Kinetic studies of exchange-correlation effect on the collective excitations of warm dense plasmas

Jiong-Hang Liang[1], Tian-Xing Hu[1], D. Wu[2],* and Zheng-Mao Sheng[1]†

[1]*Institute for Fusion Theory and Simulation, Department of Physics, Zhejiang University, 310027 Hangzhou, People's Republic of China and*

[2]*Key Laboratory for Laser Plasmas and School of Physics and Astronomy, and Collaborative Innovation Center of IFSA (CICIFSA), Shanghai Jiao Tong University, 200240 Shanghai, People's Republic of China*

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The exchange-correlation of electrons, as a fundamental effect in quantum mechanics, play an important role in the collective motions of electrons in warm dense matter. We derive the quantum kinetic equations based on the time-dependent Kohn-Sham equation. By using a temperature-dependent functional for the exchange-correlation, the excitations of electrostatic waves are analysed under the adiabatic local density approximation (ALDA). We find that the influences of exchange-correlation effect on the phase velocity of electrostatic waves can be as high as 10% when both the density and temperature are low. Moreover, we also compare the results obtained by using ALDA-based kinetic theory, exchange kinetic theory and quantum hydrodynamics, and the differences among them are discussed.

* dwu.phys@sjtu.edu.cn

† zmsheng@zju.edu.cn

I. INTRODUCTION

Due to its key roles in ICF [1] and astrophysics [2–4], warm dense matter (WDM), with temperature of $1 \sim 100$ eV and density of $10^{21} \sim 10^{28}$ cm^{-3}, has attracted wide attention of researchers. However, even for the homogeneous electron gas (HEG), as a simplified model, there are still many issues to be investigated because of the harsh conditions.

One of the most crucial research contents is the collective effect of electron-ion systems in WDM. The energy parameter $H = \hbar\omega_{\rm pe}/E_{\rm F}$ representing the ratio of plasmon energy and Fermi energy, as a measure of the strength of the collective effect, ranges from 0.3 to 3 in WDM [5]. It implies that the collective excitation energy is in the same order as the fermion ground-state energy, and the collective effect has an important impact in WDM. While classical plasma theory has provided an accurate theoretical basis for the study of collective excitation in high-temperature low-density systems, quantum plasma theory, as an effective theory bridging the gap between classical sparse matter and quantum dense matter, has also attempted to make a breakthrough within WDM [6].

The development of quantum plasma theory originated from the work of Bohm and Pines [7–9] to study the dynamic response of dense plasma. Then Lindhard analytically described the density response of free electron gas at low temperatures and thus added quantum corrections to the plasma theory [10]. Bonitz summarized the quantum effects of the kinetic theory [11] which is too complicated to solve in three-dimensional systems. Hass and Manfredi et al. simplified the Wigner equation by fluid approximation to create quantum hydrodynamics (QHD) [12] that is much easier to analyze for high-dimensional systems. However, the shortcomings of QHD have made its applicability doubtful [13] in the short-wavelength region, and QHD does not contain quantum effects other than quantum diffraction effects, such as exchange-correlation interactions, to which the nonlinear density response is highly sensitive [14].

To solve the many-body problem in quantum mechanics with the complete inter-particle interactions, the system's wave function is calculated from the basic *Schrödinger's* equation

$$\left[\sum_{i}^{N}\left(-\frac{\hbar^2\nabla^2}{2m}+v_{\rm ext}(\mathbf{r}_i,t)\right)+\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j,t\right)\right]\Psi\left(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N,t\right)=i\hbar\partial_t\Psi\left(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N,t\right) \tag{1}$$

where N is the number of electrons and $U\left(\mathbf{r}_i,\mathbf{r}_j\right)$ is the electron-electron interaction. For a Coulomb system one has

$$\hat{U}=\sum_{i<j}U\left(\mathbf{r}_i,\mathbf{r}_j\right)=\sum_{i<j}\frac{q^2}{|\mathbf{r}_i-\mathbf{r}_j|} \tag{2}$$

and $v_{\rm ext}$ represents the potential that the electron system feels, including the external field and the potential provided by ions. However, it is impossible to solve this equation in a large system due to its complex properties.

A one-to-one correspondence between electron density n and effective potential $V_{\rm eff}$ has been established by Runge-Gross theorem [15], which leads to the birth of a powerful and viable alternative – time dependent density functional theory (TDDFT). It reduces complex multi-particle problems to relatively straightforward single-particle problems and allows for a comparatively complete consideration of the most intractable exchange-correlation component of Eq.(2). TDDFT has already made many contributions to the analysis of opacity [16] and electron transport behavior [17] in WDM, and its time-free simplified model, density functional theory (DFT), has played a crucial role in the characterization of WDM [18, 19]. The results of TDDFT can also be applied to collisionless plasmas as G. Manfredi

concluded [20], and the exchange-correlation analysis has been added on the basis of TDDFT-QHD for the electrostatic waves at low temperature limit [21, 22]. Exchange kinetic theory (EKT) established by Ekman, Bordin, and Zamanian [23], which was obtained by simplifying the collision term of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy, has also shown some discrepancies in the QHD analysis of the exchange-correlation interaction [24]. Moreover, most of these completed works cannot be effectively extended to the high-energy density regime, where high temperatures significantly affect the wave-particle interactions and the exchange-correlation interactions.

