QUASI-CLASSICAL THEORY AND SIMULATION OF TWO-COMPONENT PLASMAS

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PLASMA PARAMETER IN THE QUASI-CLASSICAL REGIME

Due to the long-range nature of Coulomb forces, the regime of quasi-classical behavior of plasmas is different from that of van der Waals gases. We consider here a two-component plasma (TCP) consisting of electrons of density n_e and ions of density n_i with the charges $-e$ or $+e$ respectively, in equilibrium at the temperature T. The quasi-classical regime is defined by the conditions

$$d \gg a_0, \quad d \gg \lambda_{ij}, \quad l \gg \lambda_{ij} \tag{1}$$

by using the characteristic length parameters

$$d = (3/4\pi n_e)^{1/3}, \quad l = (e^2/kT), \quad a_0 = (\hbar^2/me^2), \quad \lambda_{ij} = \hbar/(2m_{ij}kT)^{1/2} \tag{2}$$

Under these conditions, the free charges in a plasma may be treated by quasi-classical methods, while the bound states must always be treated quantum-mechanically. This concept was already developed by Planck and Brillouin [1].

QUASI-CLASSICAL PLASMA MODELS

A first description is provided by the Debye-Hückel theory in combination with a mass-action law on the basis of the Planck-Brillouin-Larkin partition function and an appropriate choice of the the effective diameter of the charges [2, 3]. The interaction energy per particle reads in this model

$$\epsilon_{int} = -\frac{e^2}{2(r_D + \lambda_{ie}\sqrt{\pi}/4)}, \qquad r_D = \frac{kT}{8\pi n_e e^2}. \tag{3}$$

In the quasi-classical regime, this model is consistent with the exact quantum-statistical calculations up to the order $O(\hbar)$ [2]. A special property of this model is the existence of a plasma-phase transition, which can be determined analytically [2]. The critical point is located at $T_c = (e^2/8ka_0)$ and $n_c = a_0^{-3}$.

Another widely used model for quasi-classical plasmas is based on the non-singular potential [4, 5, 7, 6],

$$V_{ij} = \frac{e_i e_j}{r} \left\{ 1 - \exp\left(-\frac{r}{R_{ij}}\right) \right\} . \tag{4}$$

By generalizing an early work by Kramers, Berlin and Montroll [8] were able to derive the exact free energy density as a function of $\Gamma = e^2/kTd$ under the assumption that $R_{ij} = O(V^{1/3})$. In our earlier papers [9, 10], we used the model of gauss-distributed charges. This relatively simple model can be derived from the method of wave packet dynamics (WPD) [11]. Under the assumption that the charge e_i is gauss-distributed with radius R_i, we obtain the interaction potential

$$V_{ij} = \frac{e_i e_j}{r} \operatorname{erf}\left(\frac{r}{R_{ij}}\right) , \qquad R_{ij}^2 = R_i^2 + R_j^2 . \tag{5}$$

For this potential, one can find a lower bound for the energy per charge that corresponds to a configuration, in which the Gaussian charges are surrounded by screening clouds of opposite charge concentrated around a common center. This leads to

$$\epsilon_i = -\frac{2e_i^2}{\sqrt{\pi} R_i} . \tag{6}$$

In our quasi-classical WPD simulations [9, 10], we used the effective radii

$$R_i^2 = r_0^2 = \frac{\hbar^2}{p_0^2} = \frac{3\hbar^2}{2\, m\, \epsilon_i^{ideal}} \tag{7}$$

Our results can be approximated by the semi-empirical Debye-Hückel-type equation for the interaction energy per charge

$$\epsilon_{int} = -\frac{e^2}{2r_D + r_0\sqrt{\pi}/2} \tag{8}$$

An even simpler quasi-classical model was treated by Norman et al. [17] on the basis of molecular dynamics.

