Reduced Ionic Diffusion by the Dynamic Electron-Ion Collisions in Warm Dense Hydrogen

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The dynamic electron-ion collisions play an important role in determining the static and transport properties of warm dense matter (WDM). Electron force field (eFF) method is applied to study the ionic transport properties of warm dense hydrogen. Compared with the results from quantum molecular dynamics and orbital-free molecular dynamics, the ionic diffusions are largely reduced by involving the dynamic collisions of electrons and ions. This physics is verified by the quantum Langevin molecular dynamics simulations, which includes electron-ion collisions induced friction into the dynamic equation of ions. Based on these new results, we proposed a model including the correction of collisions induced friction (CIF) of ionic diffusion. The CIF model has been verified to be valid at a wide range of density and temperature. We also compare the results with the one component plasma (OCP), Yukawa OCP (YOCP) and Effective OCP (EOCP) models, showing the significant effect of non-adiabatic dynamics.

I. INTRODUCTION

Warm dense matter (WDM) exists widely in the inner cores of giant gas planets and the outer shells of brown and white dwarf stars1. It is also an important stage in the X-ray conversion zone and main fuel layer of implosion compression during the inertial confinement fusion (ICF)2,3 process. Moreover, it is a transient state between cold condensed matter and ideal gas plasma such that neither condensed-matter nor ideal-plasma theory assumptions work well. In the WDM regime, bound and free electrons, multiple ions, atoms, molecules and clusters coexist, leading strong coupling, partial degeneracy and partial ionization all play important roles in describing the structures and properties of WDM. The Born-Oppenheimer (BO) approximation—decouples ions from electrons to the instantaneously adjusting potential energy surface (PES) formed by fast electrons—has achieved great success on both classical molecular dynamics (CMD)4–6 and first principle method such as density function theory (DFT)7–9. It is possible to perform efficient simulations owing to BO approximation. However, at higher temperature and density such as in WDM regimes, the free electrons will collide with ions frequently, and the gap between PES of different eigenstates of electrons becomes narrow, so that ions are possible to hop out of the current PES. Here, the BO approximation breaks down, and non-adiabatic dynamic electron-ion collisions will exhibit significant effects on the equilibrium and the non-equilibrium processes10–13. With the improvement of diagnostic methods, especially the usage of X-ray Thomson scattering techniques14, electronic information of WDM can be obtained in the laboratory. To interpret the experimental data, a more precise theory beyond BO approximation is required on account of the complex environment of WDM.

The non-adiabatic effect has been considered by some methods to get more accurate interactions between electrons and ions in WDM. Derived from time-dependent Kohn-Sham equation, time-dependent density function theory (TDDFT)15 gives the relatively exact electronic structure information. Thanks to the coupling of the electrons and ions, TDDFT-Ehrenfest approach can give the results such as energy dissipation process, excitation energies and optical properties etc.16,17. However, TDDFT is extremely time-consuming, limited by finite time and size scale. Thus low frequency modes cannot be described well and the convergence of scale is required to be verified carefully. Quantum Langevin molecular dynamics (QLMD) holds a more efficient first principles computation efficiency, simultaneously regarding dynamic electron-ion collisions as frictional forces in Langevin dynamical equation of ions18. Using the QLMD method, a stronger ionic diffusive mode at low frequency has been found when the selected friction parameter becomes larger, as well as the decrease of the sound-speed19. Nevertheless, the determination of the friction parameter is a priori. Recently, Simon et al have provided ab-initio calculations of the friction tensor in liquid metals and warm dense plasma20. They obtain a non-diagonal friction tensor, reflecting the anisotropy of instantaneous dynamic electron-ion collisions. Electron force field (EFF) expresses electrons as Gaussian wave packets, so that it can include the non-adiabatic effect intrinsically in molecular dynamics simulation21,22. Lately the method has been applied to warm dense aluminum and found similar conclusions that non-adiabatic effect enhances ion modes around \(\omega = 0\), however, the effect is not sensitive to the sound speed23. Q. Ma et al have developed the EFF methodology to study warm and hot dense hydrogen24,25. They conclude that dynamic electron-ion collisions reduce the electrical conductivities and increase the electron-ion temperature relaxation times compared with adiabatic and classical framing theories. As another approach, Bohmian trajectory formalism has been applied by Ladder et al recently.26 Constructing a thermally averaged, linearized Bohm potential, fast dynamical computation with coupled electronic-ionic system is achieved26. The result also reveals different phenomenon of dynamic structure factor (DSF) and dispersion relation from DFT-MD simulation. All researches reflect that electron-ion collisions affect signif-

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icantly on the study of dynamic properties of WDM, for both electrons and ions. Nevertheless, the effect of non-adiabatic effect on the ionic transport properties such as diffusion coefficient is few studied, in both numerical simulations and analytical models.

The transport properties such as self-diffusion, mutual-diffusion and viscosity of WDM and plasma systems are important for the study of astrophysics and ICF experiments. And they are pivotal input parameters to the radiation-hydrodynamics simulations. Diffusion leads to the sedimentation of heavy elements and the formation of white dwarf stars, as well as the complex phenomenon of giant planets like phase separation. It also appears in the implosion compression of ICF process because of the mixture of fuel. Transport properties can also affect the fluid instabilities like Rayleigh-Taylor instability (RTI) and Richtmyer-Meshkov instability (RMI) which are crucial in ICF implosions. To emphasize the non-adiabatic effect, the present work will focus on the self-diffusion of the simplest element: hydrogen. Hydrogen and its isotopes are important in astrophysics and ICF, and it is a perfect system to compare the physics in different models. For ideal gas plasma, kinetic theory has a good description based on binary-collision approximation. The diffusion coefficient can be obtained from Chapman-Enskog formulas, deduced from Boltzmann equation. In parallel, Hansen et al have run massive molecular-dynamics simulations based on the classical one-component plasma (OCP) model, and given a series of transport properties over a wide range of thermodynamic states. Dagaut has systematically studied the strong collective behavior of OCP and given better fitting formulas of the diffusion and viscosity coefficient.

