Quantum dynamics of charged particles in the Wigner formulation of quantum mechanics

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Abstract. We are going to study the kinetic properties of dense hydrogen plasma by a new quantum dynamics method in the Wigner representation of quantum mechanics. This method combines the Feynman and Wigner formulation of quantum mechanics and uses for calculation the direct path integral Monte Carlo (PIMC) and molecular dynamics methods. We are going to solve the Wigner–Liouville equation for dense degenerate hydrogen with the initial condition sampled by the PIMC method from equilibrium plasma state. We hope to do calculations of the hydrogen plasma properties under extreme conditions.

1. Introduction

Hydrogen plasma is quantum-mechanical one even at high temperature and low density since the Heisenberg uncertainty principle is necessary to keep the electrons from collapsing into the ions, thus it cannot be described in the framework of classical mechanics. Nevertheless the classical molecular dynamic simulation became a traditional way of calculation of thermodynamic and transport properties of non-ideal plasma [1–3]. The main difficulty, however, since the invention of the Monte-Carlo (MC) and the molecular dynamics (MD) methods remains the treatment of bound states in dense media. This is the reason for classical methods with quantum-mechanical treatment of bound states. Kinetic properties are the most important quantities which determine the behavior of plasma. Experimental efforts for measurement of kinetic properties up to high densities revealed many quantum effects such as Pauli blocking, dynamic screening, the Debye–Onsager relaxation effect, formation of bound states etc. Molecular dynamics simulations of fully ionized classical plasma are widely used for the calculation of kinetic properties with the help of the Kubo formula [4].

In this work, we are going to generalize classical MD methods to take into account quantum effects. We use the Feynman and Wigner formulations of quantum mechanics combining with MC methods. In the paper, we describe the computational method for the calculation of kinetic properties of dense hydrogen. The Wigner–Liouville equation is solved by a combination of MD and path integral Monte-Carlo (PIMC) methods. The initial conditions are obtained using PIMC method, which allows calculating such thermodynamic quantities as the internal energy, pressure and pair distribution functions in a wide range of density and temperature. To study the influence of the interparticle interaction on the dynamic properties of dense plasmas we are going to compute the temporal correlation functions of quantum operators.
2. Wigner quantum dynamics

To calculate the electrical conductivity of dense two component Coulomb system of particles, we use quantum dynamics in the Wigner representation of quantum mechanics. As example of Coulomb system of particles, in three dimensional space (3D) we consider a two-component mass asymmetric electron–hole plasma consisting of Coulomb system of particles, in three dimensional space (3D) we consider a two-component mass asymmetric electron–hole plasma consisting of Coulomb system of particles, in three dimensional space (3D). We consider a two-component mass asymmetric electron–hole plasma consisting of Coulomb system of particles, in three dimensional space (3D).

Our starting point is the canonical ensemble-averaged time correlation function \[ C_{FA}(t) = \langle \hat{F}(0) \hat{A}(t) \rangle = Z^{-1} \text{Tr} \left\{ \hat{F} e^{i\hat{H}c/\hbar} \hat{A} e^{-i\hat{H}e/\hbar} \right\} , \] where $\hat{F}$ and $\hat{A}$ are the operators of arbitrary observables, $t_e = t - i\hbar\beta/2$ is the complex time, $\beta = 1/(k_BT)$ and

\[ Z = \text{Tr} \left\{ e^{-\beta \hat{H}} \right\} \]

is the partition function. The Wigner representation of (1) in a $\nu$-dimensional space is

\[ C_{FA}(t) = (2\pi\hbar)^{-2\nu} \int \int dpdq \, d\tilde{p}d\tilde{q} \, F(p) A(p) W(pq; \tilde{p}\tilde{q}; t; \beta) , \]

where $p$ and $q$ comprise the momenta and coordinates of all particles, $\nu = 12N$. Notations $A(pq)$ and $F(pq)$ mean Weyl’s symbols of the operators

\[ A(pq) = \int d\xi e^{-i\xi p} \left\langle q - \frac{\xi}{2} | \hat{A} | q + \frac{\xi}{2} \right\rangle \]

and $W(pq; \tilde{p}\tilde{q}; t; \beta)$ is the spectral density expressed as

\[ W(pq; \tilde{p}\tilde{q}; t; \beta) = \frac{1}{Z} \int \int d\xi d\tilde{\xi} e^{i\xi p} e^{i\tilde{\xi} \tilde{p}} \left\langle \tilde{q} + \frac{\xi}{2} \right| e^{i\hat{H}c/\hbar} \left| \tilde{q} - \frac{\xi}{2} \right\rangle \]

\[ \times \left\langle \tilde{q} + \frac{\xi}{2} \right| e^{-i\hat{H}e/\hbar} \left| \tilde{q} - \frac{\xi}{2} \right\rangle . \]