This paper is organized as follows. In Sec. II, we derive the kinetic equations on the basis of the TDDFT equations and summerize the interconnections. In Sec. III, we analyze the effect of the exchange-correlation interaction on quantum Langmuir waves and quantum ion-acoustic waves in the range of WDM parameters. In Sec. IV we compare and analyze the similarities and differences between the EKT, QHD and ALDA-based kinetic theory, and give the exchange interaction corrections for the ion-acoustic wave dispersion relation at low/high temperatures. A summary and discussion will be given in Sec. V.

II. KINETIC MODEL

We start from the time-dependent electrostatic non-interacting Kohn-Sham equation (TDKS),

$$\{-\frac{\hbar^2}{2m_\alpha}\nabla^2 + V_{\rm eff}(\mathbf{r},t)\}\psi_\alpha(\mathbf{r},t) = i\hbar\frac{\partial\psi_\alpha(\mathbf{r},t)}{\partial t}, \tag{3}$$

where the effective scale potential $V_{\rm eff}$ contains the electron-ion interaction, external field, Hatree term and exchange-correlation correction,

$$V_{\rm eff}(\mathbf{r},t) = V_{\alpha\alpha'}(\mathbf{r},t) + V_{\rm ext}(\mathbf{r},t) + V_{{\rm H}\alpha}(\mathbf{r},t) + V_{{\rm xc}\alpha}(\mathbf{r},t). \tag{4}$$

In fact, if we adopt the Born-Oppenheimer approximation and treat the ion behavior as static, the first two term can be combined into one external field. However, we split the two parts here in order to study the behavior of both electrons and ions.

To derive the quantum TDDFT-based kinetic equation, we shall take the quantum analogy of distribution function, written in second quantization,

$$f_\alpha(\mathbf{p},\mathbf{R},t) = \int \frac{d\mathbf{r}}{(2\pi\hbar)^3}\exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right)\langle\psi^*_\alpha(\mathbf{R}+\mathbf{r}/2,t)\psi_\alpha(\mathbf{R}-\mathbf{r}/2,t)\rangle. \tag{5}$$

where the brackets indicate the expectation value of the operators. To describe the time derivative of the distribution function, which can be calculated from the Heisenberg equation,

$$i\hbar\frac{\partial X}{\partial t} = [X,H], \tag{6}$$

we shall take the product $\psi^*\psi$ from the definition of the f for the operator X:

$$\frac{\partial f_\alpha}{\partial t} = \frac{1}{i\hbar}\int \frac{d\mathbf{r}}{(2\pi\hbar)^3}\exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right)\langle[\psi_\alpha^*(\mathbf{R}+\mathbf{r}/2,t)\psi_\alpha(\mathbf{R}-\mathbf{r}/2,t), H(t)]\rangle. \tag{7}$$

Futhermore, after calculating the content in the $\langle\rangle$-brackets, we have

$$\left(\frac{\partial}{\partial t}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{R}}}{m}\right)f_\alpha(\mathbf{p},\mathbf{R},t) = \frac{1}{i\hbar}\int\int \frac{d\mathbf{r}d\mathbf{p}'}{(2\pi\hbar)^3}\exp\left(\frac{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{r}}{\hbar}\right)[V_{\text{eff}}^+ - V_{\text{eff}}^-]f_\alpha(\mathbf{p}',\mathbf{R},t), \tag{8}$$

If we suppose that potential V_{eff} varies slowly in the space coordinate $\mathbf{R}$, and the exchange-correlation interaction is negligible under classical condition, we may therefore expand the effective potentials as

$$V_{\text{eff}}(\mathbf{R}\pm\mathbf{r},t) = V_{\text{eff}}(\mathbf{R},t)\pm(\mathbf{r}/2)\cdot\nabla_{\mathbf{R}}V_{\text{eff}}(\mathbf{R},t), \tag{9}$$

and we find precisely the classical collisionless Valsov equation in electrostatic fields as

$$\{\frac{\partial}{\partial t}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{R}}}{m_\alpha}-\nabla_{\mathbf{R}}V_{\text{eff}}(\mathbf{R},t)\cdot\nabla_{\mathbf{p}}\}f_\alpha(\mathbf{p},\mathbf{R},t)=0. \tag{10}$$

Now, back to Eq.(8), and assuming the field of the scale potential is sufficiently low, we can follow the usual procedure to obtain the linear response of the system,

$$f_\alpha(\mathbf{p},\mathbf{R},t) = f_{0\alpha}(\mathbf{p})+\delta f_\alpha(\mathbf{p},\mathbf{R},t), \tag{11}$$

where $f_{0\alpha}$ indicates the system is basically in equilibrium, satisfying the Fermi-Dirac distribution, and δf is the disturbance due to the absence of external fields, δV_{ext}.

According to the famous random phase approximation (R.P.A),

$$\begin{aligned}\delta f_\alpha(\mathbf{p},\mathbf{R},t) &= \delta f_\alpha(\mathbf{p},\mathbf{k},\omega)e^{i\mathbf{k}\cdot\mathbf{R}-i\omega t},\\ \delta\tilde{V}_{\text{eff}}(\mathbf{R},t) &= \delta\tilde{V}_{\text{eff}}(\mathbf{k},\omega)e^{i\mathbf{k}\cdot\mathbf{R}-i\omega t},\end{aligned} \tag{12}$$

we have the linearized kinetic equation

$$(\omega-\mathbf{k}\cdot\mathbf{p}/m)\,\delta f_\alpha = \delta\tilde{V}_{\text{eff}}[f_{0\alpha}^- - f_{0\alpha}^+]/\hbar, \tag{13}$$

where $f_{0\alpha}^\pm = f_{0\alpha}\,(\tilde{\mathbf{p}}\pm\hbar\mathbf{k}/2)$. According to the classical plasma theory, combining the linearized kinetic equation with the Poisson equation, we can get the classical electrostatic dielectric function. However, considering the complex form of effective potential V_{eff}, we need to include the correspondences between electron density and other species of potential energy as additive terms.

