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WPMD simulations of a two-component plasma

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Abstract

Using wave packet molecular dynamics simulations we calculate the dynamic structure factor $S(k, \omega)$ of a two-component plasma (TCP). The results are compared with corresponding classical molecular dynamics simulations of a model TCP with effective interactions. Both approaches agree well in the low frequency part of $S(k, \omega)$ but increasingly deviate for high frequencies. This clearly demonstrates a restriction of the method of effective potentials to static properties and low frequency phenomena.

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1. Introduction

Simple two-component plasmas (TCP), such as e.g. a proton–electron plasma, are of fundamental interest for the understanding and description of many real plasmas in particular for temperature–density regimes where strong interparticle correlations show up. They have, however, to be treated by quantum mechanics as the wave nature of the particles and their indistinguishability may be important. In the wave packet molecular dynamics (WPMD) method [1–5], which is based on a time-dependent variational principle, these quantum effects are approximately taken into account by representing the electrons by anti-symmetrized localized wave packets which have a simple analytical form and are described by only a few relevant parameters. The wave packet approach fairly well reproduces many dynamical properties of quantum many-body systems and reduces the computational amount from the solution of a partial differential equation to the much simpler case of a set of ordinary differential equations. Another very fruitful approach used for describing strongly coupled TCPs is the method of effective potentials [6] where the Coulomb interaction is regularized at short distances. Such effective interactions have been derived e.g. from the two-particle Slater sum [7, 8] and are exact in the low density limit. Their application to nonideal TCPs enables the use of classical statistics and numerical simulations such as classical molecular dynamics (MD) or Monte Carlo, see e.g. [9–16]. These simulations have shown that the concept of effective potentials is quite successful in describing equilibrium properties such

as thermodynamic functions and correlation functions of a real TCP. As based on quantum statistical considerations, it is, however, less suited to study transport properties or non-equilibrium situations. Here an extension to potentials with time-dependent parameters, as e.g. provided by the WPMD, is required. In this context, two important questions arise. First, of course, how well the classical dynamics generated within the WPMD approach can describe the dynamic properties of a quantum TCP. Second, to which extent the concept of using time-independent effective potentials is applicable for dynamic properties or truly dynamic situations. In this paper, we aim at finding answers to the second question by comparing the frequency dependence of the dynamic structure factor of a TCP of protons and electrons as obtained from WPMD simulations and classical MD simulations with time-independent effective potentials.

2. Wave packet molecular dynamics simulations

In our present application of the WPMD simulation technique to hydrogen TCPs, the N_i protons of our simulation sample are described classically, i.e. by their positions $\vec{R}_I$ and momenta $\vec{P}_I$, whereas the N_e electrons are represented by Gaussian wave packets

$$\varphi_k(\vec{x},t)=\left(\frac{3}{2\pi\gamma_k^2}\right)^{\frac{3}{4}}\exp\left[-\left(\frac{3}{4\gamma_k^2}+\frac{\mathrm{i}p_{\gamma_k}}{2\hbar\gamma_k}\right)(\vec{x}-\vec{r}_k)^2+\frac{\mathrm{i}}{\hbar}\vec{p}_k(\vec{x}-\vec{r}_k)\right], \tag{1}$$

with eight variational parameters $\{\vec{r}_k(t),\,\vec{p}_k(t),\,\gamma_k(t),\,p_{\gamma_k}(t)\}$, representing the mean values of position and momentum, and the width and its conjugate momentum. The dynamics of the system is governed by the principle of stationary action, from which one can derive equations of motion for the variational parameters $\{q_k(t)\}$ of the pseudo-Hamiltonian form

$$\sum_\beta \mathcal{N}_{\alpha\beta}\dot{q}_\beta=\frac{\partial\langle\Psi|\hat{H}|\Psi\rangle}{\partial q_\alpha},\qquad\text{with}\qquad \mathcal{N}_{\alpha\beta}=\frac{\partial}{\partial q_\alpha}\langle\Psi|\mathrm{i}\hbar\frac{\partial}{\partial q_\beta}|\Psi\rangle-\frac{\partial}{\partial q_\beta}\langle\Psi|\mathrm{i}\hbar\frac{\partial}{\partial q_\alpha}|\Psi\rangle. \tag{2}$$