As has been proved in [6–8], $W$ obeys the following integral equation:

\[ W(pq; \tilde{p}\tilde{q}; t; \beta) = \int dp_0dq_0 dp_0\tilde{q}_0 G(pq, \tilde{p}\tilde{q}; t; p_0q_0, \tilde{p_0}\tilde{q}_0, 0) W(p_0q_0, \tilde{p_0}\tilde{q}_0; t = 0, \beta) \]

\[ + \frac{1}{2} \int_0^t dt' \int ds \int dp'q' dp'\tilde{q}' G(pq, \tilde{p}\tilde{q}; t; p'q', \tilde{p'}\tilde{q'}, t') \]

\[ \times \left[ W(p' - s, \tilde{p'} - s; \tilde{p'}\tilde{q'}; t') \omega(s, \tilde{q'}) - W(p'q'; \tilde{p'} - s, \tilde{q'}; t') \omega(s, \tilde{q'}) \right] , \]

(3)

with the Green function

\[ G(pq, \tilde{p}\tilde{q}; t; p'q', \tilde{p'}\tilde{q'}; t') = \delta (\tilde{p} - \tilde{p}(t; p'q', t')) \delta (\tilde{q} - \tilde{q}(t; p'q', t')) \]

\[ \times \delta \left( \tilde{p} - \tilde{p}(t; p'q', t') \right) \delta \left( \tilde{q} - \tilde{q}(t; p'q', t') \right) , \]

which describes propagation of the spectral density along classical trajectories in positive time direction

\[ \frac{dp}{dt} = \frac{1}{2} F(\tilde{p}t), \quad \frac{d\bar{q}}{dt} = \frac{1}{2} F(\tilde{q}t), \quad \frac{d\bar{p}}{dt} = \frac{1}{2} F(\tilde{p}t) \]

and in the reverse time direction

\[ \frac{dp}{dt} = -\frac{1}{2} F(\tilde{p}t), \quad \frac{d\bar{q}}{dt} = -\frac{1}{2} F(\tilde{q}t), \quad \frac{d\bar{p}}{dt} = -\frac{1}{2} F(\tilde{p}t) . \]
into account the other terms of this iteration series may be important in a simulation of the small physical parameters is needed for the convergence. From physical point of view taking with the initial conditions fixed in between these instants, i.e., at \( t = 0 \) the spectral density is \( W(\overline{pq}; \tilde{p}_0 q_0; t = 0, \beta) = \overline{W}(\overline{pq}; \tilde{p}_0 q_0; \beta) \). The right-hand sides of equations (4) and (5) include interparticle interaction that can be arbitrary strong.

The iteration series for \( C_{\phi A}(t) = \langle \phi | W^t \rangle = \langle \phi | K_{t_1} K_{t_0}^t \overline{W}^0 \rangle + \ldots \),
\[
\begin{align*}
\phi(\overline{pq}; \tilde{p} q) \equiv F(\overline{pq}) A(\tilde{p} q) \text{ and the parentheses } (\ldots) \text{ denote integration over the phase spaces}
\{\overline{pq}, \tilde{p}_0 q_0\}, \quad \{d\overline{p} q' d\tilde{p} q'\}
\end{align*}
\]
and so on. To compute the electron electrical conductivity we calculate the electron momentum–momentum time correlation function \( C_{pp}(t) \) and then apply the Kubo formula which contains the Fourier transform of \( C_{pp}(t) \) at \( \omega = 0 \).

The iteration series for \( C_{\phi A}(t) \) can be efficiently computed with the use of MC methods. We have developed a MC scheme which provides domain sampling of the terms giving the main contribution to the iteration series, cf. [6–8]. For simplicity, in this work, we take into account only the first term of iteration series, which is related to the propagation of the initial quantum distribution \( \overline{W}^0 \) according to the Hamiltonian equations of motion. This term, however, does not describe pure classical dynamics but accounts for quantum effects [6] and, in fact, contains arbitrarily high powers of the Planck’s constant:
\[
W(\overline{pq}; \tilde{p} q; t; \beta) \simeq \int d\overline{pq} d\tilde{p} q_0 G(\overline{pq}, \tilde{p} q, t; \overline{pq}_0, \tilde{p}_0 q_0, 0) \times W^0(\overline{pq}_0; \tilde{pq}_0; \beta).
\]

As has been shown in [6], the absolute convergence of the iteration series takes place and no small physical parameters is needed for the convergence. From physical point of view taking into account the other terms of this iteration series may be important in a simulation of the tunneling quantum particles through a potential barrier in case when classically forbidden regions for particle dynamics give the main contribution.

Here the initial condition \( W^0(\overline{pq}; \tilde{pq}; \beta) \equiv W(\overline{pq}; \tilde{pq}; 0; \beta) \) for equation (3) can be presented in the form of a finite difference approximation of the Feynman path integral [7–9].

The expression for \( W \) has to be generalized to account for the spin effects. This gives rise to an additional spin part of the initial density matrix, e.g., [10,11]. Also, to improve the simulation
accuracy the pair interactions $U_{ab}$, are replaced by an effective quantum potential $U^{\text{eff}}_{ab}$, such as the Kelbg potential [12]. For details we refer to paper [9], where recent applications of the PIMC approach to correlated Coulomb systems has been discussed.