For an electron-ion system, we have the Poisson's equations respectively

$$V_{\text{ei}}(\mathbf{r},t) = -\frac{e^2}{4\pi\epsilon_0}\int\frac{n_i(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}', \tag{14}$$

$$V_{\mathrm{He}}(\mathbf{r},t)=\frac{e^2}{4\pi\epsilon_0}\int\frac{n_e(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}', \tag{15}$$

And more importantly, the exchange-correlation potential is defined as the functional derivative of the xc-action $\mathcal{A}_{\mathrm{xc}}$, which was originally proposed by Runge and Gross,

$$V_{\mathrm{xce}}(\mathbf{r},t)=\frac{\delta\mathcal{A}_{\mathrm{xc}}[n_e](\mathbf{r},t)}{\delta n_e(\mathbf{r},t)}. \tag{16}$$

The simplest concept for setting up approximations for xc-action is to turn it into locality in time and space, as the use of a stationary functional evolving in approximately adiabatic progress, which is usually called Adiabatic Local Density Approximation (ALDA),

$$\mathcal{A}_{\mathrm{xc}}^{ALDA}[n]=\int_{t_0}^{t_1}dt\int d\mathrm{r}e_{\mathrm{xc}}^{HEG}\left(n\left(\mathrm{r},t\right)\right), \tag{17}$$

where $e_{\mathrm{xc}}^{HEG}\left(n\right)$ is the xc-energy density of the homogeneous electron gas at gas density n. And the linearized xc potential can be expressed as

$$\delta V_{\mathrm{xce}}(\mathbf{r},t)=\int dt'\int d\mathbf{r}'\frac{\delta V_{\mathrm{xce}}(\mathbf{r},t)}{\delta n\left(\mathbf{r}',t'\right)}\bigg|_{n_0}\delta n\left(\mathbf{r}',t'\right). \tag{18}$$

where contains a key quantity of TDDFT in the linear response regime, called time-dependent xc kernel,

$$f_{\mathrm{xc}}(\mathbf{k},\omega)=\int dt'\int d\mathbf{r}'e^{i\mathbf{k}\cdot\left(\mathbf{r}'-\mathbf{r}\right)-i\omega\left(t'-t\right)}\frac{\delta V_{\mathrm{xce}}(\mathbf{r},t)}{\delta n\left(\mathbf{r}',t'\right)}\bigg|_{n_0(\mathbf{r})}. \tag{19}$$

The description of electron quantum kinetic equation is sufficient for high-frequency wave. And low-frequency electrostatic wave can be explored including ion dynamics, which can be described by classical Vlasov equation due to their heavy mass,

$$\{\frac{\partial}{\partial t}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{R}}}{m_i}-\nabla_{\mathbf{R}}V_{\mathrm{effi}}\cdot\nabla_{\mathbf{p}}\}f_i(\mathbf{p},\mathbf{R},t)=0, \tag{20}$$

where the effective potential $V_{\mathrm{effi}}=V_{ei}+V_{\mathrm{Hi}}+V_{\mathrm{ext}}$, $V_{ie}=-V_{\mathrm{He}}$ and $V_{\mathrm{Hi}}=-V_{ei}$.

Linearizing Eq.(20) and including the electron dynamics Eq.(13), we have the dispersion relation of electron-ion system

$$\epsilon^l=1-v\left(\mathbf{k}\right)\chi_i\left(\mathbf{k},\omega\right)-\{v\left(\mathbf{k}\right)+\left[1-v\left(\mathbf{k}\right)\chi_i\left(\mathbf{k},\omega\right)\right]f_{\mathrm{xc}}\left(\mathbf{k},\omega\right)\}\chi_e^q\left(\mathbf{k},\omega\right), \tag{21}$$

where

$$\chi_\alpha\left(\mathbf{k},\omega\right)=\int d\mathbf{v}\frac{-\mathbf{k}\cdot\nabla f_{0\alpha}}{\omega-\mathbf{k}\cdot\mathbf{v}}, \tag{22}$$

$$\chi_\alpha^q(\mathbf{k},\omega) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{1}{\hbar}\frac{f_{0\alpha}^- - f_{0\alpha}^+}{\omega - \mathbf{k}\cdot\mathbf{p}/m_\alpha}, \tag{23}$$

After that, we can also employ the ALDA for $f_{\rm xc}$,

$$\begin{aligned} f_{\rm xc}^{ALDA}(\mathbf{r},\mathbf{r}';t,t') &= \left.\frac{d^2 e_{\rm xc}^{HEG}(n)}{dn^2}\right|_{n=n_0(r)} \delta(\mathbf{r}'-\mathbf{r})\,\delta(t'-t) \\ &= \left.\frac{\delta V_{\rm xc}^{ALDA}[n](\mathbf{r},t)}{\delta n(\mathbf{r}',t')}\right|_{n=n_0(\mathbf{r})}, \end{aligned} \tag{24}$$

where the xc potential $V_{\rm xc}^{ALDA}(\mathbf{r},t) = V_{\rm xc}^{LDA}(n(\mathbf{r},t))$. The approximation supplies us with a method to connect the dispersion relation with the suitable exchange-correlation potentials at finite temperature, such as the LDA functional proposed by Perrot and Dharma-Wardana [25], $V_{\rm xc}(r_s,t_f)$, where $r_s = (3/4\pi n)^{1/3}/a_0$ is the Wigner-Seitz radius, $t_f = k_B T/E_F$ is the Fermi temperature, and a_0 is the Bohr radius.