It should be noticed that all results should be examined in WDM because of the appearance of many-body interactions, electron degeneracy and electron screening. There have been many efforts on theories and simulations to validate the above models in WDM. For example, effective potential theory (EPT) and effective screening potential have been developed to get more accurate collision integrals in a more strongly coupled region. Adding the screen parameter in OCP, Yukawa one-component plasma (YOCP) model is developed and the larger self-diffusion coefficients are found because of shielding effects. Deducing effective coupling parameter and effective charge, effective one-component plasma (EOCP) model is constructed, and it has been successfully applied in warm and hot dense plasma comparing with Kohn-Sham density function molecular dynamics (KSDFMD) and orbital-free molecular dynamics (OFMD) simulations. Binary ionic mixtures (BIMs) and multi-ionic mixtures are also common in nature and laboratories. The researches on mixing process can often be found in papers such as in Refs. However, the influence of non-adiabatic electron-ion collisions on ionic diffusion is still required to be checked, and we could image the existence of dynamic electron-ion collisions will induce new effects such as dissipation or friction. In particular, for the analytical models based on traditional BO methods, we should study the non-adiabatic dynamic collisions effect on the self-diffusion in warm dense matter, and propose a new model including collisions induced friction (CIF).

The paper is organized as follows. Firstly, details of theoretical methods and the computation of diffusion coefficient are introduced in Section II. Then, in Section III, the static and transport results of QMD, OFMD, QLMD, and (C)EFF simulations are showed and the the dynamic collisions effect is discussed. In section IV, we systematically study the collision frequency effect on ionic diffusions and the CIF model is introduced to estimate the impact of electron-ion collisions. In section V, the results are compared with the OCP, YOCP, and EOCP models. Finally, the conclusions are given in section VI. All units are in atom unit if not emphasized.

II. THEORETICAL METHODS AND COMPUTATIONAL DETAILS

A. (Constrained) electron force field methodology

EFF method is supposed to be originated from wave packet molecular dynamics (WPMD) and floating spherical Gaussian orbital (FSGO) method. Considering each electronic wave function as a Gaussian wave packet, the excitation of electrons can be included with the evolution of positions and wavepacket radius. N-electrons wave functions are taken as a Hartree product of single-electron Gaussian packet written as

$$\Psi(r) = \left(\frac{2}{s^2 \pi}\right)^{3/4} \exp\left(\left(-\frac{1}{s^2} \frac{2p_1^2}{\hbar} (r - x)^2\right)\right) \cdot \exp\left(\frac{i}{\hbar} p_\mathbf{x} \cdot r\right).$$

Where $s$ and $x$ are the radius and average positions of the electron wave packet, respectively. $p_1$ and $p_\mathbf{x}$ correspond to the conjugate radial and translational momenta. Nuclei in EFF are treated as classical charged particles moving in the mean field formed by electrons and other ions.

Substituting simplified electronic wave function in the time-dependent Schrödinger equation with a harmonic potential, equation of motion for the wave packet can be derived

$$\dot{x} = p_x/m_e,$$  

$$\dot{p}_x = -\nabla_x V,$$  

$$\dot{s} = (4/d)p_s/m_e,$$  

$$p_s = -\partial V/\partial s.$$  

Where $d$ is the dimensionality of wave packets. For a three-dimensional system, $d$ is equal to 3, and it becomes 2 in 2D systems. $V$ is the effective potential. Combining with ionic equations of motion, EFF MD simulations have been implemented in LAMMPS package.

In addition to electrostatic interactions and electron kinetic energy, spin-dependent Pauli repulsion potential is added in
the Hamiltonian as the anti-symmetry compensation of electronic wave functions. In EFF methodology, the exchange effect is dominated by kinetic energy. All interaction potentials are expressed respectively as

\[ E_{\text{nuc-nuc}} = \sum_{i<j} Z_i Z_j / R_{ij}, \quad (3a) \]

\[ E_{\text{nuc-elec}} = \sum_{i<j} \left( Z_i / R_{ij} \right) \text{erf} \left( \sqrt{2} R_{ij} / s_j \right), \quad (3b) \]

\[ E_{\text{elec-elec}} = \sum_{i<j} \left( 1 / r_{ij} \right) \text{erf} \left( \sqrt{2} r_{ij} / \sqrt{s_i^2 + s_j^2} \right), \quad (3c) \]

\[ E_{\text{Pauli}} = \sum_{i, \sigma_i \neq \sigma_j} E_{\uparrow \uparrow} \text{ij} + \sum_{i, \sigma_i = \sigma_j} E_{\downarrow \downarrow} \text{ij}, \quad (3d) \]

\[ E_{\text{Pauli}} = \sum_{i, \sigma_i \neq \sigma_j} E_{\uparrow \uparrow} \text{ij} + \sum_{i, \sigma_i = \sigma_j} E_{\downarrow \downarrow} \text{ij}. \quad (3e) \]

Where \( Z \) is the charge of nucleus, \( r_{ij} \) and \( R_{ij} \) correspond to the relative positions of two particles (nuclei or electrons). \( \text{erf}(x) \) is error function, \( \sigma \) means the spin of electrons. Pauli potential is consists of same and opposite spin electrons repulsive potentials. More details can be found in Refs. 21, 22, 52, and 53.

