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LETTER TO THE EDITOR

A new evaluation of the energy of Wigner BCC and FCC crystals

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Abstract. New expressions for energies per site for two Wigner crystals are given through Euler-type constants. Numerical values specify those known previously.

Energies per site for Wigner cubic crystals [1] (simple, body-centred and face-centred lattices) were found in [2, 3]. Recently it was shown [4], by using an analytical continuation procedure for the functions concerned, that the commonly used numerical values of energies for the BCC and FCC lattices would be changed. In [4] the model with point charges surrounded by an equal amount of opposite charge distributed over a unit cube was accepted. Satisfying the requirement of charge neutrality, the above model obviously breaks homogeneity of the charge distribution for FCC and BCC crystals. Thereby we recalculate these energies in the jellium model [1, 5] strictly taking into account both homogeneity and neutrality. Our values of energies confirm those of the paper [4] and are more precise.

First, we consider the BCC lattice. We shall find the energy site per site for a finite-size cube of length $2N$ for each edge and then take the limit $N\to\infty$. In units e^2/a (a is the lattice parameter) the interaction energy of the central site (coordinates $(0, 0, 0)$) with all other lattice sites is as follows:

$$V_{--}=6\sum_{S=1}^{N}\frac{1}{S}+12\sum_{m,n=1}^{N}\frac{1}{(m^2+n^2)^{1/2}}+8\sum_{m,n,l=1}^{N}\frac{1}{(m^2+n^2+l^2)^{1/2}}$$
$$+8\sum_{m,n,l=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2+\left(l-\frac{1}{2}\right)^2\right]^{1/2}}. \tag{1}$$

In the framework of the jellium model, we build around any site of the lattice the Voronoi polyhedron with volume $a^3/2$. Correspondingly, the density ρ of a distributed charge is equal to $2e/a^3$. Now we may define the interaction energy of the central site with a compensating charge background as

$$V_{-+}\equiv-8e\rho I=-16\frac{e^2}{a}\left\{\int\!\!\int\!\!\int_0^N+3\int_N^{N+1/4}\int\!\!\int_0^N+3\int_0^N\!\!\int\!\!\int_N^{N+(1/2\sqrt{2})}\right\}\frac{\mathrm{d}x\mathrm{d}y\mathrm{d}z}{(x^2+y^2+z^2)^{1/2}}.$$

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Expression (2) contains a contribution from the surface neutralizing layer which is asymptotically exact to within I/N. With (1) and (2) we have for the interaction energy ε per site

$$\frac{a}{e^2}\varepsilon_{BCC} = \lim_{N\to\infty}(V_{--}+V_{-+}) = \frac{\pi}{4} - 6\ln\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right) + 6\gamma_1 - 12\gamma_2 + 8\gamma_3 + 8\delta_3$$

$$= -3.377\,434\,064\,464\ldots \quad (3)$$

where γ_1 is the Euler constant ($\gamma_1 = 0.577\,215\,664\,901\,5\ldots$) and $\gamma_{2,3}$, δ_3 are analogous constants appearing in asymptotic expressions for sums of the divergent series in (1) (see the appendix).

As regards the FCC case, using the same approach as above makes it possible to obtain

$$\bar{V}_{--} = 6\sum_{S=1}^{N}\frac{1}{S} + 12\sum_{m,n=1}^{N}\frac{1}{(m^2+n^2)^{1/2}} + 8\sum_{m,n,l=1}^{N}\frac{1}{(m^2+n^2+l^2)^{1/2}}$$

$$+12\sum_{m,n=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2\right]^{1/2}} \quad (4)$$

$$+24\sum_{m,n,l=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2+l^2\right]^{1/2}}$$

$$\bar{V}_{-+} \equiv -8e\bar{\rho}\bar{I} = -32\frac{e^2}{a}\int\int\int_0^{N+1/4}\frac{\mathrm{d}x\mathrm{d}y\mathrm{d}z}{(x^2+y^2+z^2)^{1/2}};$$

$$\frac{a}{e^2}\varepsilon_{FCC} = \frac{\pi}{2} - 6\ln\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right) + 6\gamma_1 - 12\gamma_2 + 8\gamma_3 + 12\mu_2 + 24\nu_3 = -4.061\,261\,142\,971\ldots,$$

where Euler-type constants μ_2 and ν_3 are given in the appendix.

Taking another normalization [2–4], instead of (3) and (4) we obtain

$$\frac{r_s}{e^2}\varepsilon_{BCC} = \left(\frac{3}{8\pi}\right)^{1/3}\varepsilon_{BCC}\frac{a}{e^2} = -1.662\,955\,690\,79\ldots \quad (5)$$

$$\frac{\bar{r}_s}{e^2}\varepsilon_{FCC} = \left(\frac{3}{16\pi}\right)^{1/3}\varepsilon_{FCC}\frac{a}{e^2} = -1.587\,125\,912\,88\ldots. \quad (6)$$

The values (5) and (6) specify the previous results [4] ($-1.662\,96\ldots$ and $-1.587\,13\ldots$, correspondingly).

Appendix

Here we give asymptotic expansions of sums of the divergent series from (1) and (4) which are obtained by the Euler–MacLaurin method [6].

$$\sum_{m,n=1}^{N}\frac{1}{(m^2+n^2)^{1/2}}=2N\ln(1+\sqrt{2})-\ln N-\gamma_2+O\left(\frac{1}{N}\right)$$

$$\gamma_2=0.670\,908\,307\,883\,6\ldots$$

$$\sum_{m,n,l=1}^{N}\frac{1}{(m^2+n^2+l^2)^{1/2}}=3\left\{(N^2+N)\left[\ln\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)-\frac{\pi}{12}\right]-N\ln(1+\sqrt{2})+\frac{1}{4}\ln N\right\}$$

$$+\gamma_3+O\left(\frac{1}{N}\right)\qquad \gamma_3=0.581\,748\,045\,317\ldots$$

$$\sum_{m,n,l=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2+\left(l-\frac{1}{2}\right)^2\right]^{1/2}}=3N^2\left[\ln\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)-\frac{\pi}{12}\right]$$

$$+\delta_3+O\left(\frac{1}{N}\right)\qquad \delta_3=-0.034\,792\,149\,303\,7\ldots$$

$$\sum_{m,n=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2\right]^{1/2}}=2N\ln(1+\sqrt{2})+\mu_2+O\left(\frac{1}{N}\right)$$

$$\mu_2=-0.403\,885\,656\,141\,17\ldots$$

$$\sum_{m,n,l=1}^{N}\frac{1}{\left[\left(m-\frac{1}{2}\right)^2+\left(n-\frac{1}{2}\right)^2+l^2\right]^{1/2}}=(3N^2+N)\left[\ln\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)-\frac{\pi}{12}\right]$$

$$-N\ln(1+\sqrt{2})+\nu_3+O\left(\frac{1}{N}\right)\qquad \nu_3=0.129\,127\,726\,556\,69\ldots.$$

References

[1] Wigner E P 1934 *Phys. Rev.* **46** 1002
[2] Coldwell-Horsfall R A and Maradudin A A 1960 *J. Math. Phys.* **1** 395
[3] Borwein D, Borwein J M, Shail R and Zucker I J 1988 *J. Phys. A: Math. Gen.* **21** 1519
[4] Borwein D, Borwein J M and Shail R 1989 *J. Math. Anal. Appl.* **143** 126
[5] Crandall R E and Buhler J P 1987 *J. Phys. A: Math. Gen.* **20** 5497
[6] Kukhtin V V and Shramko O V 1991 *Phys. Lett.* **156A** 257