III. LONG-WAVELENGTH APPROACH

A. quantum electron Langmuir wave

Let us consider first the long-wavelength limit in which the disturbance varies so slowly in space that $\omega \gg kv_{Fe} \gg \frac{\hbar k^2}{2m_e}$. And ions cannot timely response to density disturbance due to the high frequency electron waves, so $\chi_i = 0$. Then

$$\frac{1}{\omega - \mathbf{k}\cdot\mathbf{p}/m} \approx \frac{1}{\omega}\left(1 + \frac{\mathbf{k}\cdot\mathbf{p}}{m\omega} + \frac{(\mathbf{k}\cdot\mathbf{p})^2}{m^2\omega^2} + ...\right), \tag{25}$$

We find at long-wavelength limit

$$\omega^2 = \left(1 + \frac{n_{0e}f_{\rm xc}}{m_e\omega_{\rm pe}^2}k^2\right)\left[\omega_{\rm pe}^2 + \langle v^2\rangle k^2 + \frac{\hbar^2}{4m_e^2}k^4\right], \tag{26}$$

where $\langle v^2\rangle$ represents the mean kinetic energy of electrons

$$\langle v^2\rangle = \frac{1}{n_{0e}}\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\left(\frac{p}{m_e}\right)^2 f_{0e}(\mathbf{p}). \tag{27}$$

The quantum electron Langmuir wave dispersion relation Eq.(26) corresponds to the main results of some quantum hydrodynamic papers which is offered by TDDFT [21, 26], as long as we choose the popular Hedin-Lundqvist (HL) potential to derive the xc kernel. It is understandable because the fluid equation can be straightly derived from the kinetic equation under the long-wavelength approximation. And both equations are based on the TDKS architecture.

Especially, ignoring the high-order corrections, we have the following dispersion relation

$$\omega^2 = \omega_{\rm pe}^2 + (\langle v^2\rangle + n_{0e}f_{\rm xc}/m_e)k^2 \equiv \omega_{\rm pe}^2 + (1-\alpha)\langle v^2\rangle k^2, \tag{28}$$

where $\alpha = -n_{0e} f_{\rm xc}/m_e\langle v^2\rangle$ represents the comdined effects of system temperature and exchange-correlation energy, and is also related to the group velocity of quantum Langmuir waves.

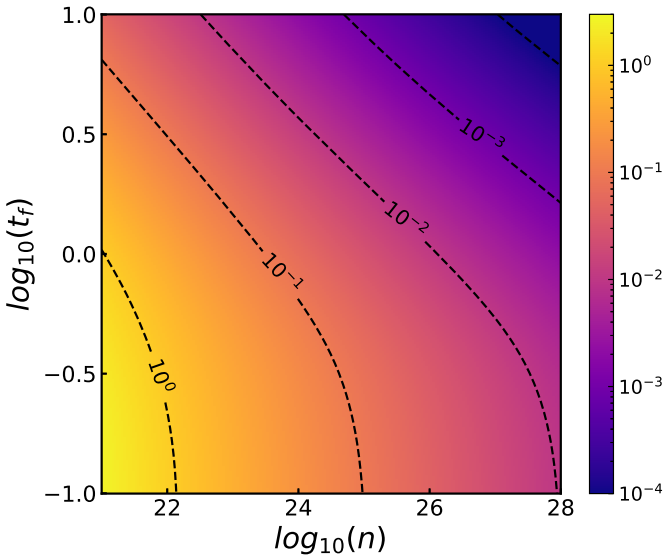


FIG. 1. The variation of α with the system density and temperature. The value is greater than 10^0 in the lower left area.

In Fig.1, the correction of exchange-correlation effects remains essentially above 1% for the entire WDM density parameter region at low temperature. More importantly when the density is below $10^{25}\mathrm{cm}^{-3}$, the correction provides a reduction of more than 10% compared to the thermodynamic term derived from the classical quantum theory. And it keeps weakening with increasing temperature, which is due to the fact that high temperature diminishes the quantum effect, including the exchange-correlation effects, quantum diffraction effects and so on. In the lower left area, Langmuir wave exhibits a negative group velocity property, which means the directions of phase and group velocity are opposite each other. This phenomenon is caused by the exchange-correlation effects and cannot be described in the classical plasma theory.

B. quantum ion acoustic wave

For the low-frequency ion oscillation mode, $ku_i \ll \omega \ll kv_{Fe}$, we can simplified the ion susceptibility as

$$\chi_i \approx -\frac{n_{0i}k^2}{m_i\omega^2}. \tag{29}$$

For the electron susceptibility, since the phase velocity ω/k is on the order of the Fermi velocity, the approximation method used for Langmuir waves is not applicable. However, we can use the static response approximation ($\omega \approx 0$) to get its contribution under the expression of Fourier expansion, and real part of the corresponding density response is

$$Re\left(\chi_e\left(\mathbf{k},0\right)\right) = -\mathcal{P}\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{1}{\hbar}\frac{f_0^- - f_0^+}{\mathbf{k}\cdot\mathbf{p}/m_e} \approx -n_{0e}\Theta_1\left(\mu\right)\tau\left(\mu,k\right), \tag{30}$$

where

$$\Theta_1(\mu) = \frac{\partial}{\partial\mu}\tilde{n}_{0e}(\mu), \tag{31}$$

$$\Theta_2(\mu) = \frac{1}{2}\frac{\partial^2}{\partial\mu^2}\tilde{n}_{0e}(\mu) + \frac{1}{9}\frac{\partial^3}{\partial\mu^3}\tilde{w}_{0e}(\mu), \tag{32}$$

$$\tau(\mu, k) = 1 - \frac{\hbar^2 k^2}{4m_e}\frac{\Theta_2(\mu)}{\Theta_1(\mu)}. \tag{33}$$