However, EFF model also suffers from the limitation of WPMD. The wave packets spread at high temperature. To avoid excessive spreading of wave packets, the harmonic constraints are often added. Recently, Constrained EFF (CEFF) method has been proposed using \( L = \lambda_D + b_0 \) as the boundary of the wave packets, getting much lower electron-ion energy exchange rate agreeing with experimental data.

B. Quantum molecular dynamics and orbital-free molecular dynamics

In QMD simulations, electrons are treated quantum mechanically through the finite temperature DFT (FT-DFT). While ions evolve classically along the PES determined by the electric density. Each electronic wave function is solved by the Kohn-Sham equation

\[ \left( -\frac{1}{2} \nabla^2 + V_{\text{KS}}[n_e(\mathbf{r})] \right) \phi_i(\mathbf{r}) = E_i \phi_i(\mathbf{r}). \quad (4) \]

Where \( E_i \) is the eigenenergy, \(-1/2\nabla^2\) is the kinetic energy contribution, and the Kohn-Sham potential \( V_{\text{KS}}[n_e(\mathbf{r})] \) is given by

\[ V_{\text{KS}}[n_e(\mathbf{r})] = V(\mathbf{r}) + \int \frac{n_e(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} d\mathbf{r'} + V_{\text{xc}}[n_e(\mathbf{r})]. \quad (5) \]

Where \( V(\mathbf{r}) \) is the external potential, the second term in the right hand of the above equation is the Hartree contribution, and \( V_{\text{xc}}[n_e(\mathbf{r})] \) represents the exchange-correlation potential. The electron density consists of single electronic wave function

\[ n_e(\mathbf{r}) = 2 \sum_i |\phi_i(\mathbf{r})|^2. \quad (6) \]

At high temperatures, the requirement of too many bands limits the efficiency of QMD method. OFMD is a good choice when dealing with high temperature conditions. Within orbital-free frame, the electronic free energy is expressed as

\[ F_e[\mathbf{R}, n_e] = \frac{1}{\beta} \int d\mathbf{r} \left\{ n_e(\mathbf{r}) \Phi[n_e(\mathbf{r})] - \frac{2\sqrt{\pi}}{3\pi^2 \beta^{3/2}} I_{3/2} \{ \Phi[n_e(\mathbf{r})] \} \right\} \]

\[ + \int d\mathbf{r} V_{\text{ext}}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r'} \frac{n_e(\mathbf{r}) n_e(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|} + F_{\text{xc}}[n_e(\mathbf{r})]. \quad (7) \]

Where \( \mathbf{R} \) is the ionic position, \( \beta = 1/\kappa_B T \) where \( T \) is the temperature and \( \kappa_B \) is the Boltzmann constant. \( I_\nu \) is the Fermi integral of order \( \nu \). \( V_{\text{ext}}(\mathbf{r}) \) represents the external or the electron-ion interaction, and \( F_{\text{xc}}[n_e(\mathbf{r})] \) is the exchange-correlation potential. The electrostatic screening potential is represented by the \( \Phi[n_e(\mathbf{r})] \) depend on electron density \( n_e(\mathbf{r}) \) only

\[ \nabla^2 \Phi[n_e(\mathbf{r})] = 4\pi n_e(\mathbf{r}) = \frac{4\sqrt{\pi}}{\pi^2 \beta^{3/2}} I_{3/2} \{ \Phi[n_e(\mathbf{r})] \}. \quad (8) \]

C. Quantum Langevin molecular dynamics

QMD and OFMD are good tools in describing static properties of warm dense matters. However, the information of electron-ion dynamical collisions is lost because of the assumption of BO approximation. In addition, electron-ion collisions are important for WDM in which electrons are excited because of the increasing temperature and density. To describe the dynamic process, QMD has been extended by considering the electron-ion collision induced friction (EI-CIF) in Langevin equation, and corresponding to the QLMD model. In QLMD, ion trajectory is performed using the Langevin equation

\[ M_I \dot{\mathbf{R}}_I = \mathbf{F} - \gamma M_I \dot{\mathbf{R}}_I + \mathbf{N}_I. \quad (9) \]

Where \( M_I \) and \( \mathbf{R}_I \) is the mass and position of the ion respectively, \( \mathbf{F} \) is the force calculated from DFT simulation, \( \gamma \) means the friction coefficient, and \( \mathbf{N}_I \) represents a Gaussian random noise. In QLMD, the force produced by real dynamics of electron-ion collisions can be replaced by the friction on account of less time scale of electronic motions comparing with that of ions. The friction coefficient \( \gamma \) is the key parameter should be determined a-priori. Generally, at high temperature such as WDM and HDM regimes, the EI-CIF dominates the friction coefficient, and can be estimated from the Rayleigh model

\[ \gamma = 2\pi m_e Z^2 \left( \frac{4\pi n_i}{3} \right)^{1/3} \sqrt{\frac{k_B T}{m_e}} \quad (10) \]
Where \( m_e \) is the electronic mass, \( Z^+ \) is the average ionization degree, and \( n_i \) means the ionic number density. There is another way to assess \( \gamma \) based on the Skupsky model\(^{60,61} \), and in this work, we adopted Rayleigh model only considering the hydrogen we studied has high density and high temperature.

To make sure that the particle velocity satisfies the Boltzmann distribution, the Gaussian random noise \( N_i \) should obey the fluctuation-dissipation theorem\(^6^{2} \):

\[
\langle N_i(0)N_j(t) \rangle = 6\gamma M_j k_B T dt.
\]  

(11)

Where \( dt \) is the time step in the MD simulation. The angle bracket denotes the ensemble average.

