Parametrization of pair correlation function and static structure factor of the one component plasma across coupling regimes

N. Desbiens, P. Arnault, J. Clérouin

CEA, DAM, DIF, F-91297 Arpajon, France.

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We present a parametrization of the pair correlation function and the static structure factor of the Coulomb one component plasma (OCP) from the weakly coupled regime to the strongly coupled regime. Recent experiments strongly suggest that the OCP model can play the role of a reference system for warm dense matter. It can provide the ionic static structure factor that is necessary to interpret the x-ray Thomson scattering measurements, for instance. We illustrate this with the interpretation of a x-ray diffraction spectrum recently measured, using a Bayesian method that requires many evaluations of the static structure factor to automatically calibrate the parameters. For strongly coupled dusty plasmas, the proposed parametrization of the Coulomb OCP pair correlation function can be related to the Yukawa one, including screening. Further prospects to parametrize the static structure of Yukawa systems are also discussed.

A realistic description of hot dense plasmas requires a model that includes all many-body interactions explicitly in contrast to weakly coupled plasmas that are well represented by only binary collisions and mean-field effects. This regime is characterized by strong interactions between ions, outweighing their thermal kinetic energy and leading to a liquid-like structure. Such strongly correlated plasmas are found in a variety of environments including planetary interiors, dwarf stars, and neutron star crusts in astrophysics, and in many experimental set-ups of dusty plasmas, colloidal suspensions, and warm dense matter (WDM) in inertial confinement fusion studies. Liquid metals are also another manifestation of high Coulomb coupling in nature.

In strongly coupled plasmas, the many-body interactions are not amenable to a theoretical approach in perturbation since there is no small parameters available. Besides very demanding state-of-the-art molecular dynamics simulations, a possible modeling comes through the definition of simpler idealized systems. These reference systems can be studied extensively by molecular dynamics once and for all, with results easily available through parametrizations and/or tabulations. The Coulomb and Yukawa one-component-plasma (OCP) systems are good candidates of such reference models.

The Coulomb OCP represents a system of interacting ions, with the pair potential $V_C(r) = Qe/r$, in a neutralizing uniform background of electrons. All its static and dynamic properties depend on only one parameter, the Coulomb coupling parameter $\Gamma = Q^2e^2/ak_BT$, where $Q$ is the ionic charge, $T$ is the temperature, and $a = (4\pi n/3)^{-1/3}$ is the Wigner-Seitz radius ($n$ is the ionic density). The Coulomb coupling parameter $\Gamma$ is a measure of the importance of correlation in plasmas as the ratio of the mean nearest neighbor interaction to the mean kinetic energy. The ideal gas-like behavior corresponds to $\Gamma \ll 1$, liquid-like short-range order appears when $\Gamma \approx 1$, and crystalline long-range order when $\Gamma \geq 180$. Analytic parametrizations in $\Gamma$ are available for the equation of state\textsuperscript{11,12} and the ionic transport coefficients, viscosity\textsuperscript{13,14} and diffusion\textsuperscript{15,16}. Interestingly, when the plasma is partially ionized, the coupling parameter $\Gamma$ can stay constant along isochores as a result of the increase of ionization compensating the increase of temperature\textsuperscript{15,16}. In plasma mixtures, the coupling parameter $\Gamma$ may be different for each species giving rise to interesting coexistences between different coupling regimes\textsuperscript{21–23}.

In the Yukawa model, the polarization of the electrons close to each ion is accounted for by a screened potential $V_Y(r) = Qe \exp(-\kappa r)/r$, where $\kappa$ is an inverse screening length. This form of the pair potential originates from a linear response treatment of the electron gas in presence of a test charge, in the small wave number (long distance) limit\textsuperscript{24} for given values of ionization, temperature, and density.

Here, we address the static structure of dense plasmas, as revealed by the pair distribution function (PDF) $g(r)$ and the static structure factor (SSF) $S(k)$\textsuperscript{25}. The PDF gives the proportion of ions around a given ion as a function of their distance, with respect to the uniform distribution of a non-interacting system. The effect of repulsive interactions on the PDF is to create a correlation void at small distance, and corresponding peaks at larger distances reflecting the emerging shell structure, that ultimately forms the crystal lattice at solidification. The PDF is an input data in different theoretical frameworks: the variational theory of fluid\textsuperscript{26,27}, the thermodynamic integration for the equation of state; the quasi-localized charge approximation\textsuperscript{38,39} for the study of wave dispersion\textsuperscript{40} in strongly coupled plasmas. This structural information is also directly observable in dusty plasma experiments\textsuperscript{41} whereas the SSF $S(k)$, representing the Fourier content of $g(r)$, is probed by neutron and x-ray diffraction in WDM.

