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## Pair distribution of ions in Coulomb lattice

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### Abstract

The pair distribution function  $g(\mathbf{r}) \equiv g(x, y, z)$  and the radial pair distribution function  $g(r)$  of ions in body-centred-cubic and face-centred-cubic Coulomb crystals are calculated within the harmonic-lattice (HL) approximation in a wide temperature range, from the high-temperature classical limit ( $T \gg \hbar w_p$ ,  $w_p$  being the ion plasma frequency) to the low-temperature quantum limit ( $T \ll \hbar w_p$ ). In the classical limit,  $g(r)$  is also calculated by the Monte Carlo (MC) method. MC and HL results are demonstrated to be in good agreement. With decreasing  $T$ , the correlation peaks of  $g(\mathbf{r})$  and  $g(r)$  become narrower. At  $T \ll \hbar w_p$  they become temperature independent (determined by zero-point ion vibrations).

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### 1. Introduction

A model of a Coulomb crystal of point charges in a uniform compensating background of opposite charge is well known in many branches of physics. For instance, it is used in solid state physics to describe electron–hole plasma (e.g., [1]), in plasma physics to describe dusty plasmas and ion plasmas in Penning traps (e.g., [2]); it is widely used in astrophysics as a model of crystals of ions in the cores of white dwarfs and the envelopes of neutrons stars (e.g., [3]). For certainty, we consider a crystal of ions immersed in a uniform electron background. We analyse the pair distribution function of ions  $g(\mathbf{r}) \equiv g(x, y, z)$  and the radial pair distribution function  $g(r)$  (i.e.,  $g(\mathbf{r})$  averaged over orientations of  $\mathbf{r}$ ).

Both distribution functions are needed for calculating the thermodynamic and kinetic properties of the crystals. In particular, they determine the Coulomb energy of the system, and they are required for a strict description of processes involving ions. The structure factors

(which are the Fourier transforms of the pair distribution functions, see equation (1)), are needed to calculate electron transport properties in Coulomb crystals (e.g., [4, 5]).

The functions  $g(\mathbf{r})$  and  $g(r)$  can be determined numerically: by classical Monte Carlo (MC) e.g., [6] and references therein, molecular dynamics (MD) e.g., [7], and also by path-integral Monte Carlo (PIMC) e.g., [8], but numerical schemes require very large computer resources. As a result, reliable calculations of  $g(r)$  have been performed only by MC for classical body-centred-cubic (bcc) and face-centred-cubic (fcc) Coulomb crystals ( $T \gg \hbar w_p$ ) at  $r/a \lesssim 7$ , where  $w_p = \sqrt{4\pi e^2 Z^2 n / M}$  is the ion plasma frequency,  $a = (4\pi n / 3)^{-1/3}$  is the ion sphere radius,  $Ze$  is the ion charge,  $M$  is its mass and  $n$  is the number density of ions.

Recently, Baiko *et al* [4, 9] constructed a semi-analytic model for calculating the correlation functions of Coulomb systems using the harmonic-lattice (HL) approximation (e.g., [10]). This model is much simpler for practical realization. It does not take into account exchange terms but describes correctly other quantum effects.

Baiko *et al* [9] compared the HL function  $g(r)$  with MC results for classical bcc crystals ( $T \gg \hbar w_p$ ). The agreement was very good for  $1.5 \lesssim r/a \lesssim 7.3$ . In addition, the HL  $g(r)$  was calculated for a quantum bcc crystal at one particular temperature  $T = 0.1 \hbar w_p$ . Here, we present the HL calculations of  $g(\mathbf{r})$  and  $g(r)$  for bcc and fcc crystals. We also present more accurate MC  $g(r)$  for classical crystals and study the HL  $g(\mathbf{r})$  and  $g(r)$  in the quantum and intermediate (classical–quantum) cases.

