

# Formalism of compound particles for simulation of the heavy ions in a stationary nonequilibrium warm dense matter

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**Abstract.** The screened interaction potential between two compound particles, compound particle and charged particle (ion or electron) in multipole approximation for simulation of nonequilibrium warm dense matter are discussed. The density and temperature range has been considered at which the formalism of compound particles can be used. It is proposed that the presented screened potential can be useful for the simulation of the heavy ions in the presence of streaming electrons. Discussions about the implication of a compound particle picture for consideration of the dynamics of the beam of the charged particles in plasmas are given. The proposed model of interaction between heavy ions consists of dipole terms and the short range repulsion due to the Pauli exclusion principle.

## 1. Introduction

Plasma consists of different particles types both charged and neutral. Usually, different species of particles have a large difference in physical properties such as mass and charge. The difference in the mass between particles of different species, e.g between electron and ion in usual two component plasma, leads to the different characteristic time scales of plasma components. In this regard, the subsystem of particles with similar values of the mass and charge can be considered within so called one component plasma model with neutralizing background. In the case of the weak electron-ion coupling, the electrons can be treated within linear response theory and the ions by molecular dynamics or Monte-Carlo simulation as has been proposed by Ludwig et al. [1]. This approach is also useful for the simulation of so called complex or dusty plasma (see, for example, [5] and references therein) where the subsystem of strongly coupled nano- or micro-sized dust particles with ideal electrons and ions as a background can be investigated in the framework of the one component plasma model. The idea of Ludwig et al. [1] has been used by Graziani et al. to decouple the electron kinetic equation using the Singwi-Tosi-Land-Sjölander scheme [2] or a recently derived extension [3,4].

For simulation of the heavy component of the plasma, which can be nonideal, the collective screening effect due to mobile component (electrons) of plasma has to be taken into account properly in the effective screened interaction potential [6,7]. The effective screened interaction

potentials can be obtained by methods based on the kinetic equations and the formalism of the dielectric response function. However, these methods are not useful for derivation of the screened potential if considered particles have a dipole moment, as a dipole field does not have spherical symmetry. In the recent work [8] it has been shown that the multipole expansion method allows to find screened interaction potentials between compound particles with dipole moments, if one knows the screened potential of single charged particle at a given plasma parameters. In this case the problem of finding the effective interaction potential is reduced to the problem of finding derivatives.

In this paper some problems related to the calculation of the screened interaction potential between particles with non zero dipole moment by standard way are discussed and the formalism of the compound particles for the simulation of the heavy component of the plasma in presence of the streaming of particles of mobile component relatively to the inert ones are proposed. We consider interaction model of heavy ions in the presence of streaming electrons in warm dense matter and in the case when ion beam penetrates into the plasma. The temperature and density range is discussed at which the formalism of compound particles is applicable.

## 2. Interaction potential between compound particles in nonequilibrium plasmas

The key of the multiscale approach is to absorb the fast particle kinetics into the effective screened interaction potential  $\Phi$  of the heavy particles with charge  $Q$  where the screening is provided by the mobile particles (electrons in two component plasma) via a dielectric function  $\epsilon$ , e.g. [1]

$$\Phi(\mathbf{r}) = \int \frac{d^3k}{2\pi^2} \frac{Q^2}{k^2 \epsilon(\mathbf{k}, \omega = 0)} e^{i\mathbf{k}\cdot\mathbf{r}} \quad , \quad (1)$$

taken in the static limit. The effect of streaming electrons (ions) is important in warm dense matter. Then one have dynamically screened potential and the frequency argument becomes  $\omega = \mathbf{k}\mathbf{u}$  which leads to wake effects, that are well investigated theoretically and experimentally for dusty plasmas, e.g. [9–11] and quantum plasmas, e.g. [12] and references therein.

In the case of quantum plasmas, an accurate calculation of dynamically screened potential of an ion takes from few minutes for zero temperature limit up to several hours for finite temperature case. Therefore it is important to have simple analytical model which takes into account wake effect for simulation of the inert particles in nonequilibrium plasma. Such interaction model can be proposed knowing properties of the dynamically screened potential.