Despite many theoretical efforts to find analytical approximations of the OCP static structure from the integral equations of fluid theory\textsuperscript{9,25,31} accurate enough SSF are only available as tabulations produced in the 80s\textsuperscript{32}. An alternative approach consists in using brute force to parametrize results of microscopic simulations. Recently,
Ott et al. performed large scale molecular dynamics simulations to extract analytic fits for the height of the first peak $g_{\text{max}}$ of the Coulomb and Yukawa PDFs $g(r)$ and the radius of the correlation hole $r_{1/2}$, defined as the nearest distance to an ion where $g(r) = 1/2$, reflecting the mutual repulsion of ions at short distance.

In this paper, we present a parametrization of the PDF and the SSF of the Coulomb OCP, as functions of the Coulomb coupling parameter $\Gamma$, based on extensive molecular dynamics simulations covering the whole fluid phase across coupling regimes ($0 \leq \Gamma \leq 180$). The PDF of the Yukawa system depends on the screening parameter $\kappa$ in addition to the coupling parameter $\Gamma$. Nevertheless, a correspondence between the Coulomb and Yukawa PDFs was evidenced recently. It defines an effective coupling parameter $\Gamma_{\text{eff}}$, depending on $\Gamma$ and $\kappa$, that produces almost the same PDF. Indeed, we shall see that our parametrization of the OCP PDF can be used as well for the Yukawa systems.

The paper is organized as follows. The molecular dynamics simulations are first described in Sec. II. Then, the parametrizations of PDF (Sec. III) and SSF (Sec. IV) are presented and their accuracy is assessed by direct comparison with simulations. Further constraints are also examined with the calculations of the equation of state using either the PDF or the SSF (Sec. V). The relationship between Yukawa and OCP static structures is illustrated in Sec. VI by the comparison of PDFs and SSFs corresponding to the same effective coupling parameter $\Gamma_{\text{eff}}$, with emphasis on the limitations of the present parametrization of $\Gamma_{\text{eff}}$ in the weak to moderate coupling regime. Finally, an example is given in Sec. VII of the usefulness of our parametrization in the interpretation of x-ray Thomson scattering measurement. In this example, we use a Bayesian method to quantify the accuracy of this OCP-based representation of the ion feature. Lastly, a summary and some prospects to extend the parametrization to the Yukawa system are presented in the conclusion (Sec. VIII).

### I. MOLECULAR DYNAMICS SIMULATIONS

We used the ESPRESSO code to perform molecular dynamics simulations of the Coulomb OCP. This code allows one to use reduced units. In our simulations, the space variable $r$ is scaled by the Wigner-Seitz radius $a$, leading to a constant density of $n = 3/4\pi$. The time unit is the inverse plasma frequency $\omega_p^{-1} = [4\pi n Q^2 e^2/m]^{-1/2}$, where $m$ is chosen as the unit of mass for the ions. When the energy unit is chosen as $k_B T$, the pair potential energy reduces then simply to:

$$U_C(r) = \frac{\Gamma}{r}. \quad (1)$$

We placed $N$ ions in a cubic box, that is periodically duplicated in each direction. Their dynamics is followed solving the Newton equations by a velocity Verlet algorithm with (NVT ensemble) or without (NVE ensemble) a Berendsen thermostat. The long-range Coulomb forces between the ions, including their periodic images, are computed using the particle-particle-particle-mesh method that scales as $N \log N$. This method, also known as the P3M method, is efficiently parallelized in the ESPRESSO code, using one-dimensional fast Fourier transforms.