Here, Similar to the quantum diffraction term in the linear dispersion relation of Langmuir waves, the second term in τ is proportional to k^2, which means that it is a high-order correction term, and can be indeed ignored in the linear discussion. The imaginary part can be found by the theoretical approach

$$Im(\chi_e(k,\omega)) = \frac{2m_e^2}{4\pi\beta\hbar^4 k}\ln\left|\frac{1+\exp[\beta\mu - \frac{\beta}{E_k}(\hbar\omega + E_k)^2]}{1+\exp[\beta\mu - \frac{\beta}{E_k}(\hbar\omega - E_k)^2]}\right|, \tag{34}$$

where $E_k = \hbar^2k^2/2m$ represents the electron kinetic energy, and the parameter μ and β represent, respectively, the chemical potential and temperature of the system. It should be noted that the xc kernels are analytical functions in the upper half of the complex ω-plane. Due to the $Im(\chi_e) \ll Re(\chi_e)$ and $Im(f_{\rm xc}) \ll Re(f_{\rm xc})$ at long-wavelength limt, we can reduce the real part of dispersion relation Eq. (21) as

$$\omega^2 = \frac{C_s^2k^2(1/\tau - n_{0e}Re(f_{\rm xc})\Theta_1)}{1+\frac{C_s^2k^2}{\omega_{\rm pi}^2}(1/\tau - n_{0e}Re(f_{\rm xc})\Theta_1)} \equiv \frac{C_s^2k^2\nu}{1+\lambda_{\rm qe}^2k^2\nu}, \tag{35}$$

where the ion-acoustic velocity $C_s = 1/\sqrt{-(m_i\Theta_1)}$, and $\lambda_{\rm qe}^2 = {C_s}^2/\omega_{\rm pi}^2$. At zero temperature, the velocity of ion-acoustic is given by

$$C_s^2 = \frac{m_e}{3m_i}v_{\rm F}^2, \tag{36}$$

which is known as the Bohm-Staver relation [27]. And if we consider the influence of the exchange-correlation correction, the quantum ion-acoustic velocity should be as $C_s^q = \sqrt{\nu}C_s$, where ν contains both the quantum diffraction (τ, and $\tau \approx 1$ in the linear analyze) and exchange-correlation effects.

In Fig.2, we have evaluated the exchange-correlation effects on the ion-acoustic velocity with the help of the temperature-dependent LDA functional, and found two interesting effects. First of all,similar to the effect on quantum Langmuir waves, since the xc kernel $f_{\rm xc}$ is inversely proportional to the density n (which should actually be $n^{4/3}$) and temperature T (in the high-temperature limit, the functional is much more complicated at low temperatures [25]), the influence of the exchange-correlation effect diminishes with increasing density and temperature of the system. Secondly, there exits a density and temperature limited region satisfied $|f_{\rm xc}| < 1/(n_0|\Theta_1|)$ in which the ion-acoustic velocity appears as a pure imaginary number. It also means that the ion-acoustic waves cannot propagate in the

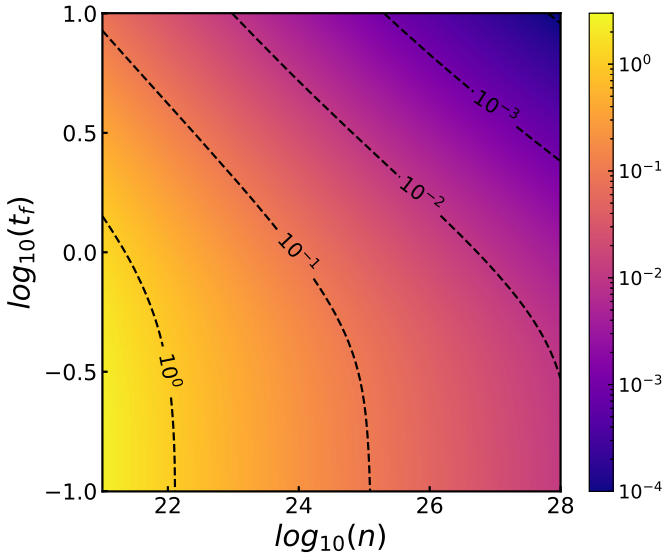


FIG. 2. The variation of exchange-correlation correction parameter $1-\nu$. The value is greater than 10^0 in the lower left area of density and temperature.

system that take values in this region.