Here $\Psi=\hat{A}\prod_k\varphi_k(\vec{x}_k,t)$ is the many-particle wavefunction in Hartree–Fock approximation ($\hat{A}$ indicates the anti-symmetrization) and $\hat{H}$ is the Hamilton operator ($e'^2=e^2/4\pi\varepsilon_0$)

$$\hat{H}=\sum_I\frac{P_I^2}{2M}+\sum_k\frac{\hat{p}_k^2}{2m}+\sum_{I<J}\frac{e'^2}{|\vec{R}_I-\vec{R}_J|}+\sum_{k<l}\frac{e'^2}{|\hat{\vec{x}}_k-\hat{\vec{x}}_l|}-\sum_{I,k}\frac{e'^2}{|\vec{R}_I-\hat{\vec{x}}_k|} \tag{3}$$

for the proton–electron TCP at hand. Further details on the WPMD method with full anti-symmetrization are given in [4, 5, 15]. As we are here mainly interested in diffraction effects, we restrict ourselves to systems with temperatures T well above the Fermi temperature T_F and thus consider the much less demanding case of the Hartree wavefunction $\Psi=\prod_k\varphi_k(\vec{x}_k,t)$. Now the equations of motion take the usual symplectic form

$$\dot{\vec{r}}_k(t)=\frac{\partial\mathcal{H}}{\partial\vec{p}_k},\qquad \dot{\vec{p}}_k(t)=-\frac{\partial\mathcal{H}}{\partial\vec{r}_k},\qquad \dot{\gamma}_k(t)=\frac{\partial\mathcal{H}}{\partial p_{\gamma_k}},\qquad \dot{p}_{\gamma_k}(t)=-\frac{\partial\mathcal{H}}{\partial\gamma_k}, \tag{4}$$

where the expectation value $\mathcal{H}=\langle\Psi|\hat{H}|\Psi\rangle$ is given by $\mathcal{H}=\mathcal{H}_\mathrm{ee}+\mathcal{H}_\mathrm{ei}+\mathcal{H}_\mathrm{ii}$ with

$$\mathcal{H}_\mathrm{ee}+\mathcal{H}_\mathrm{ei}=\sum_k\left(\frac{p_k^2}{2m}+\frac{p_{\gamma_k}^2}{2m}+\frac{9\hbar^2}{8m\gamma_k^2}\right)+\sum_{k<l}\frac{e'^2}{r_{kl}}\mathrm{erf}\left(\frac{r_{kl}}{\sigma_{kl}}\right)-\sum_{I,k}\frac{e'^2}{r_{Ik}}\mathrm{erf}\left(\frac{r_{Ik}}{\sigma_{Ik}}\right), \tag{5}$$

$\mathcal{H}_\mathrm{ii}=\sum_I P_I^2/2M+\sum_{I<J}e'^2/|\vec{R}_I-\vec{R}_J|$ and $r_{kl}=|\vec{r}_k-\vec{r}_l|$, $\sigma_{kl}^2=2\left(\gamma_k^2+\gamma_l^2\right)/3$, $r_{Ik}=|\vec{R}_I-\vec{r}_k|$, $\sigma_{Ik}^2=2\gamma_k^2/3$.

To avoid an infinite growth of the widths γ_k of unbound electrons, we confine every wave packet in an external harmonic-oscillator potential which moves together with the centre of mass of the electrons by adding $\hat{H}_{\mathrm{ext}} = \left(9\hbar^2/8m\gamma_0^4\right)\sum_k(\hat{\vec{x}}_k - \langle\hat{\vec{x}}_k\rangle)^2$ to equation (3). The parameter γ_0 adjusts the mean width of *unbound* electrons. It is usually chosen much larger than the typical width of a bound electron, e.g. in an atom or molecule. This 'confinement potential' results in an additional term $\mathcal{H}'_{\mathrm{ee}} = \left(9\hbar^2/8m\gamma_0^4\right)\sum_k \gamma_k^2$ in equation (5) and the corresponding Hamiltonian for *free* electrons thus takes the form

$$\mathcal{H}_{\mathrm{ee}} = \sum_k \left[\frac{p_k^2}{2m} + \frac{p_{\gamma_k}^2}{2m} + \frac{9\hbar^2}{8m\gamma_0^2}\left(\frac{\gamma_0^2}{\gamma_k^2} + \frac{\gamma_k^2}{\gamma_0^2}\right)\right]. \tag{6}$$