### 2.1. Dynamically screened ion potential in two component quantum plasmas

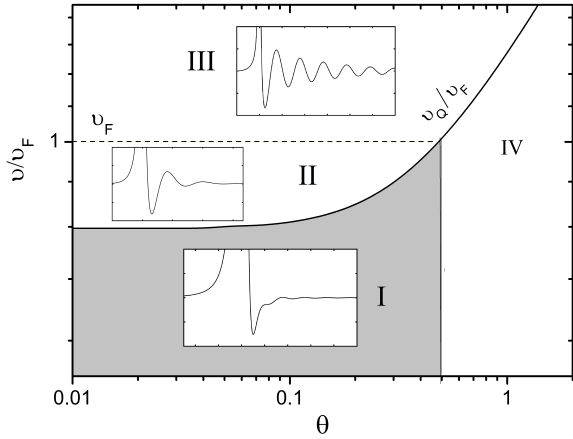
Recently, we have done detailed analysis of the dynamically screened ion potential in warm dense matter and dense plasmas [12–14] as a function of the electrons degeneracy parameter and so called streaming parameter (Mach number) which is in fact dimensionless velocity of streaming electrons or of the ion penetrating into plasma. In particular, the transition from the high temperature regime (classical) to the low temperature regime (quantum) was investigated. Strong deviations from the static Yukawa type potential [6] as well as a possibility of an attraction between like-charged ions were shown. The conditions have been found at which streaming of the plasma background is giving rise to a dynamically screened charge field with a negative trailing potential minimum behind considering ion, which may lead to the attraction between like-charged ions. The physical mechanism is that the streaming fast particles gives rise to a deflection of the latter and, eventually, to an excess density behind the test particle. This interpretation was directly confirmed by computing the electron density perturbation which reveals a clear enhancement behind the ion [12]. In figure 1 the summary of the analysis of dynamically screened ion potential is presented at  $(u/u_F; \theta)$  plane in the form of the diagram, where  $u_F$  is the Fermi velocity,  $u$  electrons streaming velocity (or projectile velocity), and

$\theta = k_B T / E_F$  is the degeneracy parameter of electrons. In figure 1 the characteristic quantum velocity reads:

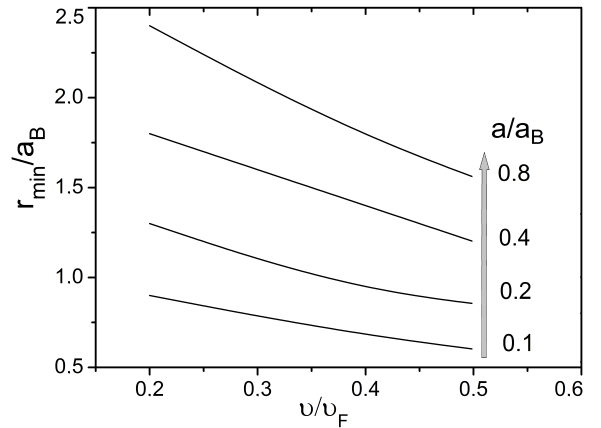
$$v_Q^2 = \frac{2 \langle K \rangle_Q}{m} = \frac{3}{2} v_F^2 \theta^{5/2} \int_0^\infty dy \frac{y^{3/2}}{\exp(y - \beta\mu) + 1}. \quad (2)$$

This diagram was recently used with a special focus on anomalous wake effects [13]. Here we use this diagram to present at which parameters the formalism of compound particles can be used. In the regions II and III, the dynamically screened potential has oscillations with more than one negative minima. In these regions the dynamically screened potential probably can not be presented by a relatively simple analytical formula. In the region IV, the dynamically screened potential can have negative minimum, but the distance between the ion and this negative minimum is more large than the mean interparticle distance (if neglect Friedel oscillations [12]). In this region, the screening length behind and ahead of the ion different from each other and rescaling of the screening length can be used [15–18]. In the region I the ion wake field possesses only one main potential minimum. *At these plasma parameters we have a positively charged point like ion and a negatively charged cloud of the focused electrons. One can consider this as one compound particle with non zero total charge and dipole moment.* Therefore, in the region I, the dynamically screened ion potential can be replaced by the statically screened potential of a compound particle.

In figure 2 the distance between an ion and a negative trailing potential minimum behind considering ion for different values of the mean interparticles distance of electrons  $a = (4\pi n_e/3)^{-1/3}$  as a function of the streaming velocity (or projectile velocity) at  $\theta = 0.01$  is shown. With increase of the degeneracy parameter up to  $\theta \simeq 0.1$  this distance remains nearly constant [12]. Further increase in the degeneracy parameter up to  $\sim 0.5$  can increase the distance from an ion to the negative minimum of the dynamically screened ion potential no more than 1.5 times [12, 13].