D. Self-diffusion coefficient

In MD simulations, the self-diffusion coefficient is often calculated from the velocity autocorrelation function (VACF) using Green-Kubo formula\(^5^{3} \):

\[
D = \lim_{t \to \infty} D(t),
\]

(12a)

\[
D(t) = \frac{1}{3} \int_0^t dt \langle v_i(t) \cdot v_i(0) \rangle.
\]

(12b)

In which \( v_i(t) \) is the center of mass velocity of the \( i \)th particle at time \( t \), and the angle bracket represents the ensemble average. Generally, the integral is computed in long enough MD trajectories so that the VACF becomes nearly zero and has less contribution to the integral. All the same species of particles are considered in the average to get faster convergent statistical results.

In practical, it is impossible to get a strict convergent result because the infinite simulation is forbidden. Thus, we usually use an exponential function \( \langle v(t) \cdot v(0) \rangle = a \exp(-t/\tau) \) to fit the VACF to get the self-diffusion coefficient \( D = a \cdot \tau \). Where \( a \) and \( \tau \) are fitting parameters determined by a least-squares fit. \( \tau \) corresponds to the decay time. In moderate and strong coupling regimes, a more sophisticated fitting expression is needed to be considered\(^6^{5} \). In the exponential function fitting, the statistical error can be estimated by

\[
\varepsilon = \sqrt{\frac{2\tau}{NK_{traj}}}.
\]

(13)

Where \( N \) is the number of particles, \( T_{traj} \) is the total time in the MD simulation.

III. RESULTS AND DISCUSSION

A. Computational details

We have performed (C)EFF, QMD, and OFMD simulations to study the static and transport properties of warm dense hydrogen at the density of \( \rho = 5g/cm^3 \) and \( \rho = 10g/cm^3 \). The

temperatures are from 50kK to 300kK. The ionic coupling parameters \( \Gamma = Z^+ e_v^2 / (r_i k_B T) \) is larger than 1 in all regimes we studied, here \( r_i = (3/(4\pi n_i))^{1/3} \) is the Wigner-Seitz radius. The electronic degeneracy parameter \( \Theta = T/T_F \) describes the quantum effect of electrons, here \( T_F = (3\pi^2 n_e)^{2/3} / 2 \) is electronic Fermi temperature. For all density and temperature in this work, \( \Theta \) is always less than 1, revealing that the quantum effects play important roles in these states.

QMD simulations have been performed using Quantum-Espresso (QE) open-source software\(^6^{5} \) the electron-ion interaction is described as plane wave pseudopotential. The electron-electron exchange-correlation potential is represented by the Perdew-Burke-Ernzerhof (PBE) functional\(^6^{6} \) (PBE) in the generalized-gradient approximation (GGA). The velocity Verlet algorithm\(^6^{7} \) is used to update positions and velocities of ions. In our simulations, we used supercells containing 256 H atoms. The time step is set from 0.05fs to 0.1fs at different temperature to ensure convergence of energy. The cutoff energy is tested and set from 100 Ry to 150 Ry. The number of bands is sufficient for the occupation of electrons. Only the \( \Gamma \) point \((k = 0)\) is sampled in the Brillouin-zone. Each density and temperature point is performed for at least 4000-10000 time steps in the canonical ensemble, and the ensemble information is picked up after the system reaches equilibrium. The OFMD simulations are performed with our locally modified version of PROFESS\(^6^{8} \). The PBE functional\(^6^{6} \) is also used to treat the exchange-correlation potential. 256 atoms are also used in the supercell. The kinetic energy cutoff is 7000eV when the density \( \rho = 5g/cm^3 \), and 10000eV at \( \rho = 10g/cm^3 \). The time step is set from 0.04fs to 0.15fs with the temperature increasing. The size effect has been tested in all MD simulations.

In the EFF simulations, the real electron mass is used so that we choose the time step as small as 0.2as. 1000 ions and 1000 electrons are used in the simulation. 5ps microcanonical ensemble with a fixed energy, volume, and number of particles (NVE) has been performed to calculate statistical average after 10ps simulations with fixed temperature, volume, and number of particles (NVT). When temperature and density become higher, CEFF is applied to avoid packets spreading.

B. Static and transport properties

We firstly calculate the radial distribution function (RDF) \( g(r) \) of H-H, as shown in Fig. 1. It is shown that the RDFs from OFMD calculations agree well with RDFs of QMD results. Moreover, the RDFs calculated from (C)EFF reflect similar microscopic characteristics with QMD and OFMD results, especially when the temperature is relatively low, where the electron-ion collisions are not so important. For these cases, it is appropriate to show the intrinsic different physics between static and transport properties if the RDFs shown are very close to each other. It should be noticed that the RDFs of (C)EFF model shows a little more gradual than QMD’s and OFMD’s with the increase of temperature. It is deduced that the non-adiabatic effect play little role in the static structures.
of warm dense hydrogen shown here, which is similar to the effects of Langevin dynamics on the static structures, in which the choice of friction coefficients has little effect on the RDFs.

However, non-adiabatic effects on dynamic properties are significant. We calculated the self-diffusion coefficients for warm dense hydrogen by integrating the VACF. To get a convergent value, a simple exponential function mentioned in Section II is applied. The self-diffusion coefficient varies with temperature at 5g/cm$^3$ and 10g/cm$^3$ are shown in Fig. 2 using different methods of (C)EFF, QMD, and OFMD.