After an equilibration of the system in NVT ensemble during $100 \omega_p^{-1}$, the PDF and the SSF are collected and averaged in NVE ensemble over a duration of $1000 \omega_p^{-1}$. Without thermostat (NVE), we also collect the velocity autocorrelation functions for a future study. As the temperature fluctuates in NVE, the targeted coupling is realized with a relative accuracy of $\Delta \Gamma/\Gamma = 1\%$. The Table I gives for the different values of the coupling parameter $\Gamma$, the number $N$ of ions and the time step $\tau$ used. Finite size effects have been checked by varying the timestep and the number of particles.

| $\Gamma$ from to step | $N$ | $\tau$ ($10^{-3}\omega_p^{-1}$) |
|-----------------------|-----|-------------------------------|
| 0.04 0.09 0.01 | 15000 | 1 |
| 0.1 0.9 0.1 | 15000 | 1 |
| 1 4 0.15 | 2500 | 5 |
| 5 155 5 | 2500 | 5 |

**TABLE I:** Ranges of Coulomb coupling parameter $\Gamma$ studied in this work together with the number of particles $N$ and the timestep $\tau$ used in the MD simulations ($\omega_p$ is the plasma frequency).

### II. PAIR DISTRIBUTION FUNCTION

We used different functional forms to parametrize the PDF $g(r)$ at weak and strong couplings. For Coulomb coupling parameter $\Gamma$ less than 5, the weak coupling form $g_{\text{weak}}(r)$ contains a non-linear Debye-Hückel contribution whereas at higher coupling, the strong coupling form $g_{\text{strong}}(r)$ accounts for the oscillations after the first peak of $g(r)$ and their attenuations. The latter form is inspired from the works of Matteoli, Mansoori, and Lai et al.

$$g_{\text{weak}}(r) = \begin{cases} g_{\text{weak}}(r) & \text{for } \Gamma \leq 5, \\ g_{\text{strong}}(r) & \text{otherwise,} \end{cases} \quad (2a)$$

$$g_{\text{weak}}(r) = e^{-\frac{r}{\lambda(r)}} + \frac{\lambda(r)}{\lambda(r)} (2b)$$

$$g_{\text{strong}}(r) = \begin{cases} \sigma \cdot e^{-\mu(-x)^r} & \text{for } x \leq 0, \\ 1 + (\sigma - 1) \cdot \frac{\cos(\alpha x + \beta \sqrt{x})}{\cos(\alpha x)} & \text{otherwise,} \end{cases} \quad (2c)$$
parameters of strong coupling are:

$$\begin{align*}
\zeta &= 1.634 + 7.934 \times 10^{-3} \sqrt{\Gamma} + \left( \frac{1.608}{\Gamma} \right)^2, \\
\sigma &= 1 + 1.093 \times 10^{-2} (\ln \Gamma)^3, \\
\mu &= 0.246 + 3.145 \Gamma^{3/4}, \\
\nu &= 2.084 + \frac{1.706}{\ln \Gamma}, \\
\alpha &= 6.908 + \left( \frac{0.860}{\Gamma} \right)^{1/3}, \\
\beta &= 0.231 - 1.785 e^{-\Gamma/60.2}, \\
\gamma &= 0.140 + 0.215 e^{-\Gamma/14.6}, \\
\delta &= 3.733 + 2.774 \Gamma^{1/3}, \\
\epsilon &= 0.993 + \left( \frac{33.0}{\Gamma} \right)^{2/3}.
\end{align*}$$

III. STATIC STRUCTURE FACTOR

The SSF $S(k)$ is related to the Fourier transform of the correlation function, $h(r) = 1 - g(r)$, by the following relation:

$$S(k) = 1 + n \int dr \, e^{-i k \cdot r} [g(r) - 1].$$

In the reduced units introduced in Sec. III, an integration over angles leads to the quadrature to be used with our
parametrization:

\[ S_i(k) = 1 + 3 \int_0^\infty r^2 [g(r) - 1] \frac{\sin(kr)}{kr} \, dr. \] (6)

In the latter equation, and in the following, the wave number \( k \) is in units of \( a^{-1} \).