## 2. Harmonic-lattice method

The HL formalism has been known for a long time (e.g., [10]). We discuss its implementation for Coulomb crystals (e.g., [4, 9, 10]). As can be shown, e.g., from the results of Baiko *et al* [4], the static ion–ion structure factor is given by

$$S(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R} - 2W(k) + v_{\alpha\beta}(\mathbf{R})k_{\alpha}k_{\beta}} - (2\pi)^3 n \delta(\mathbf{k}) \quad (1)$$

where the sum is over direct lattice vectors  $\mathbf{R}$ ,  $e^{-2W(k)}$  is the Debye–Waller factor, and

$$W(k) = \frac{\hbar k^2}{2m} \left\langle \frac{1}{w_{\nu}} \left( \bar{n}_{\nu} + \frac{1}{2} \right) \right\rangle_{\text{ph}} \quad (2)$$

$$v_{\alpha\beta}(\mathbf{R}) = \frac{3\hbar}{2m} \left\langle \frac{e_{\nu\alpha} e_{\nu\beta}}{w_{\nu} \tanh(z_{\nu}/2)} e^{i\mathbf{q} \cdot \mathbf{R}} \right\rangle_{\text{ph}}. \quad (3)$$

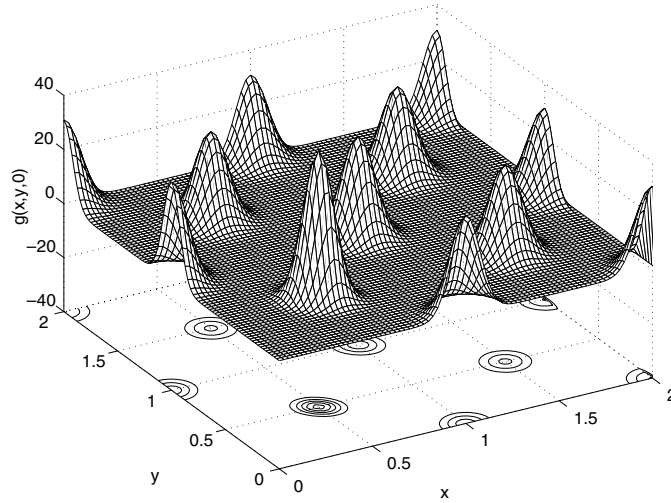
Here,  $\nu \equiv (\mathbf{q}, s)$  denotes phonon branches;  $\mathbf{q}$ ,  $e_{\nu}$  and  $w_{\nu}$  are, respectively, the phonon wave vector, polarization vector and frequency;  $\bar{n}_{\nu} = (e^{z_{\nu}} - 1)^{-1}$  is the mean number of phonons in a mode  $\nu$ ,  $z_{\nu} = \hbar w_{\nu} / T$ . The brackets  $\langle \cdots \rangle_{\text{ph}}$  denote averaging over the phonon spectrum, which can be performed numerically, e.g., [5]. Equation (2) is exact at least for bcc and fcc crystals. For these crystals,  $W(k) = r_T^2 k^2 / 6$ , where  $r_T$  is the rms displacement of a vibrating ion.

We are interested in the pair distribution function

$$g(\mathbf{r}) = 1 + \frac{1}{n} \int \frac{d\mathbf{k}}{(2\pi)^3} [S(\mathbf{k}) - \mathbf{1}] e^{-i\mathbf{k} \cdot \mathbf{r}}. \quad (4)$$

Using equation (1) we have

$$g(\mathbf{r}) = \frac{1}{n} \sum'_{\mathbf{R}} \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{r}) - 2W(k) + v_{\alpha\beta}(\mathbf{R})k_{\alpha}k_{\beta}}. \quad (5)$$



**Figure 1.**  $g(\mathbf{r})$  as a function of  $x$  and  $y$  in units of basic cube lengths at  $z = 0$  for a classical fcc crystal at  $\Gamma = 180$ . The bottom plane shows isolines of  $g(\mathbf{r})$ .