It is very interesting that three methods give consistent results when temperature is relatively low. And the OFMD and QMD results have close values even with the increase of temperature. However, the (C)EFF simulations have a distinct reduce on the self-diffusion coefficients comparing with QMD and OFMD results. And the difference becomes more obvious at higher temperature. We boil it down to the non-adiabatic electron-ion dynamic collisions, which is lost in the framework of BO approximation such as QMD and OFMD. Regarding the electron as a Gaussian wave packet, (C)EFF methodology implements the electron-ion dynamics simulations, in which the dynamic coupling and collisions can be naturally included. As shown in Fig. 2, with the temperature increase, more electrons are excited or ionized and become free electrons. These free electrons lead continual and non-negligible electron-ion collisions, supplying drag forces for the motion of ions, and giving rise to much lower diffusion coefficients. The collision rate increases with the temperature, showing lower diffusive properties for ions, significantly affects the transport properties of WDM.

The lost of dynamic collisions can be introduced into the QMD model by considering electron-ion collision induced friction in Langevin equation. Here, we use the Rayleigh model to estimate the friction coefficient $\gamma$, and the QLMD simulations have been performed. It is very exciting that the QLMD results, showed in Fig. 2, agree well with (C)EFF simulations. The greatest difference between the two models is 12%, but mostly within 6%. This suggests that the reduction in ionic diffusion from (C)EFF simulations does indeed come from electron-ion dynamic collisions. We believe the small difference belongs to the choice of friction coefficient $\gamma$. Since the prior parameter should be determined artificially in QLMD simulations, we are encouraged to do quan-

FIG. 1. The RDFs of H-H at 5g/cm$^3$ (a) and 10g/cm$^3$ (b). The ordinate is differentiated by adding factors at different temperatures. Blue double dots lines represent the results from (C)EFF simulation. Black solid and red dashed lines are the QMD and OFMD results, respectively.

FIG. 2. The self-diffusion coefficients of H as a function of temperature at 5g/cm$^3$ (a) and 10g/cm$^3$ (b), calculated by QMD, OFMD, QLMD, and (C)EFF methods. Black squares represent the QMD results, red circles are the results of OFMD’s, and the (C)EFF results are represented by blue triangles. The QLMD results are represented by purple diamonds.
titative analysis about the electron-ion collisions effect using the (C)EFF results as benchmark for the results of all adiabatic methods and analytical models.

IV. ELECTRON-ION COLLISIONS EFFECT ASSESSMENT

As shown above, we should figure out the mechanism how does the dynamic collisions work on the ionic transport? We can find a clue from the Landau-Spitzer (LS) electron-ion relaxation rate \( \nu_{ei} \):

\[
\nu_{ei} = \frac{8\sqrt{2\pi n_i Z^2 e^4}}{3m_e m_i} \left( \frac{k_B T_e}{m_e} + \frac{k_B T_i}{m_i} \right)^{-3/2} \ln \Lambda \quad (14)
\]

Where \( m_e (m_i) \), \( n_e (n_i) \) and \( T_e (T_i) \) are the mass, number density and temperature of electrons(ions), respectively. The Coulomb logarithm \( \ln \Lambda \) can be calculated by the GMS model\(^7\). In Eq. 14, it is obvious that with the increase of density and temperature (the Coulomb logarithm also varies with the density and temperature), the collision frequency becomes higher, leading the diffusion coefficients reduce more significantly. The results of QMD and (C)EFF simulations showed in Fig. 2 exhibit the same behaviors.

As shown in Eq. 14, the electron-ion relaxation rate \( \nu_{ei} \) is the function of temperature and density. However, the thermodynamic state also changes with temperature and density, therefore it is difficult to distinguish the electron-ion collisions effect. For this purpose, we can change the effective mass of electrons in the (C)EFF simulation without altering the intrinsic interactions in the Hamiltonian of the system\(^22,71\). Since the mass of ions is much greater than that of electrons, we can find a simple relationship between the electron-ion collision frequency \( \nu_{ei} \) and the mass of the electron \( m_e \) from Eq. 14

\[
\nu_{ei} = f(\rho, T) m_e^{1/2} \quad (15)
\]

When the dynamic electron mass is larger, the motion of effective electrons exhibit more classical, and the collisions between electrons and ions become stronger. By this way, we can study the influence of electron-ion collisions by adjusting electronic mass in (C)EFF simulations. The VACFs and self-diffusion coefficients of H at different dynamic electron mass are showed in Fig. 3.

From the VACF results we can see, The change of dynamic electron mass does not alter the thermodynamic states of ions. While, dynamic collisions reduce the correlation of particles, showing lower decay time with the increase of dynamic electron mass, as well as the electron-ion collision frequency. Dffusions reflect similar trends, and more interestingly, the diffusion of ions is inversely proportional to the log of electronic mass as showed in Fig. 3(b). The inverse ratio relation reflects the reduction of the diffusion due to electron-ion collisions, and the slope determines the magnitude of this influence. In Fig. 3(b), it is shown that the influence of electron-ion collisions becomes stronger with the increase of temperature, since the electrons are more classical at higher temperature.

To quantitatively describe the relationship between diffusion and collision frequency, we performed more intensive simulations on dynamic electron mass as showed in Fig. 4. Here, the QMD results are used as the value at reference point, corresponding to no dynamic electron-ion collisions, since \( m_e \) can not be zero.

