle, the generalized quantum ion-acoustic speed from Eq. (35) could vanishes, in view of the negative contribution from exchange-correlation ($V_{\rm XC}$ should always be an increasing function of density). We can assume HL potential from Eq. (13), as well as the equation of state for the ideal Fermi gas. This yields

$$c_s^2 = \frac{2E_F}{3M}\left(1 - f(H)\right)\,, \quad H = \frac{\hbar\omega_e}{E_F}\,, \quad f(H) = c1 H^2 \left(1 + \frac{c_2}{1 + c_3/H^2}\right)\,, \tag{37}$$

where $c_1 = 0.188, c_2 = 0.625, c_3 = 10.081$. The function $f(H)$ is the exchange-correlation correction. In fully degenerate plasma, the parameter $H = \hbar\omega_e/E_F \sim n_0^{-1/6}$ is a measure of the collisional effects [9, 41]. Hence, degenerate plasma tends to be more ideal for increasing density. More exactly, we can define a graininess parameter $g = U_p/<K>$, where $U_p = e^2/(4\pi\varepsilon_0 r_s)$ is a rough estimate of the average electrostatic energy per

particle, $r_s = [3/(4\pi n_0)]^{1/3}$ is the Wigner-Seitz radius and $<K>= (3/5)E_F$ is the average kinetic energy per particle. A quick calculation gives $g = 1.02H^2$. From Eq. (37), we see that the relative role of the correlation effects (proportional to $c_2 < 1$) tends to be smaller for larger density, being always a correction to the exchange effects. In addition, from Eq. (37) we have that the exchange-correlation correction is as expected an increasing function of the density, with $c_s^2 < 0$ for $H > 2.11$, or equivalently $n_0 < 1.23 \times 10^{28}\,\mathrm{m}^{-3}$, corresponding to strongly coupled plasma, formally beyond the present treatment [41]. Nevertheless, the exchange-correlation correction can be significant even for $H < 1$, as depicted in Figs. 1 and 2. In terms of the effective potential (13), one finds the estimate $10^{30}\,\mathrm{m}^{-3} < n_0 < 10^{31}\,\mathrm{m}^{-3}$ in order to have both $H < 1$ and a quantum ion-acoustic speed exchange-correlation correction above 10%, as shown in Fig. 3. Such densities are clearly already experimentally accessible to laboratory experiments, keeping in mind also the strong degeneracy $\kappa_B T << E_F$ assumption. Finally, from Eq. (36) we find that the relative importance of quantum diffraction (the ratio between the third term proportional to $\hbar^2 k^2$ and the second term proportional to $c_s^2 k^2$) is

$$\frac{\hbar^2\omega_i^2}{36Mmc_s^4} = \frac{H^2}{16}\,\frac{1}{(1-f(H))^2}\,. \tag{38}$$

Although the role of quantum diffraction is by construction a second order correction, it can be enhanced if the characteristic function $f(H)$ becomes of order unity.

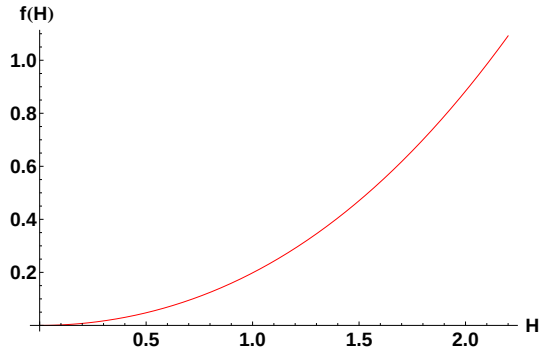

Figure 1. Exchange-correlation correction $f(H) \equiv c1H^2[1 + c2/(1 + c_3/H^2)]$ to the quantum ion-acoustic speed, from Eq. (37), where $H = \hbar\omega_e/E_F, c_1 = 0.188, c_2 = 0.625, c_3 = 10.081$.