The prime over the sum means that the central ( $\mathbf{R} = 0$ ) lattice vector is excluded. It is natural to introduce the matrix  $V_{\alpha\beta}(\mathbf{R}) = r_T^2 \delta_{\alpha\beta}/3 - v_{\alpha\beta}(\mathbf{R})$  and its inverse:  $N_{\alpha\beta}(\mathbf{R}) = (V^{-1})_{\alpha\beta}$ . Integrating then over  $\mathbf{k}$  we obtain the expression convenient for numerical evaluation

$$g(\mathbf{r}) = \sum_{\mathbf{R}}' \frac{\sqrt{N(\mathbf{R})}}{8\pi^{3/2}\eta} e^{-N_{\alpha\beta}(\mathbf{R})(R_\alpha - r_\alpha)(R_\beta - r_\beta)/4} \quad (6)$$

where  $N(\mathbf{R}) = \det\{N_{\alpha\beta}(\mathbf{R})\}$ . Thus,  $g(\mathbf{r})$  is the sum of (typically narrow) Gaussian peaks centred at direct lattice vectors  $\mathbf{R}$ .

Now the radial pair distribution function is

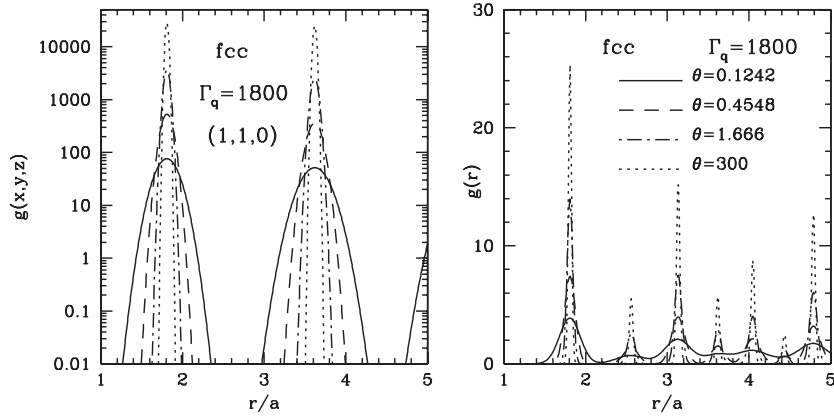
$$g(r) = \frac{1}{4\pi} \int d\Omega g(\mathbf{r}) = \sum_{\mathbf{R}}' g_{\mathbf{R}}(r) \quad (7)$$

where  $d\Omega$  is the solid angle element in the direction of  $\mathbf{r}$ , and  $g_{\mathbf{R}}(r)$  is the contribution from an ion in a lattice site  $\mathbf{R}$ . Using equation (6) one can obtain several representations of  $g_{\mathbf{R}}$  which we do not present here.

The distribution functions  $g(\mathbf{r})$  and  $g(r)$  depend on the lattice type and two parameters: the classical ion-coupling parameter  $\Gamma = Z^2 e^2 / (aT)$  and the quantum parameter  $\theta = \hbar w_p / T$  that measures the importance of zero-point lattice vibrations. It is also useful to introduce a density parameter  $\Gamma_q = Z^2 e^2 / (a\hbar w_p) = \Gamma / \theta$ .

### 3. Results

Figure 1 shows the HL  $g(\mathbf{r})$  for a classical fcc Coulomb crystal at  $\Gamma = 180$  (i.e., close to the melting value  $\Gamma_{\text{melt}} \approx 175$ ; see, e.g., [11]). Vector  $\mathbf{r}$  varies in the plane containing lattice sites. One can observe Gaussian correlation peaks centred at these lattice sites. The peaks are high and narrow, i.e., they do not overlap. The peak widths are determined by thermal vibrations of ions in a lattice. The plane at the bottom of the figure displays isolines of  $g(\mathbf{r})$ . The isolines for neighbouring ions (close to the origin of the coordinate system), turn out to be ellipsoidal, but they become circular for distant ions.



**Figure 2.** Pair distribution functions for fcc crystal at  $\Gamma_q = 1800$  and four values of  $\theta$ . Left panel:  $g(\mathbf{r})$  in direction  $(1, 1, 0)$ . Right panel: radial distribution  $g(r)$ .