COMPARISON WITH PATH-INTEGRAL SIMULATIONS

Already in [9], we could show for the OCP that quasi-classical WPD simulations with the potential (5) yield good agreement with the interaction energy obtained in the classical QMC work by Ceperley and Alder [12]. Now we will to compare results of our WPD simulations [10] for mass-symmetrical TCP with new path-integral Monte Carlo calculations (PIMC). PIMC simulations [13,14,15,16] have been proven to be a powerful and accurate technique to study the static properties of quantum systems. The comparison was performed in order to advance a dynamic simulations model, which can reproduce the essential PIMC results with a reasonable accuracy and which then can be used to study dynamic plasma properties. The interaction energies for two densities $n_e = 10^{22}\mathrm{cm}^{-3}$ and $n_e = 10^{23}\mathrm{cm}^{-3}$ and several temperatures are shown in figure 1, in which ϑ denotes the degeneration parameter $\vartheta = T/T_F$. We also included results from analytical approximations by means of Padé formulae [18] and the chemical picture (PACH) [3, 18]. The comparison shows a satisfactory agreement between the PIMC results and the PACH approximations. The WPD simulations shows qualitatively agreement with the other methods but the quantitative agreement is still not sufficing.
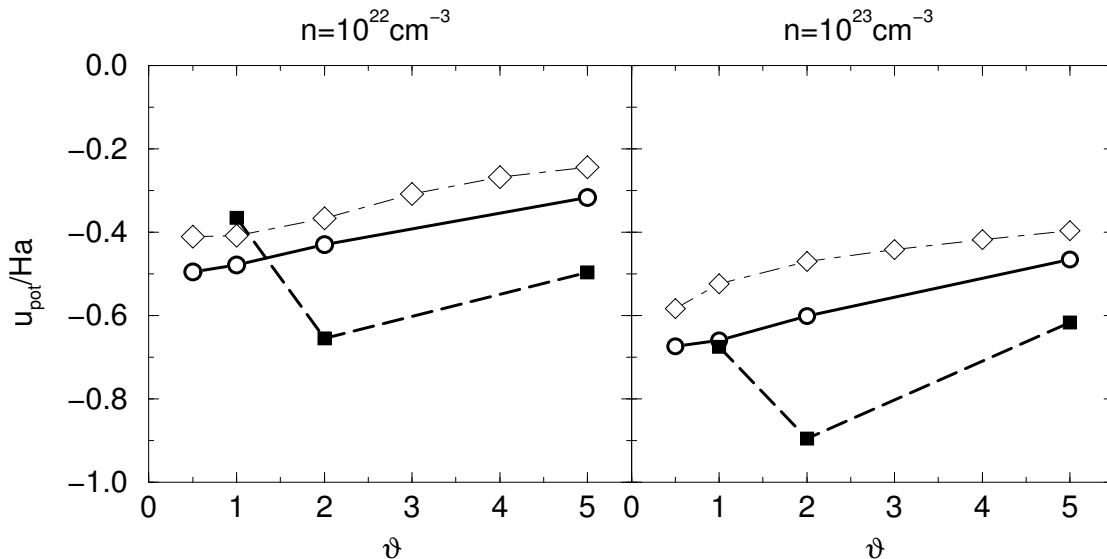
Figure 1. Interaction energy of the electron-positron plasma per pair of particles from wave packet dynamics simulations (dashed line), from path-integral Monte Carlo simulations (solid line) and Padé approximations in the chemical picture (dot-dash line) are compared at the two densities $n = 10^{22}$cm^{-3} ($T_F = 19\,600$ K) and $n = 10^{23}$cm^{-3} ($T_F = 91\,100$ K) as a function of $\vartheta = T/T_F$

This is partly caused by a too strong interaction potential eqn. (5,7). Hence, the agreement can be improved by adjusting the length parameter R_{pe}. In particular, this is true for the region where $d < \lambda < l$ corresponding to rather low densities and high temperatures. This point however needs a more careful investigation.