It is relevant to have a comparison between the fluid and kinetic approaches. For this purpose, consider the Vlasov equation for ions,

$$\frac{\partial f_i}{\partial t} + \mathbf{v}\cdot\nabla f_i - \frac{e}{M}\nabla\phi\cdot\frac{\partial f_i}{\partial \mathbf{v}} = 0\,, \tag{39}$$

where $f_i = f_i(\mathbf{v}, \mathbf{r}, t)$ is the ions probability distribution function. Equations (11) and (39) together with Poisson's equation

$$\nabla^2\phi = \frac{e}{\varepsilon_0}\left(\int d\mathbf{v} f(\mathbf{v},\mathbf{r},t) - \int d\mathbf{v} f_i(\mathbf{v},\mathbf{r},t)\right) \tag{40}$$

constitute a quantum kinetic model taking into account exchange-correlation for electrons, in the weak coupling approximation.

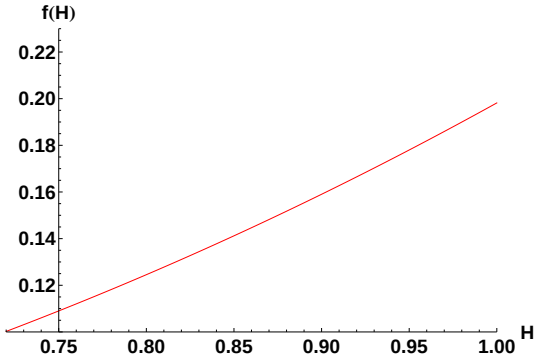

Figure 2. Same as Fig. 1, focusing in the region where $H < 1$ and $f(H) > 1/10$.

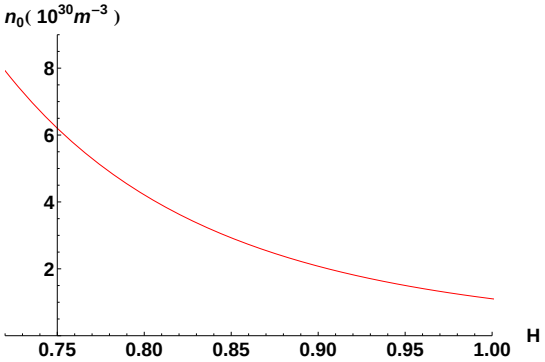

Figure 3. Number densities corresponding to Fig. 2, where $H < 1$ and $f(H) > 1/10$.

The system of Eqs. (11), (39) and (40) can be linearized for plane wave perturbations around the equilibrium $f = f_0(\mathbf{v})$, $f_i = n_0\delta(\mathbf{v})$ (for cold ions), $\phi = 0$. The dispersion relation is $\epsilon(\mathbf{k}, \omega) = 0$, where

$$\epsilon(\mathbf{k},\omega) = 1 - \frac{\omega_i^2}{\omega^2} - \frac{1}{n_0}\left[\omega_e^2 + \frac{n_0 k^2}{m}\left(\frac{dV_{\mathrm{XC}}}{dn}\right)_0\left(\frac{\omega_i^2}{\omega^2} - 1\right)\right] \times$$
$$\times \int \frac{d\mathbf{v} f_0(\mathbf{v})}{(\omega - \mathbf{k}\cdot\mathbf{v})^2 - \hbar^2 k^4/(4m^2)} \,. \tag{41}$$

In the special case $f_0(\mathbf{v}) = \alpha$ for $v < v_F$ and $f_0(\mathbf{v}) = 0$ for $v > v_F$, corresponding to strong electron degeneracy, and considering the static response approximation ($\omega \approx 0$ in the integral in Eq. (41)) which is appropriate to ion-acoustic waves, the result is

$$\epsilon(\mathbf{k},\omega) = 1 - \frac{\omega_i^2}{\omega^2} + \frac{3}{k^2 v_F^2}\left[\omega_e^2 + \frac{n_0 k^2}{m}\left(\frac{dV_{\mathrm{XC}}}{dn}\right)_0\left(\frac{\omega_i^2}{\omega^2} - 1\right)\right] \times$$
$$\times \left(1 - \frac{\hbar^2 k^2}{12 m^2 v_F^2}\right) , \tag{42}$$

up to the leading quantum diffraction correction, see [40, 42] for details about the algebra for the static response. For the sake of comparison with fluid theory, the integral in Eq. (41) was taken in the principal value sense, ignoring the contribution from the poles. As remarked in [42], Landau damping on quantum ion-acoustic waves described by the usual Wigner-Poisson system is not a serious issue as long as the ionic temperature is

much smaller than the electrons Fermi temperature, being a higher order correction $\sim \sqrt{m/M} \ll 1$. Finally, solving $\epsilon(\mathbf{k},\omega) = 0$ from Eq. (42) in the long wavelength limit $kc_s \ll \omega_i \ll 1$ gives the same linear dispersion relation from the fluid model, as shown in Eqs. (35) and (36), as it should be.