The left panel of figure 2 exhibits  $g(\mathbf{r})$  at the density parameter  $\Gamma_q = 1800$  as a function of  $r$  in one direction  $x = y, z = 0$  for four values of the quantum parameter:  $\theta = 0.1242, 0.4548, 1.666$  and  $300$ . The two lowest values of  $\theta$  correspond to the classical limit, the third value is intermediate, while the highest  $\theta$  corresponds to the quantum limit. One can see the two closest correlation peaks and the wing of the third one;  $g(\mathbf{r})$  varies with  $r$  by many orders of magnitude; the values of  $g(\mathbf{r})$  outside the peaks are extremely small.

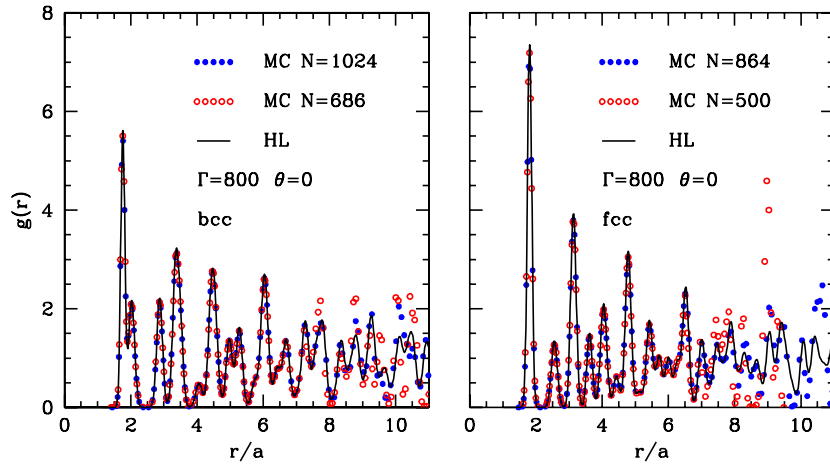
In a classical crystal ( $\theta \lesssim 1$ ) the pair distribution is actually determined by the only parameter  $\Gamma = \Gamma_q \theta$ . The peak heights grow with decreasing  $T$  (increasing  $\theta$  and  $\Gamma$ ) as  $\propto \Gamma^{3/2}$ , and the peak widths decrease as  $\Gamma^{-1/2}$ .

In the quantum regime, the rms ion displacements are determined by zero-point ion vibrations, independent of temperature. The pair distribution becomes ‘frozen’ (temperature independent) being solely determined by the density parameter  $\Gamma_q$ . The peak heights in this regime scale as  $\Gamma_q^{3/2}$  and the peak widths scale as  $\Gamma_q^{-1/2}$ .

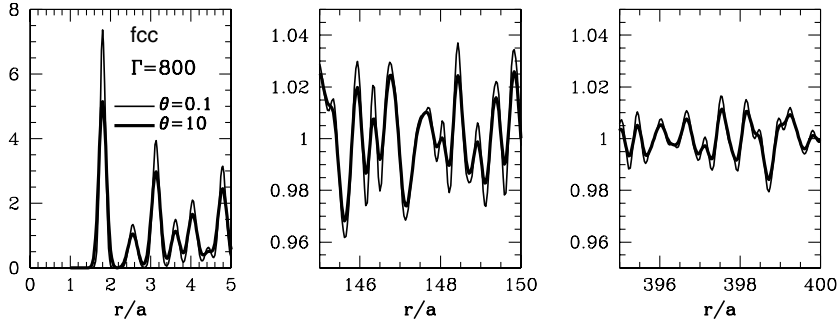
The right panel of figure 2 presents HL  $g(r)$  calculated for the same parameters as on the left panel. The peak heights of  $g(r)$  are naturally much lower than those of  $g(\mathbf{r})$  because of averaging over directions of  $\mathbf{r}$ . The evolution of  $g(r)$  with increasing  $\theta$  (i.e., with decreasing  $T$  at a given density) reflects the evolution of  $g(\mathbf{r})$ : the peaks are seen to become higher and narrower due to decreasing rms amplitude,  $r_T$ , of ion vibrations. In the classical regime, the peak heights evolve as  $\sqrt{\Gamma}$ , and the peak widths as  $\Gamma^{-1/2}$ . In the quantum crystal  $g(r)$  is independent of  $T$ ; the peaks acquire their maximum heights and minimum widths (the heights behave as  $\sqrt{\Gamma_q}$  and the widths as  $\Gamma_q^{-1/2}$ ).