In order to prevent artificial oscillations occurring in the quadrature at low \( k \) for high values of \( \Gamma \) and to recover the low-\( k \) behavior \( k^2/(k^2 + 3\Gamma) \), the SSF calculation is slightly modified according to:

\[
S_{\text{fit}}(k) = \begin{cases} 
S_H(k) & \text{if } \Gamma \geq 60, \\
S_L(k) & \text{otherwise},
\end{cases}
\] (7a)

\[
S_H(k) = \begin{cases} 
S_i(k) & \text{if } k \geq k_m, \\
S_{\text{high}}(k) & \text{otherwise},
\end{cases}
\] (7b)

\[
S_L(k) = S_i(k) \cdot W(k) + S_{\text{low}}(k) \cdot (1 - W(k)),
\] (7c)

\[
S_{\text{high}}(k) = \frac{S_m \left( \frac{k}{k_m} \right)^2}{1 + \omega \cdot (k - k_m)^2},
\] (7d)

\[
S_{\text{low}}(k) = \frac{k^2}{k^2 + 3\Gamma},
\] (7e)

\[
W(k) = \frac{1}{2} \left( 1 + \tanh \left( \frac{k - k_t}{\delta k} \right) \right),
\] (7f)

The good agreement of the parametrized SSFs with the ones obtained in simulations is illustrated for five values of \( \Gamma \) spanning weak to strong coupling in Fig. 4. The average and maximum discrepancies between the parametrization and the simulation results as functions of \( \Gamma \) are also reported in Fig. 5. The mean with respect to \( \Gamma \) of the average and maximum discrepancies are \( 1.7 \times 10^{-3} \) and \( 3.3 \times 10^{-2} \).

The height \( S_{\text{max}} \) of the first peak of the SSF can be
FIG. 6: Relative deviations in percent between reduced excess internal energy $U_{ex}$, per particle in unit of $k_BT\Gamma$, obtained in the simulations and computed using the parametrization of the pair distribution functions (red plus) or the static structure factors (black circles), for each studied value of the coupling parameter $\Gamma$.

fitted as a function of $\Gamma$ by:

$$S_{\text{max}} = 1 + 5.86 \times 10^{-3} \ln (\Gamma + 1)^{3.56},$$

with a maximum error of 0.039 and an average error of $1.5 \times 10^{-4}$.

IV. EQUATION OF STATE

We further assess the accuracy of the parametrization of the PDF and the SSF by computing the reduced excess internal energy $U_{ex}$ per particle in unit of $k_BT\Gamma$. It is related to the Coulomb interaction energy $U_C$, that is obtained directly from simulations, according to:

$$U_{ex} = -\frac{U_C}{N k_BT\Gamma}.$$  \hspace{1cm} (10)

This coulomb energy can also be computed from the PDF $g(r)$ or the SSF $S(k)$ with:

$$\frac{U_C}{N} = n \int dr \ U_C(r) \ [g(r) - 1],$$  \hspace{1cm} (11)

$$= \frac{1}{2} \int \frac{dk}{(2\pi)^d} \ U_C(k) \ [S(k) - 1].$$  \hspace{1cm} (12)

Using the reduced units introduced in Sec. I, these expressions simplify to:

$$U_{ex} = -\frac{3}{2} \int_0^{\infty} r \ [g(r) - 1] \ dr,$$  \hspace{1cm} (13)

for the PDF route and to:

$$U_{ex} = -\frac{1}{\pi} \int_0^{\infty} [S(k) - 1] \ dk,$$  \hspace{1cm} (14)

for the SSF route. The Figure 6 shows the relative deviations between the excess energy $U_{ex}$ obtained from the simulation results and computed with the parametrization following the PDF-route (Eq. 13) or the SSF-route (Eq. 14). In average, the relative accuracy is around 1-2%. This gives a supplemental measurement of the quality of the fitted PDF and SSF proposed in this work.

V. YUKAWA STATIC STRUCTURE

The Yukawa static structure depends on two parameters: the Coulomb coupling parameter $\Gamma$ and the screening parameter $\kappa$. This renders any parametrization of the PDF and the SSF more complicated than in the case of the OCP static structure that only depends on $\Gamma$. A promising way to circumvent this difficulty was recently advanced by Ott et al. with the definition of an effective coupling parameter $\Gamma_{\text{eff}}$ that establishes a correspondence between the PDFs of the OCP and Yukawa systems, at least at short-range. This effective coupling parameter $\Gamma_{\text{eff}}$ was parametrized as a function of $\Gamma$ and $\kappa$ according to:

$$\Gamma_{\text{eff}} = \left(1 - 0.309 \kappa^2 + 0.0800 \kappa^3\right) \Gamma,$$  \hspace{1cm} (15)

for $0 \leq \kappa \leq 2$ and $1 \leq \Gamma_{\text{eff}} \leq 150$.