We can compare the present results with the findings from recent quantum kinetic models [28]-[30], where exchange effects were included considering from the beginning the antisymmterization of the $N-$particle density matrix, without correlation or (using a long wavelength limit) quantum diffraction effects. Ion-acoustic waves in the dilute plasma limit ($\kappa_B T \ll E_F$) have been considered, yielding

$$\omega/k = c_{sc}\left[1 + 0.8\left(\frac{\hbar\omega_e}{mv_T^2}\right)^2 - i\,\left(\frac{\pi m}{8M}\right)^{1/2}\left(1 - 3\left(\frac{\hbar\omega_e}{mv_T^2}\right)^2\right)\right], \tag{43}$$

as shown in Eq. (16) of [28], where $c_{sc} = \sqrt{m/M}\,v_T$ is the classical ion-acoustic speed assuming cold ions, v_T is the electrons thermal speed. The parameter $[\hbar\omega_e/(mv_T^2)]^2$ plays the role of a coupling parameter on non-degenerate plasma. On the opposite limit of strong degeneracy, one has from Eq. (11) of [29]

$$\omega/k = \left(\frac{2E_F}{3M}\right)^{1/2}\left(1 - 0.62H^2(1 + 0.59i)\right), \tag{44}$$

see also Eq. (26) of [30]. According to Eq. (43), exchange effects increase the phase speed of the otherwise classical ion-sound waves, while from Eq. (44) these effects have the opposite influence in completely degenerate plasma. Moreover, while in the dilute limit one has a Landau damping of order $\sqrt{m/M} \ll 1$, in the fully degenerate plasma one apparently can have from inspection of the imaginary part in Eq. (44) a strong damping due only to exchange effects provided H is reasonable high. On the other hand, the present quantum kinetic theory as well as the fluid model from [19] give a smaller phase speed due to exchange effects, as shown in Eq. (37), with some discrepancy on the numerical factors in comparison with Eq. (44). For a proper comparison, c_2 must be set to zero in Eq. (37) because correlation effects are not included in Eq. (44). Moreover, Eq. (41) gives no strong Landau damping due to exchange, since a separate calculation following [42] shows a $\sim \sqrt{m/M}$ correction in this regard. Finally, applying Eq. (41) together with a Maxwellian equilibrium would be inappropriate, since the HL exchange-correlation potential is based on an homogeneous zero-temperature Fermi gas.

5. Conclusion

We have deduced a quantum kinetic equation starting from a quantum statistical ensemble with exchange-correlation potentials. Quantum plasma hydrodynamics was found from the moments of the resulting generalized Wigner-Moyal equation (11). Closure of the fluid equations was obtained assuming a local velocity-shifted quasi-equilibrium Wigner function and small quantum diffraction effects, or, equivalently, the weak coupling assumption. By definition, as in classical plasma, the isothermal quasi-equilibrium assumption tends to work better for low frequency waves. The case

of linear quantum ion-acoustic waves in completely degenerate plasma was worked out. The precise conditions for reasonably large exchange-correlation effects compatible with the weak coupling assumption were discussed, indicating possible experiments to check the accuracy of the present theory, as well as of alternative approaches [28]-[30]. Similarly, the HL form of the exchange-correlation potential can be also checked against experiments on low frequency electrostatic waves in quantum plasma, since this parametrization is a key ingredient in the resulting wave dispersion. Several extensions of the kinetic equation (11) and the associated hydrodynamics are also desirable, considering for instance finite-temperature effects, gradient corrections for the exchange-correlation potential, spin polarization and magnetized plasmas. Finally, a more profound comparison with time-dependent density functional and quantum kinetic theories with collisional operators such as the Lenard-Balescu one and others is also highly indicated [43, 44, 45, 46].

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