As showed in Fig. 4, the change of diffusion coefficients decrease much steeper when the electron dynamic mass becomes smaller, revealing more significant effect of electron-ion collisions. Another decaying function as \( D = a \log (1 + b m_e^c) + d \) can well describe this relation of diffusion varying with the dynamic electron mass \( m_e \). This function can transit to the linear form when \( m_e \) is large. Here, we have found the approximate relationship between ionic diffusion coefficient \( D \) and electron-ion collision rate \( \nu_{ei} \) taking Eq. 15 into the fitting function.
vanishes, and within this consideration, the total diffusion coefficient can be obtained via

\[ D = f_1(\rho, T) \log \left(1 + f_2(\rho, T) v_{ei}^{f_3(\rho, T)}\right) + f_4(\rho, T) \]  

(16)

Where \( f_1(\rho, T) \), \( f_2(\rho, T) \), \( f_3(\rho, T) \), \( f_4(\rho, T) \) are the function of the density \( \rho \) and temperature \( T \). If \( v_{ei} \) is set to zero, the first term in the right hand of Eq. 16 vanishes, and \( D = f_3(\rho, T) = D_0 \). Here, the remaining term \( D_0 \) represents the diffusion without electron-ion collisions. We call the first term as collisions induced friction (CIF) of the ionic diffusion \( D_{CIF} \). Within this consideration, the total diffusion coefficient can be obtained via

\[ D = f_1(\rho, T) \log \left(1 + f_2(\rho, T) v_{ei}^{f_3(\rho, T)}\right) + D_0 \]

\[ D = D_{CIF} + D_0 \]  

(17)

For \( D_0 \), plenty of models have been developed to study on it, such as QMD and OFMD which are based on BO approximation. In this paper, the diffusion coefficient including non-adiabatic effect has been calculated using (C)EFF method. As the collision frequency is a small term, the equation can be simplified as \( D_{CIF} = D - D_0 = f(\rho, T) v_{ei}^{f(\rho, T)} \). \( D \) and \( D_0 \) can be obtained from (C)EFF and QMD simulations, respectively. We develop an empirical fitting function from the available data as the assessment of electron-ion collisions induced the decrease of ionic diffusions

\[ D_{CIF} = \frac{v_{ei}^{0.25}}{a \rho / T^{3/2} + b \rho + c / T^{3/2} + d} \]  

(18)

where the fitting coefficient \( a = -8.942 \times 10^{-3} \), \( b = 1.585 \times 10^{-3} \), \( c = 6.849 \), and \( d = -4.195 \). The corrected QMD results by the CIF model, which are shown in Fig. 5, agree well with (C)EFF simulations. To verify the accuracy of the fitting function, we calculate self-diffusion of H and He at some other temperatures and densities. The results are listed in Table I.

In Table I, the ionic self-diffusion coefficients obtained from the QMD model can be corrected by adding the CIF factor as the compensation of electron-ion collisions. The results are in good agreement with the (C)EFF and QLMD results, showing that our CIF correction can be applied to warm dense matter. It needs to be emphasized that the CIF correction is independent of other models, therefore, any model based on the adiabatic framework can use it to offset the loss of the electron-ion collisions.

V. COMPARISON WITH ANALYTICAL MODELS

The expensive computational costs of first principles simulations make it difficult to apply online or generate large amount of data. On the contrary, some analytical models based on numerical simulations have been proposed, supplying promising approaches to the establishment of database.
The OCP is a widely used model to describe a single species of ion surrounded by a uniform, neutralizing background of electrons. All properties of OCP model are dependent on the coupling parameter \( \Gamma \). However, the validity of OCP model in describing WDM should be examined as shown in the previous work\(^ {72} \). Daligault has given a rational function to calculate the reduced self-diffusion and viscosity.\(^ {36,73} \) The function is fitted based on a mass of MD simulations on condensed matter

\[
D^* = D/D_0 = \sum_{i=0}^{3} a_i \Gamma^i / \sum_{i=0}^{3} b_i \Gamma^i \tag{19}
\]

where \( D^* \) is the reduced self-diffusion and \( D_0 = \omega_0 a^2 \). \( \omega_0 = (4\pi n_i Z^2 e^2/m_0)^{1/2} \) is the plasma frequency and \( r_i \) is anionic Wigner-Seitz radius. \( a_i \) and \( b_i \) are fitting parameters as given in Table II.

In this work, we use the form proposed by Arnault\(^ {41} \) to fix the discontinuity of Daligault’s parametrizations at the threshold of \( \Gamma = 2 \) as

\[
D^*_{OCP} = \begin{cases} 
D_0^*, & \text{if } \Gamma < 1.5, \\
1.834 \Gamma^{-1.26}, & \text{if } 1.5 \leq \Gamma < 2.5, \\
D_0^*, & \text{if } \Gamma \geq 2.5.
\end{cases} \tag{20}
\]

Here, the Yukawa potential has been applied replacing the bare Coulomb interactions.\(^ {28,74,75} \) In this way, the screening effect is included in YOCP model as a development of OCP model. In the YOCP framework, the inverse screening length \( \kappa \) also affects the structures and properties of matters. Usually, \( \kappa \) is defined as the reciprocal of the Thomas-Fermi (TF) screening length\(^ {14} \)

\[
\lambda_{TF} = \left( \frac{\pi}{12Z} \right)^{1/3} \sqrt{r_i} \tag{21}
\]

where \( Z \) is the ionic charge, and \( r_i \) is the Wigner-Seitz radius, respectively. The self-diffusion can be obtained using Yukawa potential \( u(r) = q^2 e^{-kr}/r \) on MD simulations. Daligault has applied it in a wide range of \( \kappa \) and over the entire fluid region.\(^ {59} \) In the gas-like small coupling regime, the reduced self-diffusion coefficients model can be extended from the Chapman-Spitzer results as\(^ {39} \)

\[
D^*(\kappa, \Gamma) = \frac{1}{\sqrt{3}} \frac{1}{\alpha(\kappa) \Gamma^{5/2} \ln \Lambda(\kappa, \Gamma)} \tag{22}
\]