The width thus evolves dynamically according to the equations of motion, but now restricted to values about the minimum of the 'potential energy' $\left(9\hbar^2/8m\gamma_0^2\right)\left(\gamma_0^2/\gamma_k^2 + \gamma_k^2/\gamma_0^2\right)$ at $\gamma_k = \gamma_0$. For the present application, γ_0 was chosen as $\gamma_0 = 0.64\lambda_{\mathrm{th}}$ with the thermal wavelength $\lambda_{\mathrm{th}} = \hbar/(mk_{\mathrm{B}}T)^{1/2}$, see [4] for details. As was recently shown [6], such a confinement of the width and a resulting $\mathcal{H}_{\mathrm{ee}}$ like (6) can also be obtained in a more consistent way by appropriate additional phase factors of the wave packets (1).

Equations (4)–(6) are solved by the MD simulation technique as used and described in [11–14], here for $N = N_{\mathrm{i}} + N_{\mathrm{e}} = 500$ particles. The actual simulations are performed in the microcanonical ensemble. It is generated by a previous simulation which starts from random positions and velocities and relaxes towards the equilibrium distribution of desired temperature by dynamical propagation with velocity rescaling.

3. Results

The quantity of interest in the present study is the dynamic structure factor

$$S(k,\omega) = \frac{1}{N}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\langle\rho_k(t)\rho_k(0)\rangle, \tag{7}$$

where $\rho_k(t) = \sum_\alpha q_\alpha \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\alpha(t))$ is the microscopic fluctuating charge density. It is sampled for a given wave number k from the positions $\{\vec{r}_\alpha(t)\}$ ($\alpha = 1,\ldots,N$) of protons and electrons ($q_\alpha = \pm e$) during the simulation runs. For more details on the dynamic structure factor of a TCP see [11, 12, 14]. To determine $S(k,\omega)$ for a proton–electron TCP within the WPMD method, numerical simulations based on equations (4)–(6) have been performed for various densities and temperatures. Figure 1 shows results for $S(k,\omega)$ (left and centre) at different coupling parameters $\Gamma = e^2/(4\pi\epsilon_0 a k_{\mathrm{B}}T) = 0.5, 1$ and 2 ($a = (3/4\pi n)^{1/3}, n = n_{\mathrm{i}} = n_{\mathrm{e}}$) and fixed $T/T_{\mathrm{F}} = 7$, that is, for non-degenerate systems. The wave number is $k = 2\pi/L = 0.62a^{-1}$ which is the smallest accessible value for $N_{\mathrm{i}} = N_{\mathrm{e}} = 250$ protons and electrons in a box of volume L^3.

In the present implementation of the WPMD, quantum effects are entirely contained and described by the additional degrees of freedom $\gamma_k(t)$, $p_{\gamma_k}(t)$ associated with the variable widths of the (Gaussian) wave packets. This results in a replacement of the Coulomb interaction in the original Hamiltonian (2) by the effective interactions $V_{\mathrm{ee}} \propto \mathrm{erf}(r_{\mathrm{ee}}/\sigma_{\mathrm{ee}})/r$, $V_{\mathrm{ei}} \propto \mathrm{erf}(r_{\mathrm{ei}}/\sigma_{\mathrm{ei}})/r$ in the final equations of motion (4) and (5), with, however, fully time-dependent $\sigma_{\mathrm{ee}}, \sigma_{\mathrm{ei}}$ according to the time evolution of the widths $\gamma_k(t)$. The related equilibrium distributions of the width as sampled from $\gamma_k(t)$ during the WPMD simulation runs are plotted in the right panel of figure 1. They are concentrated about the minimum of the potential energy of equation (6), i.e. at $\gamma_0 = 0.64\lambda_{\mathrm{th}}$, and are almost identical in all given cases having only slightly different mean values $\langle\gamma\rangle$ (as denoted in the figure). These mean values are now taken for additional simulations with fixed $\gamma_k = \langle\gamma\rangle$. This corresponds to an entirely classical MD