IV. EXCHANGE-KINETIC THEORY COMPARISON

It is necessary for us to compare the kinetic model based on TDDFT with the equation obtained in other ways, such as the simplification of BBGKY chain equations, to verify its reliability. Ekman, Zamanian, and Brodin [23, 24] has derived a kinetic model, where exchange correction were included considering the beginning the antisymmetrization of the N-particle density matrix. They wrote the dispersion relation as

$$1 + D_i + D_e + D_x = 0, \tag{37}$$

where the terms are respectively the classical ion term, the classical electron term and exchange correction term. They are given by

$$D_i = -\omega_{\mathrm{pi}}^2/\omega^2, \tag{38}$$

$$D_e = \frac{3\omega_{\mathrm{pe}}^2}{2k^2 v_{\mathrm{F}}^2} \int_{-1}^{1} \frac{z\,dz}{z - \omega/kv_{\mathrm{F}}}, \tag{39}$$

$$D_x = \left(9\hbar^2\omega_{\mathrm{pe}}^4/16m^2k^2v_{\mathrm{F}}^6\right) I\left(w\right), \tag{40}$$

$$I(\mathrm{w}) = \int_{-1}^{1} dx \int_{-1}^{1} dy \frac{xy}{\mathrm{w}-y} \frac{sgn(x-y)}{(\mathrm{w}-(x+y)/2)^2}, \tag{41}$$

where $\mathrm{w} = \omega/kv_{\mathrm{F}}$ is the normalized phase velocity. And they compared the exchange correction term $I(\mathrm{w})$ with the electron exchange contribution of the hydrodynamic version, $I^h(\mathrm{w})$, where

$$I^h(\mathrm{w}) = \frac{0.445}{(\mathrm{w}^2 - 3/5)^2}. \tag{42}$$

A. High-frequency comparison

Exchange-kinetic theory (EKT) concluded that when $\mathrm{w} \lesssim 1.4$, the sign of the exchange correction would change and manifested as a strong enhancement for Langmuir waves, which cannot be reflected in the hydrodynamic model. However, is this due to the error caused by the fluid approximation, or the inapplicability of the ALDA spirit at short-wavelength region, or even the both? To find the answer, we can also distinguish the quantum effect including the exchange(-correlation) effect from the classical term in the ALDA-based quantum kinetic theory,

$$D_x' = [v(\mathbf{k}) + f_{\mathrm{xc}}]\chi_e^q(\mathbf{k},\omega) - v(\mathbf{k})\chi_e(\mathbf{k},\omega), \tag{43}$$

$$I^A(\mathrm{w}) = \frac{16m^2k^2v_{\mathrm{F}}^6}{9\hbar^2\omega_{\mathrm{pe}}^4} D_x'(\mathrm{w}). \tag{44}$$

It should be noted that the zero temperature assumption was made during the derivation of exchange-kinetic theory and neglected the two-particle correlations. Thus, we choose also the Dirac exchange correction V_{X} for the homogeneous electron gas,

$$V_{\mathrm{X}}^0 = -g_{\mathrm{D}}\left(\frac{n}{n_0}\right)^{1/3}, \qquad f_{\mathrm{x}} = -\frac{g_{\mathrm{D}}}{3n_0}, \qquad g_{\mathrm{D}} = 0.985\frac{\left(3\pi^2\right)^{2/3}}{4\pi}\frac{\hbar^2\omega_{\mathrm{pe}}^2}{mv_{\mathbf{F}}^2} \approx 0.375H^2\varepsilon_{\mathrm{F}}. \tag{45}$$

And we have

$$I^A(\mathrm{w}) = \left(\frac{0.667}{\mathrm{w}^2}\gamma^2 - \frac{10.667}{H^2}\right)\int_0^1 dy\int_{-1}^1 dx \frac{y^2}{(\mathrm{w}-xy)^2 - H^2\gamma^2/16\mathrm{w}^2} + \frac{10.667}{H^2}\int_0^1 dy\int_{-1}^1 dx\frac{y^2}{(\mathrm{w}-xy)^2}. \tag{46}$$

where the parameter $\gamma = \omega/\omega_{\mathrm{pe}}$ represents the ratio of wave frequency and electron oscillation frequency. Substituting Eq.(45) into Eq.(28), we have

$$\omega^2 \approx \omega_{\mathrm{pe}}^2 + \left(0.6 - 0.0625H^2\right)v_{\mathrm{F}}^2k^2. \tag{47}$$

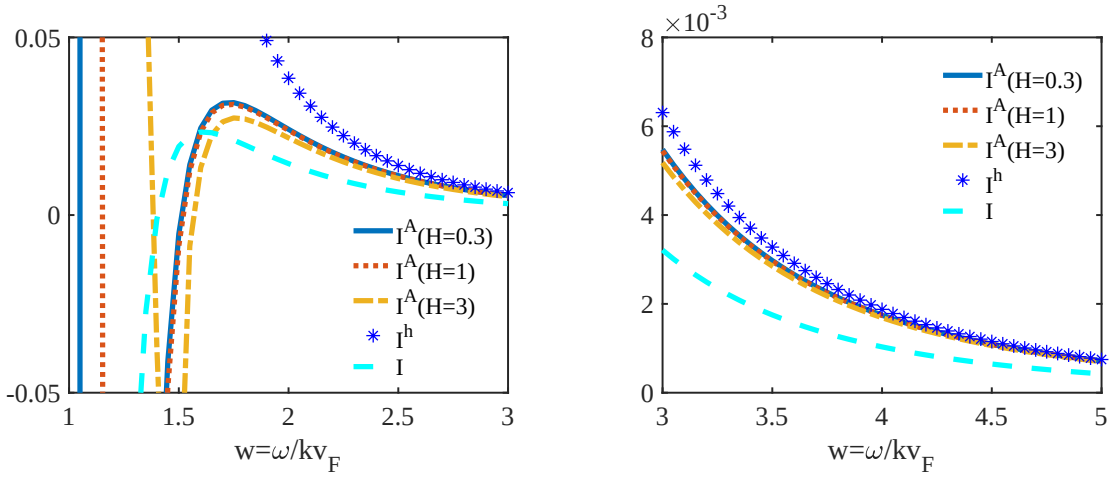
Compared with the quantum Langmuir wave dispersion relation obtained by EKT in the long-wavelength approx-