The generalized Coulomb logarithm \( \ln \Lambda(\kappa, \Gamma) \) is expressed as

\[
\ln \Lambda(\kappa, \Gamma) = \ln \left( 1 + B(\kappa) \frac{\lambda_D}{b_c} \right) = \ln \left( 1 + \frac{B(\kappa)}{\sqrt{3 \Gamma^{3/2}}} \right) \tag{23}
\]

where \( \lambda_D \) is the Debye length \( \lambda_D = \sqrt{4\pi q^2 nZ^2 k_B T} \) and \( b_c \) is the classical distance of closest approach \( b_c = Zq^2/k_BT \). \( \alpha(\kappa) \) and \( B(\kappa) \) are fitting parameters dependent on \( \kappa \) only

\[
\alpha(\kappa) = \frac{1}{\Gamma^2} \frac{1}{\pi a_0 + a_1 \kappa^{2}} \tag{24}
\]

\[
B(\kappa) = b_0 + b_1 \text{erf} \left( b_2 \kappa^{b_3} \right) \tag{25}
\]

All coefficients are listed in Table II. The self-diffusion coefficient is obtained according to \( D = D^* \omega a^2 \), and \( \omega = (4\pi n_i Z^2 e^2/m_i)^{1/2} \) is the plasma frequency. \( Z^* \) can be estimated using average atom (AA) model\(^ {76} \), in which the energy level broadening effect is considered. The comparison between the results of different models are shown in Fig. 6. The QMD results and the CIF correction of QMD’s are also showed as the benchmarks.

It is shown in Fig. 6 that the self-diffusion coefficients from YCOP model are much larger than those of OCP model. It is because that when we consider the screening of electrons, the repulsive interactions between ions become weaker, so that ions exhibit more free and diffusive. For warm dense hydrogen at the density of 5g/cm\(^3 \), YOCP model can excellently reproduce results from the QMD simulations. However, at higher density, the YOCP model overestimates the diffusion compared with QMD results. The reason for the phenomenon is that the Yukawa model underestimates the ionic interactions at short distances.\(^ {77} \) When the density and temperature are higher, the electronic charges around the ions overlap, and the Pauli principle makes electrons more repulsive. A short-range repulsion (SRR) should be added to Yukawa model as a correction. In the YOCP model, we attribute the lost of SRR to the over-shielding of Thomas-Fermi (TF) screening. An empirical parameter can be introduced to correct the TF screening length. For 10g/cm\(^3 \) hydrogen, we use \( \kappa^* = 1/\lambda_{TF} = 1/(1.27\lambda_{TF}) \) instead of the TF inverse screening length and the results from the modified YOCP (MYOCP) model are in good agreement with the QMD results. Similar situations are shown in Ref.\(^ {78} \) and 79. There is another scheme to deal with larger ionic coupling systems, in which we can reduce effective volumes of particles so that the collision frequency can be increased and the ionic transportation

**TABLE I.** The self-diffusion coefficients calculated by QMD, QLMD and (C)EFF models. The QMD results corrected by the CIF model is also listed in the table.

| species | density(g/cm\(^3\)) | temperature(K) | \( D_{\text{QMD}} \)(cm\(^2\)/s) | \( D_{\text{QLMD}} \)(cm\(^2\)/s) | \( D_{\text{CIF}} \)(cm\(^2\)/s) | \( D_{\text{QMD+CIF}} \)(cm\(^2\)/s) |
|---------|---------------------|----------------|-------------------------|-------------------------|-------------------------|-------------------------|
| H       | 8                   | 100000         | 0.0155                  | 0.0133                  | 0.0122                  | 0.0123                  |
| H       | 8                   | 200000         | 0.0386                  | 0.029                   | 0.0264                  | 0.0284                  |
| H       | 15                  | 200000         | 0.0237                  | 0.0181                  | 0.0182                  | 0.0183                  |
| H       | 15                  | 300000         | 0.0396                  | 0.0289                  | 0.0289                  | 0.0278                  |
| He      | 10                  | 100000         | 0.00757                 | 0.0066                  | 0.00598                 | 0.00596                 |
| He      | 10                  | 200000         | 0.0181                  | 0.016                   | 0.0108                  | 0.0128                  |

The Chapman-Spitzer results as the Wigner-Seitz radius. All properties of OCP model are dependent on the coupling parameter \( \Gamma \). However, the validity of OCP model in describing WDM should be examined as shown in the previous work. Daligault has given a rational function to calculate the reduced self-diffusion and viscosity. The function is fitted based on a mass of MD simulations on condensed matter.
TABLE II. Coefficients from OCP and YOCP models as in Ref. 36 and 73.

|        | $a_0$     | $a_1$     | $a_2$    | $a_3$    | $b_0$    | $b_1$    | $b_2$    | $b_3$    |
|--------|-----------|-----------|----------|----------|----------|----------|----------|----------|
| OCP($\Gamma \leq 2$) | -0.732599 | 3.89667   | 0.489336 | -0.271605 | 0.0426862 | -0.501987 | 1.34111  | 0.741386 |
| OCP($\Gamma > 2$)   | 59.7446   | 3.1094    | 1.37071 $\times 10^{-3}$ | -2.40269 $\times 10^{-5}$ | -32.1103 | 56.2554  | 1.24087  | 0.0371926 |
| YOCP               | 1.55273   | 1.10941   | 1.36909  |          |          |          |          |          |

FIG. 6. Comparison of QMD and modified QMD simulations with different analytical models for self-diffusion coefficients of warm dense H at 5g/cm$^3$ (a) and 10g/cm$^3$ (b). The black solid squares and circles represent the results calculated by QMD and QMD with CIF correction, respectively. The red and blue solid lines are the results of the OCP model and YOCP model respectively. The purple lines represent the results from the EOCP models. The effective coupling parameters of the EOCP model are obtained from the RDFs of QMD.