The Figure 7 shows that the PDFs of the Coulomb and Yukawa systems corresponding to the same value of the effective coupling parameter $\Gamma_{\text{eff}}$ are indeed quite close to each others. However, there is still room for improvements especially at low coupling where the parametrization of $\Gamma_{\text{eff}}$ is extrapolated.

Actually, this correspondence between the Coulomb and Yukawa systems is no longer possible for the long-range correlations, as revealed in the limit of vanishing wave number of the SSFs (see Figure 8). This was expected since the value of the SSF in this limit is proportional to the compressibility of the system, which
effective coupling parameter $\Gamma$ between their static structure through the definition of an Yukawa system renders impossible a perfect match between their static structure through the definition of an effective coupling parameter $\Gamma_{\text{eff}}$ (0.1, 1 and 10), which is a function of $\Gamma$ and $\kappa$ given in Eq. (15).

vanishes for the OCP but stays finite for the Yukawa systems.

This fundamental difference between the OCP and Yukawa system renders impossible a perfect match between their static structure through the definition of an effective coupling parameter $\Gamma_{\text{eff}}$. Nevertheless, it is still desirable to get the best approximate parametrization of $\Gamma_{\text{eff}}$ as a function of $\Gamma$ and $\kappa$ from the viewpoint of a simple parametrization of the static structure of both systems. To this end, our choice to parametrize separately the short wave number range of the SSF should allow to pass from the OCP static structure to the Yukawa one. Interestingly, the SSFs observed in quantum molecular dynamics simulations exhibit both the behavior of the Yukawa SSF at small wave number and the OCP behavior at higher wave number.

Because it is out of the scope of the present paper, we postpone the extension of our parametrization to the Yukawa system for a future study.

VI. X-RAY DIFFRACTION INTERPRETATION

The role played by the OCP and Yukawa models as reference systems can be evidenced in the interpretation of experimental results. In this respect, the recent measurements of x-ray Thomson scattering gives unprecedented insights into the microscopic structure of WDM.

Very recently, x-ray diffraction was measured simultaneously with x-ray diffusion giving access to the static structure of aluminum ions together with the electronic plasmon spectrum. The frequency-resolved spectra give the density via the shift of the plasmon peak and the temperature via the ratio of intensities between the elastic scattering and the plasmon. The simultaneous measurement of the wave number-resolved spectrum allows for an independent check of the thermodynamic state producing the static structure factor.

The wave number-resolved spectrum is also known as the ion feature $W(k)$. It is related to the SSF $S(k)$ by:

$$W(k) = |f(k) + q(k)|^2 S(k), \quad (16)$$

where $f(k)$ and $q(k)$ are the form factors of bound and free electron densities at an ion. Both the form factors and the SSF, to be used in x-ray Thomson scattering interpretation, are the subjects of active current research involving innovative developments in quantum molecular dynamics simulations.

Here, we propose a simple strategy to tackle the problem of the interpretation of x-ray diffraction from WDM, prior to more involved treatments. The SSF is taken as the OCP one depending on density $\rho$ and temperature $T$ via the coupling parameter $\Gamma$ and the wave number $k$ in units of $\text{Å}^{-1}$, i.e. a function of $\rho$. The form factor is parametrized using a simple exponential dependence:

$$f(k) + q(k) = Z \exp(-\lambda k), \quad (17)$$

where $Z$ is the atomic number of the element.

| $\rho$ (g cm$^{-3}$) | $|\beta|$ | $\sigma_\beta$ | $\sigma_\beta/\beta$ (%) |
|----------------------|--------|-------------|----------------|---|
| 6.813                | 0.038  | 0.6         | 0.6           |   |
| $T$ (eV)             | 2.25   | 0.06        | 2.7           |   |
| $\lambda$ (Å)        | 0.138  | 0.001       | 0.7           |   |
| $\sigma_{\text{mod}}$ | 1.6    | 0.4         | -             |   |

TABLE II: Best parameters $\hat{\beta}$ (mean and standard deviation) obtained by bayesian calibration and model uncertainty $\sigma_{\text{mod}}$. 
We illustrate the efficiency of this approach with the interpretation of the x-ray diffraction spectrum on aluminum measured by Fletcher et al.\textsuperscript{43} (see Fig. 9). We performed a Bayesian calibration\textsuperscript{48–50} of the three parameters $\beta = \{\rho, T, \lambda\}$, assuming the ionization $Q = 3$ close to the melting curve. Such a procedure requires many on-the-fly calculations of the SSF for different $\Gamma$ as presented above.