imation

$$\omega^2 = \omega_{\rm pe}^2 + \left(\frac{3}{5} - \frac{3}{80}H^2\right) v_{\rm F}^2 k^2, \tag{48}$$

the ALDA-based kinetic theory would be a somewhat overestimate for the exchange correction. And we have

$$\gamma^2 \approx \frac{\mathrm{w}^2}{\mathrm{w}^2 - (0.6 - 0.0625H^2)}. \tag{49}$$



(a) (b)

FIG. 3.

Fig.3 illustrates that in the long-wavelength range, the three approximation methods have the same trend, although EKT describes a slightly lower exchange effect than the other two methods. In contrast, in the short-wavelength range, when $w \approx 1.5$, the exchange correction obtained by the ALDA-based kinetic theory shows the same sign change as EKT, which deviates significantly from QHD. The deviation implies that the mutual coupling effect between the exchange correction and the kinetic higher-order corrections leads to a modification of the dispersion relation when $w \lesssim 2$. This effect is neglected in the fluid approach, leading to the inaccuracies in the short-wavelength range.

However, it is worth to be noted that the ALDA-based kinetic theory exhibits two properties that are distinguished from the exchange kinetic theory. Firstly, the exchange correction given by the ALDA-based kinetic theory is associated with H, and the effect of the exchange correction deviates more from EKT when H takes a larger value. Secondly, when $w \lesssim 1.5$, the exchange correction given by the ALDA-based kinetic theory characterizes a different variational trend from that of EKT.

In fact, both differences arise because the exchange kinetic theory does not reflect the quantum diffraction effect well. From Eq.(41) we know that the exchange correction integral has singularities when $w < 1$, i.e., which characterizes the entry into the resonant absorption region. However, based on the solution of the Wigner approach [5], we have

the kinetic resonance relation with resonance frequency ω_r and wave number k_r

$$\mathrm{w_r} = \frac{\omega_r}{k_r v_\mathrm{F}} = 1 + \frac{k_r}{2k_\mathrm{F}}, \approx 1 + \frac{\gamma H}{4\mathrm{w_r}} \tag{50}$$

$$\mathrm{w_r} \approx \left(1 + \sqrt{1+H}\right)/2, \tag{51}$$

It actually implies the resonance effect occurring between the waves with phase velocity up to the Fermi velocity and Fermi-surface particles, and the total energy/ momentum conservation of the absorption or emission processes between the radiative quantum waves and fermions [28]. Differing from EKT, it is reflected in the existence condition of the singularity of the Eq.(46).

It is the quantum fluctuation effect that leads to a significant deviation between the two theories in the short wavelength region. In Fig.2, I^A curves show two exchange interaction 'zeros', meaning that the exchange interaction can be neglected under certain phase velocity conditions, one in the non-resonance absorption region and the other in the resonance absorption region. It is different from the previous EKT conclusion that there is only one zero point in the non-resonant absorption region. Moreover, comparing the two zero-point values in the non-resonance absorption region, the results of ALDA-based kinetic theory are also significantly larger than those of EKT.

B. low-frequency comparison

Here, we compare the low-frequency ion-acoustic waves dispersion relation obtained by ALDA-based kinetic theory, exchange-kinetic theory and classical plasma theory.

1. low-temperature

Considering the Fermi-Dirac distribution, we have the real part of density response function

$$Re\left(\chi_e^F\left(\mathbf{k},0\right)\right) = \frac{3}{2}\frac{n_{0e}}{E_F}\left(1 - \frac{1}{12}\frac{k^2}{k_\mathrm{F}^2}\right), \tag{52}$$

and according to the Lindhard dispersion relation [10], we have the imaginary part

$$Im\left(\chi_e^F\right) = -\frac{m_e^2\omega}{2\pi\hbar^3 k}. \tag{53}$$

And we have the imaginary part of quantum ion-acoustic wave dispersion relation

$$\begin{aligned} Im\left(\epsilon_e^F\right) &= \left(\frac{\omega_\mathrm{pe}^2 m_e}{k^2} + \left(1 - \frac{\omega_\mathrm{pi}^2}{\omega^2}\right) Re\left(f_\mathrm{xc}\right)\right) Im\left(\chi_e^F\right) + \left(1 - \frac{\omega_\mathrm{pi}^2}{\omega^2}\right) Im\left(f_\mathrm{xc}\right) Re\left(\chi_e\right) \\ &= -\frac{\omega_\mathrm{pe}^2 m_e^3 \omega}{2n_0\hbar^3 k^3}\left(1 + \left(1 - \frac{\omega_\mathrm{pi}^2}{\omega^2}\right)\frac{n_{0e}k^2}{m_e\omega_\mathrm{pe}^2} Re\left(f_\mathrm{xc}\right)\right) + \frac{3}{2}\frac{n_{0e}}{E_F}\left(1 - \frac{1}{12}\frac{k^2}{k_\mathrm{F}^2}\right)\left(1 - \frac{\omega_\mathrm{pi}^2}{\omega^2}\right) Im\left(f_\mathrm{xc}\right). \end{aligned} \tag{54}$$