3. Transport coefficients
A natural way to obtain transport coefficients is use of the quantum Green–Kubo relations [4]. These relations give the transport coefficients in terms of integrals of equilibrium time-depended correlation functions. According to equation (8) the electron conductivity $\sigma$ is the integral over the velocity autocorrelation function

$$\sigma_e = e^2 n_e \beta \lim_{t \to \infty} \frac{1}{3} \int_0^t d\tau \langle v(0) \cdot v(\tau) \rangle_e,$$

where $\langle \cdot \rangle_e$ denotes the ensemble average of $v$ and trajectories in positive (bared) and inverse (tilded) time directions are defined by equations (4) and (5), respectively.

Calculations of autocorrelation functions in the canonical ensemble have been performed by the combination of the MC sampling of the initial conditions $\vec{p}_i q_0$ and $\tilde{\vec{p}}_i q_0$ for trajectories and solving the system of dynamic Hamiltonian equations (4) and (5). The initial conditions $\vec{p}_i q_0$ and $\tilde{\vec{p}}_i q_0$ for the trajectories are sampled by MC method accordingly to the modulus of probability $W_0(\vec{p}_i q_0; \tilde{\vec{p}}_i q_0; \beta)$, while sign of the $W_0(\vec{p}_i q_0; \tilde{\vec{p}}_i q_0; \beta)$ is accounted for as weight function at calculations average values [9]. Important dependence of the electron conductivity on temperature and other thermodynamic parameters arises through the function $W_0(\vec{p}_i q_0; \tilde{\vec{p}}_i q_0; \beta)$ as can be seen from formulas (1) and (3).

Analogously, the Green–Kubo relation can be applied for other transport coefficients. For example, the shear viscosity is the integral over the autocorrelation function of the stress–energy tensor

$$\eta = \lim_{t \to \infty} \eta(t), \quad \eta(t) = \frac{1}{VT} \int_0^t d\tau \langle \sigma_{xy}(0) \sigma_{xy}(\tau) \rangle,$$

$$\langle \sigma_{xy}(0) \sigma_{xy}(\tau) \rangle = (2\pi)^{-6N} \int d\vec{p} q d\tilde{\vec{p}} q W(\vec{p} q; \tilde{\vec{p}} q; \beta) \sigma_{xy} (\vec{p} q(\tau)) \sigma_{xy} (\tilde{\vec{p}} q(\tau)),$$

where the off-diagonal stress-energy tensor is

$$\sigma_{xy} (pq(\tau)) = \sum_{i=1}^{N} \frac{p_{ix}(\tau) p_{iy}(\tau)}{m_i^2} - \frac{1}{2} \sum_{i \neq j}^{N} q_{ij,x}(\tau) \frac{\partial U(q)}{\partial q_{ij,x}}(\tau),$$

here $q_{ij} = q_i - q_j$, and $U$ is the sum of the Kelbg potentials [12].

The autocorrelators (11) and (13) as a function of time have to be calculated along the trajectories (4) and (5), which themselves are computed by means of a numerical scheme for solution of a system of ordinary differential equations of the first order. We are going to use the explicit numerical scheme with automatically adapted time step. To check correctness of the calculations we have to control the full energy. Usually several thousands of generated trajectories are required for convergence of the antiderivative of the autocorrelation function up to accuracy of 5%. The convergence is fast enough because the autocorrelation function includes averaging-out (i.e., summation) over all particles.
Details of our PIMC simulations have been discussed in a number of papers and review books, see, e.g., papers [3, 9] and references therein. For simulation we use the standard Metropolis algorithm. We use a cubic simulation box with periodic boundary conditions. The main idea of the simulations consists in constructing a Markov chain of different particle states in the phase space.

Errors of MC calculations of thermodynamic quantities related to the finite particle number \(N\) in the system with periodic boundary conditions are of the order of \(1/N\) [3]. However, too large number of particles presented by discrete trajectories described a large number of 3D-points (beads) requires too large computer resources. In practical calculations we try to keep the total number of particles not exceeding \(N = 126\) and the number of beads \(n = 20\) for each particle is used. Our choice of particle and bead numbers is a compromise between acceptable accuracy and available computer resources.

To avoid the well known sign problem in our MC simulations of Fermi particles we used effective pair pseudopotential depending on coordinates, momenta and degeneracy parameter of particles and taking into account Pauli blocking of fermions in phase space. The agreement between the our calculations and the analytical Fermi distributions is good enough up to parameter of the electron degeneracy equal to \(n\Lambda^3 = 10\) \((T/E_F = 0.141)\), while the integral characteristics such as energy are practically equal to each other \([9, 10]\). The degeneracy of electrons in our calculations is moderate, i.e., the degeneracy parameter is of order of several units.

4. Conclusion
According to the quantum Kubo formula we have derived a new method for calculation of electrical conductivity of dense hydrogen plasma. This method combines the Feynman and Wigner formulations of quantum mechanics and uses for calculation the direct PIMC and MD methods. We are going to apply this method to treatment of hydrogen plasma.

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