**Figure 1.** In the region I the ion wake field possesses only one main potential minimum and the dynamically screened ion potential can be replaced by statically screened potential of the compound particle.



**Figure 2.** Distance from ion to the negative minimum of the dynamically screened ion potential for different values of the ratio of the mean interparticle distance of the electrons to the first Bohr radius at  $\theta = 0.01$ .

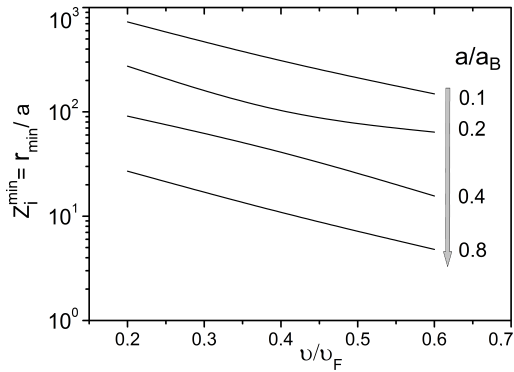
From quasi-neutrality condition, for density of ions we have  $n_i = n_e / Z_i$ , where  $Z_i$  is the ion charge in units of the electron charge (ion charge number). For applicability of the compound particle formalism within multipole approximation the mean distance between ions has to be

larger than the linear size of the compound particle. Therefore, we have condition:

$$Z_i \gg (r_{\min}[v, \theta]/a)^3, \quad (3)$$

here it is emphasized that  $r_{\min}$  depends on both streaming velocity  $v$  and the degeneracy parameter of the electrons  $\theta$ .

In figure 3, minimal values of the heavy ion charge  $Z_i^{\min}$  obtained from equation (3) are presented. As it was mentioned, the formalism of compound particles can be used when  $Z \gg Z_i^{\min}$ . In experiments on warm dense matter, the ion charge can be of order ten. Therefore, as it is seen from figure 3, the formalism of compound particles is justified if  $a/a_B \gtrsim 0.8$  (here  $a$  is the electrons mean interparticle distance). This corresponds to the number density of electrons  $n_e \gtrsim 3 \times 10^{23} \text{cm}^{-3}$ . The temperature of the electrons related to the degeneracy parameter and mean interparticle distance as  $T \simeq \frac{\theta}{(a/a_B)^2} 0.58 \times 10^6 (K)$ . Using this relation one can obtain the maximum value of the temperature  $T_{\max} \sim 4.5 \times 10^5 K$  up to which the formalism of compound particles can be used.



**Figure 3.** The minimal value of the heavy ion charge  $Z_i^{\min}$  obtained from equation (3) at different values of  $a/a_B$ .

Up to now, the interaction between ions in the presence of streaming electrons has been considered. In the case of the ion beam – plasma interaction, the density of the beam ions  $n_i^{\text{beam}}$  much less than that of plasma  $n_e$  (electrons). As the result, the formalism of compound particles can be used at higher densities of the plasma for simulation of the interaction of beam ions with each other and with the plasma ions. In this case the following condition must be satisfied :

$$\frac{n_i^{\text{beam}}}{n_e} \ll (r_{\min}[v, \theta]/a)^3. \quad (4)$$

In the high energy ion beam experiments, the ion beam density can be up to  $n_i^{\text{beam}} \sim 10^{14} \text{cm}^{-3}$  [20]. From data presented in figure 3 it is clearly seen that in the case of the ion beam – plasma interaction the formalism of compound particles can be used almost at any plasma density if  $\theta = k_B T/E_F \leq 0.5$ .

## 2.2. Screened interaction potential between compound particles with the strong repulsion at short distance

After consideration plasma parameters at which the formalism of compound particles can be used, we turn to the model of interaction between compound particles with nonzero total charge and dipole moment. As it has been discussed, the formalism of compound particles can be used for the simulation of the heavy ion component with  $Z_i > 1$ . In this case a strong additional repulsion between ions due to bound electrons must be taken into account [19,21]. This repulsion between ions appears at short distance as a result of the Pauli exclusion principle when shells of ions start to overlap. In [21] the following screened ion-ion interaction potential with a strong

repulsion at short distance for the simulation of the ion component of an equilibrium warm dense matter was proposed:

$$\Phi_Y(r; n, T) = \frac{Z_i e}{r} e^{-k_Y r} + \frac{a}{r^6}, \quad (5)$$

here  $a$  defines the strength of short range repulsion and can be understood as a radial extension of the ion,  $k_Y^2 = k_{TF}^2 \theta^{1/2} I_{-1/2}(\eta)/2$  is the screening length which interpolates between Debye and Thomas-Fermi expansions,  $I_\nu$  is the Fermi integral of order  $\nu$ ,  $\eta = \mu/k_B T$  is the chemical potential of electrons, and  $\theta = k_B T/E_F$  is the degeneracy parameter which defines whether plasma degenerate or classical.