The damping rate of ion-acoustic waves is

$$\begin{aligned}\gamma_e^F = -\frac{Im\left(\epsilon_e^F\right)}{\partial Re\left(\epsilon\right)/\partial\omega} = -\frac{\pi^2}{4}\frac{\nu C_s k}{\left(1+k^2{\lambda_{\rm qe}^F}^2\right)^2}\sqrt{\frac{m_e}{3m_i}}\left(1+3\left(1-\frac{\omega_{\rm pi}^2}{\omega^2}\right)\frac{n_{0e}k^2{\lambda_{\rm qe}^F}^2}{m_e v_{\rm F}^2}Re\left(f_{\rm xc}\right)\right)\\ +3\sqrt{\nu}C_s k^3\frac{n_{0e}Im\left(f_{\rm xc}\right)}{m_i\omega_{\rm pi}^2}\left(1-\frac{1}{12}\frac{k^2}{k_{\rm F}^2}\right)\left(1-\frac{\omega_{\rm pi}^2}{\omega^2}\right).\end{aligned} \tag{55}$$

where ${\lambda_{\rm qe}^F}^2 = v_{\rm F}^2/3\omega_{\rm pe}^2$ represents the quantum shield length. And due to the relation that $\omega \ll \omega_{\rm pe}$, we have $k\lambda_{\rm qe}^F \to 0$. Thus the damping rate approaches

$$\gamma_e^F \approx -\frac{\pi^2}{4}\nu C_s k\sqrt{\frac{m_e}{3m_i}}. \tag{56}$$

The dispersion relation for ion-acoustic waves with exchange-correction is then

$$\omega^2 \approx C_s^2 k^2 \nu\left(1 - i\frac{\pi^2}{2}\sqrt{\nu\frac{m_e}{3m_i}}\right), \tag{57}$$

where

$$\nu \approx \left(1 - 0.187H^2 + 0.0833\frac{k^2}{k_F^2}\right). \tag{58}$$

Compared to the dispersion relation derived by EKT,

$$\omega^2 = C_s^2 k^2\left[1 - H^2\left(1.24 + 0.59i\right)\right], \tag{59}$$

we find that the value of the frequency shift deviates significantly from our result. If we make the adjustment $0.985 \to 6.52$ of the numerical prefactor in (45), the real part is conformable as mentioned by the authors. But even if we apply such an adjustment, the imaginary part is still not compatible. In our result, the damping rate is proportional to the electron-ion mass ratio, and decreases in the change scale as H^2, which also differs from the result of EKT.

2. high temperature

In contrast to EKT which breaks down in the high temperature limit, the ALDA-based kinetic theory is suitable for solving the ion-acoustic dispersion relation at high temperature conditions, as long as we replace the distribution function with a Maxwellian type.

The density response function is

$$\chi_e^M\left(\mathbf{k},0\right) = \beta n_{0e}\left(1 - \frac{7}{36}\frac{k^2}{k_{\rm T}^2}\right), \tag{60}$$

where $k_{\rm T}^2 = 2m_e/\hbar^2\beta$ is the wave number corresponding to the thermal velocity. Coupling with the exchange potential

at high-temperature limit [25],

$$V_{\mathrm{X}}^{T}=\frac{2}{3t_f}V_{\mathrm{X}}^{0}, \tag{61}$$

where the imaginary part can be negligible due to the weakness of exchange correction at high temperature limit. Thus, we have

$$\omega^2\approx C_s^2k^2\left(1-\frac{0.0833}{t_f^2}H^2+0.1944\frac{k^2}{k_T^2}\right)\left(1-i\sqrt{\frac{\pi m_e}{2m_i}}\right). \tag{62}$$

Since the exchange correction is inversely proportional to the Fermi-temperature, Eq.(62) can degenerate into the classical ion-acoustic wave dispersion relation at high temperature limit.

V. CONCLUSION

In the present paper, we have derived the quantum dispersion relation of electron-ion system using the ALDA-based kinetic theory, which is based on the time-dependent density functional theory. With the help of the temperature-dependent functional, we have given a kinetic treatment of exchange-correlation effects covering the full electrostatic waves region. We found that the exchange-correlation effect on the electrostatic wave phase velocity exceeds 10% at low density conditions ($n<10^{25}cm^{-3}$), and under relatively low temperature ($t_f<1$) and sparse density conditions ($n<10^{22}cm^{-3}$), the high-frequency Langmuir waves could exhibit the negative group velocity due to the exchange-correlation effect. Moreover, the low-frequency ion-acoustic waves could also exhibit imaginary frequencies in the similar region.

Another important goal of this study is to compare the ALDA-based kinetic theory with the exchange kinetic theory (EKT) as well as quantum hydrodynamics (QHD). It is concluded that the ALDA-based kinetic theory with the addition of wave-particle interactions to QHD can be consistent with EKT in a certain short wavelength range, and can also show the sign change of the exchange component of Langmuir waves. However, in addition to certain numerical deviations, there are also differences between the ALDA-based kinetic theory and EKT for the description of quantum diffraction effects under the condition that the phase velocity is close to the Fermi velocity. EKT ignores the quantum diffraction effects due to the model simplification, and thus cannot point out the exact resonance absorption boundary. Although the model deficiency of ALDA may lead to an inaccurate description in the resonance absorption region, it actually provides us with a way to improve the resonance boundary by using better functional forms such as GGA with the addition of density gradient correction [29], time-dependent functions considering non-adiabatic processes [30], etc., to study the kinetic processes of the electron-ion system more precisely.

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