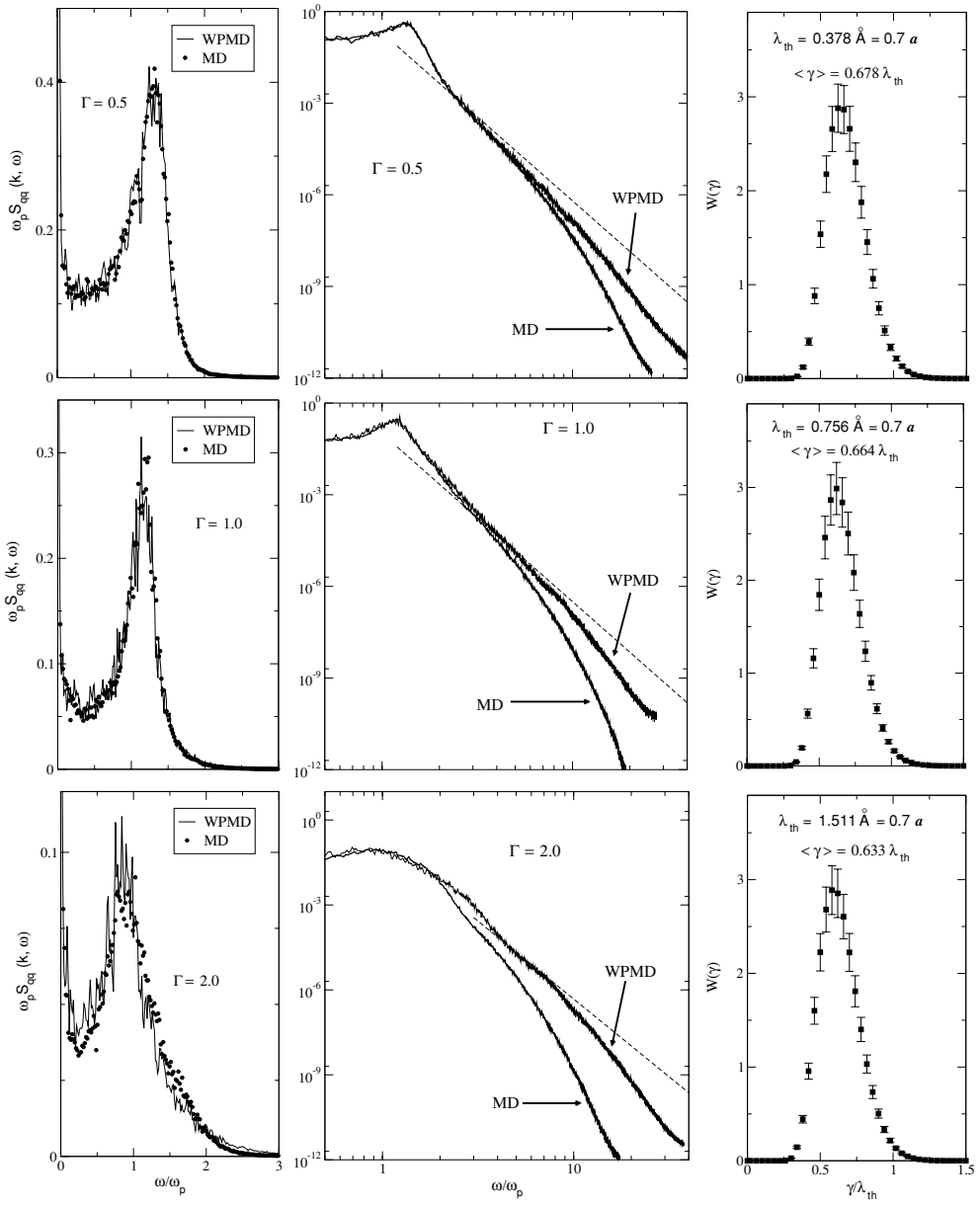

Figure 1. Left and centre: dynamic structure factor $S(k, w)$ for a proton–electron plasma as a function of ω in units of the electron plasma frequency ω_p at fixed degeneracy $T/T_F = 7$, wave number $k = 0.62a^{-1}$ and different coupling parameters $\Gamma = 0.5$ (top), 1 (centre) and 2 (bottom). Compared are results from the WPMD simulations and MD simulations using effective potentials. The dashed curves in the central panel show a functional dependency $\propto 1/\omega^{5.5}$ as expected for $S(k, w \to \infty)$ of a system with pure Coulomb interactions. Right: distribution $W(\gamma)$ of the widths γ (scaled in units of the thermal wave-length) of the wave packets as sampled from the WPMD simulations.