If we decrease the number density of ions (equivalently, increase  $\Gamma_q$ ) the quantum peaks will become higher and narrower. In contrast, if we were to increase the number density of ions the peaks in the quantum regime would become smaller and broader. At very high densities they would start overlapping. Under these conditions, our consideration would fail because the exchange effects which we ignore would become important. Note that under these conditions zero-point ion vibrations may be sufficiently strong to prevent the crystallization of Coulomb liquid (e.g., [3]).

In figure 3 we compare the HL  $g(r)$  in the classical limit with the results of the extensive MC simulations. The MC method is described, e.g., in [6]. The figure shows three sets of calculated  $g(r)$  data for bcc and fcc crystals at  $\Gamma = 800$ . The solid line represents the HL



**Figure 3.**  $g(r)$  for classical bcc (left panel) and fcc (right panel) Coulomb crystals at  $\Gamma = 800$ . Filled and open dots show MC results with larger and lower numbers of particles  $N$ ; solid line: HL.



**Figure 4.** Radial pair distribution function of an fcc crystal at  $\Gamma = 800$  and  $\theta = 0.1$  (thin lines) and 10 (thick lines) in three intervals of  $r$  up to  $r = 400a$ .

curve. Open circles in the left-hand panel exhibit MC data obtained with  $N = 686$  particles over nearly  $10^8$  MC configurations already reported by Baiko *et al* [9]. The MC results for  $g(r)$  are limited to half the size of the basic cell containing the  $N$  charges due to the bias from particles in the image cell adjacent to the basic cell. For  $N = 686$ , the basic cell length is about  $14.2a$ . Accordingly, the MC  $g(r)$  for this simulation is valid only up to  $r \approx 7.3a$  while  $g(r)$ , given by the HL model, remains accurate as  $r \rightarrow \infty$ . However, as discussed in [9], at small particle separations,  $r \lesssim 1.5a$ , the HL model is less accurate than the MC (and MC data are available down to  $r \gtrsim 1.1a$ ). Filled circles show our new MC  $g(r)$  obtained with  $N = 1024$  particles. As expected, larger  $N$  extends the validity of MC results from  $r \approx 7.3a$  to  $r \approx 8.3a$ .

The right-hand panel of figure 3 is similar to the left panel but refers to the fcc crystal. We present the results of our two MC runs obtained with  $N = 500$  and 864. In the first case, the MC  $g(r)$  is accurate at  $r \lesssim 6.4a$  while in the second case it is accurate to about  $r \lesssim 7.7a$ . The peaks for the fcc lattice are slightly more pronounced than those for the bcc lattice.

Let us emphasize once more the simplicity of the HL model which allows us to calculate  $g(r)$  and  $g(r)$  to very large  $r$  using very modest computer resources. For instance, in figure 4 we present HL  $g(r)$  for the fcc crystal at  $\Gamma = 800$  and two values of  $\theta = 0.1$  (classical regime)

and 10 (quantum regime) evaluated up to  $r = 400a$ . The peak structure is quite pronounced even for  $r \sim 400a$  although the peak heights decrease gradually with  $r$ . The classical peaks are higher and narrower (for a fixed  $\Gamma$ ).

#### 4. Conclusions

We have calculated the pair distribution functions  $g(r)$  and  $g(r)$  in the HL approximation for bcc and fcc Coulomb crystals in a wide temperature range, from the classical high-temperature limit to the quantum low-temperature limit. In the classical limit, we have compared the HL  $g(r)$  with the results of MC calculations at different numbers of ions  $N$  and find a good agreement of MC and HL results.

Let us stress that the quantum effects cannot be taken into account in a classical MC scheme. They can be explored using PIMC but such studies require very powerful computers. At present, the HL model gives the only simple method for exploring ion correlations in quantum Coulomb crystals.

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