In the case of nonequilibrium warm dense matter, the interaction potential between compound particles has additional terms which responsible for charge-dipole and dipole-dipole interactions. Screened interaction potential between compound particles with additional dipole terms was derived in recent work [8]. Using this potential and adding the short range repulsion we have:

$$\begin{aligned} \Phi(\mathbf{R}) = & \frac{Q_1 Q_2}{R} \exp(-Rk_Y) + \frac{(Q_2 \mathbf{d}_1 - Q_1 \mathbf{d}_2) \cdot \mathbf{R}}{R^3} (1 + Rk_Y) \exp(-Rk_Y) + \\ & + \frac{[(\mathbf{d}_1 \mathbf{d}_2) R^2 - (\mathbf{d}_1 \mathbf{R})(\mathbf{d}_2 \mathbf{R}) (3 + Rk_Y)] (1 + Rk_Y) + (\mathbf{d}_1 \mathbf{R})(\mathbf{d}_2 \mathbf{R}) Rk_Y}{R^5} \exp(-Rk_Y) + \frac{a}{r^6}. \end{aligned} \quad (6)$$

here  $Q_1$  and  $Q_2$  are charges of ions under consideration.

In the case of parallel dipole moments of compound particles (expected in the case of stationary nonequilibrium state), additional dipole-dipole interaction leads the stronger repulsion in perpendicular to dipole moment direction in comparison with the Yukawa potential without dipole terms [22]. In parallel to dipole moment direction, the screened interaction potential has region with attraction between compound particles [8]. In this direction, the short range repulsion  $\sim 1/r^6$  prevents collapse due to dipole-dipole attraction.

The repulsion constant  $a$  was determined fitting the structure factor obtained from density functional theory by hypernetted chain calculation or molecular dynamics simulation on the basis of potential (5). The value of  $a$  obtained for equilibrium case can be used for nonequilibrium warm dense matter as a repulsion due to quantum symmetry effect does not affected by dynamic screening. The value of the dipole moment depends on the electron stream velocity or projectile velocity and can be obtained by fitting the depth and position of the negative minimum of the dynamically screened ion potential. The maximum absolute value of the depth of the negative minimum for considering parameters (region I in figure 1) is of order  $\sim Z_i^2 \times 0.1 [Ha]$  in atomic units (see figure 5 (a) in [12]).

### 3. Conclusion

We have proposed the interaction model between heavy ions within formalism of compound particles for simulation of stationary nonequilibrium warm dense matter. This model can be used, for example, in the simulation of the ions using molecular dynamics. The proposed model has two parameters the dipole moment  $d$  of the compound particle and the radial extension  $a$  of the heavy ion. The radial extension for a silicon ion was considered in [19, 21]. The dipole moment can be varied taking into account the maximal absolute value of the negative minimum obtained from calculation of the dynamically screened ion potential. The density and temperature range at which the formalism of compound particles can be used has been discussed. It has been shown that the density and temperature have to be  $n_e \lesssim 3 \times 10^{23} cm^{-3}$  and  $T \lesssim 4.5 \times 10^5 K$ , respectively. Additionally, the degeneracy parameter has to be  $\theta \leq 0.5$ . These parameters corresponds to the warm dense matter regime.

The formalism of compound particles was used successfully for understanding properties of the charged dust particles in complex plasmas [23–29]. In the case of the complex plasma, the negatively charged dust particle injected into the plasma with streaming ions creates a focused ion cloud [24, 25] and the dust particle together with the ion cloud can be considered as one compound particle [26]. It was shown that additional charge-dipole and dipole-dipole interaction has strong impact on both structural and dynamical properties of the dusty plasma [22, 27–29]. Therefore, it is expected that the formalism of compound particles can be useful for the investigation of the warm dense matter.

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