description of the TCP at hand using the effective interactions $V_{ee}(r) = e'^2 \mathrm{erf}(\sqrt{3}r/2\langle\gamma\rangle)/r$ between electrons and $V_{ei}(r) = -e'^2 \mathrm{erf}(\sqrt{3}r/\sqrt{2}\langle\gamma\rangle)/r$ between protons and electrons.

The resulting $S(k, \omega)$ is shown as well in figure 1 (left and centre). In the low frequency part $\omega \lesssim \omega_p$ (left panel), where the prominent plasmon peak shows up around the electron plasma frequency ω_p, the MD and WPMD agree almost perfectly within the fluctuations. For higher frequencies $\omega \gtrsim 2\omega_p$ (centre) and increasing coupling Γ, increasing deviations show up. Particularly interesting is here the observed slower decay of $S(k, \omega)$ at high frequencies in the WPMD treatment. For a TCP with the effective potentials of equation (5) and with fixed time-independent $\gamma_k = \langle\gamma\rangle$, theoretical studies [17] predict an asymptotic behaviour of the dynamic structure factor at high frequencies like $S(k, \omega) \sim \exp(-\alpha\omega)/\omega^{11/2}$ (with some numerical factor α), in very good agreement with the simulation results reported in [12]. For a real TCP with Coulomb interaction, the predicted asymptotic is $S(k, \omega) \sim \omega^{11/2}$ [17, 18], showing a much weaker and non-exponential decay. This asymptotic is expected to be observed in a fully quantum mechanical description of a proton–electron plasma. The present WPMD simulations clearly show a tendency towards this asymptotic behaviour. But to draw final conclusions on this issue, a more comprehensive simulation study with higher time resolution and better statistics is needed.

4. Discussion and conclusions

The presented results definitely indicate an increasing deviation of both simulation treatments starting at a certain frequency. We are thus looking for a typical frequency which separates a high frequency domain from the low frequency regime where time-independent effective potentials and the WPMD treatment coincide. As an estimate for this characteristic frequency in the case of the WPMD we consider the typical time scale for oscillations in the effective potential for the width, equation (6). Expanding $\left(9\hbar^2/8m\gamma_0^2\right)\left(\gamma_0^2/\gamma_k^2 + \gamma_k^2/\gamma_0^2\right)$ to second order in γ about its minimum at $\gamma_k = \gamma_0$ results in a characteristic frequency $\omega_\gamma^2 = 9\hbar^2/m^2\gamma_0^4$ which yields for the present choice and settings, i.e. $\gamma_0 = 0.64\lambda_{th}$ and $\lambda_{th} = 0.7a$ (corresponding to $T/T_F = 7$), the relation $\omega_\gamma/\omega_p \approx 6/\sqrt{\Gamma}$. This is in fairly good agreement with the frequencies which can be deduced from figure 1 (centre) as the point where the WPMD and the MD results start to deviate substantially.

Comparing the frequency dependence of the dynamic structure factor obtained by the WPMD approach and by MD simulations with time-independent effective potentials, we have explicitly shown that the time-dependent dynamically varying widths of the wave packets will strongly affect the high frequency, short-time behaviour of the density fluctuations. This starts at a characteristic frequency associated with the temporal variation of the width of the wave packets. It is assumed that the temporal variation of the actual wave-function(s) in a real quantum TCP will have a similar strong influence on the short-time dynamics. This supports that the method of time-independent effective potentials is in fact, as supposed, only appropriate to describe static properties of a quantum TCP or time-dependent processes at sufficiently low frequencies. In the high frequency domain or in truly dynamical situations, a more elaborate scheme is needed to map the required time-dependent quantum treatment into a classical dynamics. Based on a variational formulation of the Schrödinger equation, the concept of WPMD might be a promising candidate. But here further investigations are necessary.

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