The pair correlation function for PIMC simulation are shown in figure 2. Comparing the correlation function for electrons with parallel and anti-parallel spins, one can study the effects of the Pauli exclusion principle, which is realized in PIMC by introducing nodal surfaces [14]. It leads to a stronger repulsion of electrons in the same spin state.

From the peak structure in the electron-positron correlation function in figure 2, one can deduce the existence of bound states [15,16]. The population of the ground state can be evaluated by studying the radial direct correlation function $r^2(g_{ep}(r) - 1)$, which is plotted in figure 3. The height of the peak is a direct measure of the number of bound electron-positron pairs. They dominate the structure in the left graph of figure 3 for the lower density, whereas the minor peak in the high density case is caused by the attraction of free electrons and positrons, which leads to Debye screening but not to binding. The effect of thermal ionization can be seen in the left graph of figure 3. The pressure ionization can be studied by comparing the low at high density graph. The reader should keep in mind that we compare at constant ϑ and not at constant temperature.

In conclusion, we state that the symmetrical two-component plasmas are a fairly useful system for testing the accuracy of analytical theories and numerical simulations. On the basis of our comparison, we deduce that the WPD method needs further improvements in order to achieve a level of correctness, which already has been reached for the electron gas.
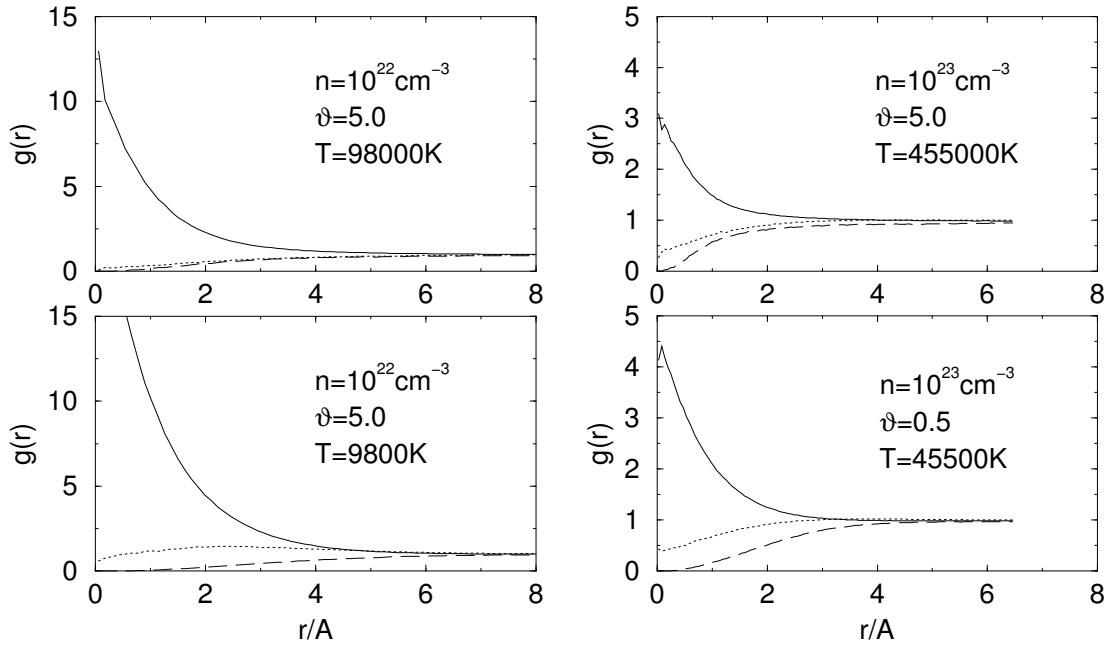
Figure 2. The pair correlation functions $g_{pe}(r)$ (solid line), $g_{ee\uparrow\downarrow}(r)$ (dotted line) and $g_{ee\uparrow\uparrow}(r)$ (dashed line) are shown for two different densities and ϑ values.
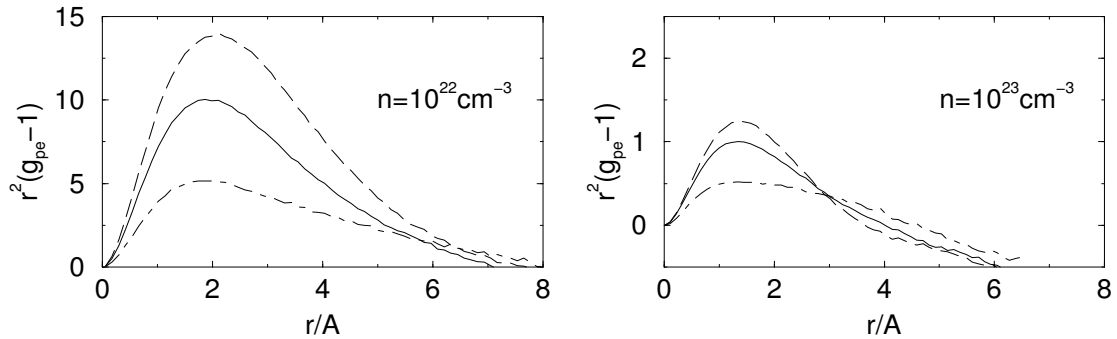