This is not the scope of this paper to explain the Bayesian technique, so we only recall the few main points. We suppose that the $W(k)$ experimental data are subject to an uncertainty $\epsilon_{\text{exp}}$ distributed according to a Gaussian distribution with a zero mean and a standard deviation $\sigma_{\text{exp}}$ of 2.5 (this value is estimated from the noise affecting the measured spectrum in Fig. 9). Our model is not perfect and hence reproduces the experimental data with an uncertainty $\epsilon_{\text{mod}}$ distributed according to a Gaussian distribution with a zero mean and a standard deviation $\sigma_{\text{mod}}$. The aim is to solve the Bayesian inference of the experimental dataset $[W(k) + \epsilon_{\text{exp}}]$ with our model $[W_{\text{mod}}(k) + \epsilon_{\text{mod}}]$. The Bayesian equation is sampled by use of a Markov Chain Monte Carlo (MCMC) procedure\textsuperscript{48–50}.

This method provides three informations: 1) the best parameters $\hat{\beta}$ for our model, 2) the uncertainty on the $\hat{\beta}$ parameters and the correlations between them and 3) the model uncertainty $\sigma_{\text{mod}}$, which is a measure of the quality of the model. These results are reported in Table [1]. The uncertainty on the best parameters $\hat{\beta}$ are of the order of one percent. We checked that they are almost uncorrelated. The model uncertainty $\sigma_{\text{mod}}$ is less than the experimental uncertainty $\sigma_{\text{exp}}$, meaning that the model perfectly reproduces the experimental data. Indeed, the agreement between both experimental and theoretical ion features is excellent as appears in Fig. 9. The simple exponential form factor with the best value of $\lambda$ is consistent with different theoretical computations already published\textsuperscript{43} (see also Ref. [51]).

The Bayesian method has allowed us to measure the accuracy of the OCP-based interpretation. However, a simple least-square fit method would provide roughly the same $\hat{\beta}$ parameters but without any information about the uncertainty on these $\hat{\beta}$ parameters nor any information about the global accuracy of the model.

Further confrontations with experimental results are still necessary to consolidate the status of the OCP model as a reference system for WDM. Some other examples of our OCP-based interpretation of x-ray Thomson scattering measurements can be found in Ref. [51].

VII. CONCLUSION

We have filled a gap in the corpus of rapidly available properties of the OCP model with the parametrization of its pair distribution function and its static structure factor. The whole fluid phase is covered from weak to strong coupling. The accuracy of the fits was assessed by direct comparisons with molecular dynamics simulations and by calculations of the equation of state.

Recent experiments on warm dense matter revealed the role of reference system the OCP model can play. This prompts us to provide a rapid evaluation of its static structure factor, since it is part of the ion feature in x-ray Thomson scattering measurements. As an illustration, we have used it to successfully interpret the recent x-ray diffraction experiment performed by Fletcher et al.\textsuperscript{43} to get the wave number-resolved spectrum of aluminum ion feature.

The extension of this work concerns the Yukawa model, more appropriate to dusty plasma. In recent experiments\textsuperscript{44} the pair distribution function is directly measured, and there is a pressing need to compare it with the Yukawa system. Ott et al.\textsuperscript{33} suggested that an effective coupling parameter $\Gamma_{\text{eff}}$ can be define as a function of the Coulomb coupling parameter $\Gamma$ and the screening parameter $\kappa$ to characterize the strength of the interaction in Yukawa system. It relies on the short-range structure of the plasma and establishes a correspondence between the OCP and the Yukawa pair distribution functions. We have shown that indeed using the fit of $\Gamma_{\text{eff}}$ proposed by Ott et al.\textsuperscript{33} one can use our parametrization of the OCP pair distribution function for the Yukawa system. Nevertheless, we have also emphasized the limitations of this correspondence, especially in the weakly coupled regime.

We plan to improve the fit of $\Gamma_{\text{eff}}$ at weak coupling and to investigate how the OCP and Yukawa static structure factors can be related. This latter issue highlights a fundamental difference between both models, since the static structure factor at vanishing wave number is proportional to the compressibility which is zero for the OCP and stays finite for the Yukawa system.

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