VI. CONCLUSION

We have performed QMD, OFMD, and (C)EFF simulations to determine the RDFs and the ionic self-diffusion coefficients of warm dense hydrogen at the densities of 5g/cm$^3$ and 10g/cm$^3$ and temperatures between 50kK to 300kK. The results from (C)EFF-MD method are carefully compared with

screening and electron-ion collisions. In WDM regimes, the influence of dynamic electron-ion collisions matches screening effects. The ions feel the friction caused by the electrons, leading changes in transport properties. With the increase of density and temperature, the collision becomes more violent and this non-adiabatic effect will more dominate the transport of ions. This leads to the offset of screening by dynamic electron-ion collisions, and the agreement between OCP and modified QMD predictions. But we should also notice that in OCP model, it is difficult to divide the dynamic collisions from the screening effect. For example, for the case of He at 10g/cm$^3$ and 100000K, OCP gives lower diffusion coefficients about 20% comparing with CEFF calculation because of stronger electronic screening comparing with electron-ion collisions, and the model fails.

It is shown in Fig. 6 that, the EOCP model has a better description in all density and temperature range we studied with the QMD simulations. In EOCP model, The effective coupling parameter $\Gamma_e$ and ionization $Q_e$ are introduced as the correction of the OCP model to reproduced the static structures of the OFMD’s. The model also works well on transports properties such as diffusion and viscosity. In this paper, we set $\Gamma_e$ by the procedure developed by Ott et al as

$$\Gamma_e = 1.238 \exp \left( 1.575 r_{1/2}^3 \right) - 0.931, \quad \left( r_{1/2} < 1.3 \right) \quad (26)$$

where $r_{1/2}$ is obtained from the RDFs $g(r)$ at $g(r) = 0.5$. The distance is expressed in the Wigner-Seitz radius unit. The effective average charge $Q_e$ is defined as $Q_e = \sqrt{T_e \alpha k_b T / e}$. We use the RDFs of QMD’s as the input of EOCP model, the results agree well with those extracted from long time MD simulations, especially when temperature is low. However, the predictions overestimate ionic diffusions compared with modified QMD results. This is because of the insensitivity of static properties as showed in Fig 1. The good reproduction of QMD simulations for the EOCP model reflects the importance of acquiring precise effective interactions. While, the difference between the modified QMD results and EOCP predictions reminds us again to pay attention to the instantaneous dynamic collisions which is lost in those static potentials.

However, all the interactions in YOCP models are static that dynamic electron-ion collisions are already lost. This is why the results obtained from modified QMD are much smaller than the YOCP results, as well as the QMD’s. On the contrary, the self-diffusion coefficients for OCP model looks closer to the modified QMD results. We conclude that the coincidence is the result of the competition between electron can be draged or dissipative. The model has successfully improved the transport properties of strongly coupled plasmas in the range $1 \leq \Gamma \leq 30$. The effective coupling parameter $\Gamma_e$ and ionization $Q_e$ are introduced as the correction of the OCP model to reproduced the static structures of the OFMD’s. The model also works well on transports properties such as diffusion and viscosity. In this paper, we set $\Gamma_e$ by the procedure developed by Ott et al as

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where $r_{1/2}$ is obtained from the RDFs $g(r)$ at $g(r) = 0.5$. The distance is expressed in the Wigner-Seitz radius unit. The effective average charge $Q_e$ is defined as $Q_e = \sqrt{T_e \alpha k_b T / e}$. We use the RDFs of QMD’s as the input of EOCP model, the results agree well with those extracted from long time MD simulations, especially when temperature is low. However, the predictions overestimate ionic diffusions compared with modified QMD results. This is because of the insensitivity of static properties as showed in Fig 1. The good reproduction of QMD simulations for the EOCP model reflects the importance of acquiring precise effective interactions. While, the difference between the modified QMD results and EOCP predictions reminds us again to pay attention to the instantaneous dynamic collisions which is lost in those static potentials.

VI. CONCLUSION

We have performed QMD, OFMD, and (C)EFF simulations to determine the RDFs and the ionic self-diffusion coefficients of warm dense hydrogen at the densities of 5g/cm$^3$ and 10g/cm$^3$ and temperatures between 50kK to 300kK. The results from (C)EFF-MD method are carefully compared with
the results from QMD/OFMD methods based on the BO approximation. In EFF method, the static properties are insensitive to electron-ion collisions, however, the diffusion of ions decreases significantly with the increase of electron-ion collisions. The ionic diffusion coefficients calculated from (C)EFF agree well with the QLMD results, but largely differ from QMD or OFMD simulations, revealing key role of electron-ion collisions in warm dense hydrogen. Most importantly, we proposed a new analytical model which introduces the electron-ion collisions induced friction (CIF) effects, constructing a formula to calculate self-diffusion coefficients without doing non-adiabatic simulations. The CIF model has been verified to be valid over a wider range of temperature, density and materials. However, since the CIF model is derived from the fitting of simulation results, whether it can be applied for more complex elements should be verified further. We also show the results from analytical models of OCP, YOCP and EOCP. The YOCP model shows good agreement with QMD results at the density of 5g/cm³, while overestimates electronic screening at higher density. Dynamic collisions suppress the motion of ions, partly offsetting the electronic screening, make the prediction of OCP model close to the modified QMD results. However, the effect of screening and dynamic collisions can not be distinguished in OCP model. Based on the static information, EOCP model reproduces QMD simulations better, but worse for modified QMD results, suggesting that non-adiabatic dynamic collisions affect significantly on the transport properties of WDM.

VII. ACKNOWLEDGMENTS

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VIII. DATA AVAILABLE

The data that support the findings of this study are available within the article.

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