Figure 3. The direct radial electron-positron correlation function $r^2(g_{pe}(r) - 1)$ is shown for two different densities at $\vartheta = 5$ (dashed line), $\vartheta = 2$ (solid line) and $\vartheta = 0.5$ (dot-dash line). The strong peak in the left graphs corresponds to the population of ground state $\psi_0(r) \propto \exp(-r/2a_0)$.

REFERENCES

1. L. Brillouin, Statistique Quantique, Paris (1932); Russ. transl. Gostekhisdat Kiev (1934)
2. W. Ebeling, W.D. Kraeft, and D. Kremp, Theory of Bound States and Ionization Equilibrium in Plasmas and in Solids, Akademie-Verlag Berlin (1976)
3. D. Beule, W. Ebeling, A. Förster, Physica A (1997), in press
4. G. Kelbg, Ann. Physik 12:219 (1963); 12:354 (1964); 14:394 (1964)
5. C. Deutsch, Phys. Lett. A 60:317 (1977)
6. C. Deutsch, M. Gombert, and H. Minoo, Phys. Rev A 23:924 (1981)
7. J.-P. Hansen, and I.R. McDonald, Phys. Rev A 23:2041 (1981)
8. T.H. Berlin, and E.W. Montroll, J. Chem. Phys. 29:75 (1952)
9. W. Ebeling, and F. Schautz, Phys. Rev. E 56, N0 1 (1997)
10. W. Ebeling, B. Militzer, and F. Schautz, Contr. Plasma. Phys. 37:137 (1997)
11. D. Klakow, C. Toepffer, and P.-G. Reinhardt, Phys. Lett. A 192:55 (1994)
12. D.M. Ceperley, and B.J. Alder, Phys. Rev. Lett. 45:466 (1980)
13. D. M. Ceperley, Rev. Mod. Phys. 67:279 (1995).
14. D. M. Ceperley, Path integral Monte Carlo methods for fermions, *in* "Monte Carlo and Molecular Dynamics of Condensed Matter Systems", Ed. K. Binder and G. Ciccotti, Bologna, Italy (1996).
15. W. R. Magro, D. M. Ceperley , C. Pierleoni, and B. Bernu, Phys. Rev. Letts. 76:1240 (1996).
16. B. Militzer, W. Magro, and D. Ceperley, this volume.
17. G. Norman, A. Kaklyugin, and A. Valuev, this volume
18. H. Lehmann, and W. Ebeling, Phys. Rev. E 54:2451 (1996)