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Screened Wigner-lattice model

Mirabeau Dias and A. N. Chaba
Departamento de Física, Universidade Federal da Paraíba,
58.000 João Pessoa, Paraíba, Brasil
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Recently Medeiros e Silva and Mokross proposed the screened Wigner-lattice model which consists of negative point charges on a Bravais lattice interacting through the screened Coulomb potential $-Q\exp(-\lambda r)/r$ and the positive charge background with the density $(Q/\Omega)\exp(-\lambda r)$. We point out the drawbacks of this model and show that by modifying the background charge density to $(Q\lambda^2/4\pi)\sum_{\vec{\tau}}\exp(-\lambda|\vec{r}-\vec{\tau}|)/|\vec{r}-\vec{\tau}|$ the screened Coloumb form of the potential emerges naturally as a consequence. Further, this modified screened Wigner-lattice model is free from the defects of the other model.

A Wigner[1] lattice (WL) is a model composed of point charges $-Q$ $(Q>0)$ on a Bravais lattice with a uniform neutralizing positive charge background. In order to explain the experimental observations[2,3] of phase transitions in systems consisting of polystyrene spheres in aqueous suspensions and motivated by the suggestion of Williams, Crandall, and Wojtowicz,[3] Medeiros e Silva and Mokross[4,5] (MM) proposed the screened Wigner-lattice (SWL) model which consists of negative point charges $-Q$ located at the lattice points (of a Bravais lattice) interacting through the screened Coulomb potential $\phi_1(r)$ given by

$$\phi_1(r)=-Q\exp(-\lambda r)/r\ , \tag{1}$$

and the positive charge background with density $\rho_1(r)$, where

$$\rho_1(r)=(Q/\Omega)\exp(-\lambda r)\ , \tag{2}$$

Ω being the volume of the system per lattice point. Also, MM calculated the electrostatic energy of the body-centered cubic (bcc) and face-centered cubic (fcc) lattices and showed the existence of a phase transition. Now we wish to make the following comments on the SWL model described above and point out its drawbacks:

(a) According to the model of MM, the charges on the Bravais lattice are point charges and so each one of them can produce only the pure Coulomb potential and not the screened Coulomb potential. Only a distribution of discrete or continuous charges may produce other forms of potential (including the screened Coulomb potential). So we feel that the assumptions of point charges at the lattice points and the screened Coulomb potential produced by each one of them are inconsistent with each other.

(b) As the charge density of the background is the sum of the terms such as $(Q/\Omega)\exp(-\lambda r)$ around (and "associated with," as we shall refer to it) every lattice point (so that the system is translationally invariant with respect to any lattice vector), therefore, in the limit of $\lambda\to 0$, this model does not reduce to the WL model (because the background charge density does not reduce to Q/Ω) in contradiction to the claim made by MM.[5]

(c) The form of the density of the background does not assure neutrality of the system as a whole, in general. For the system to be neutral, it is necessary that $\int\rho_1(r)d^3r=Q$, and this leads to the condition $\lambda=(8\pi/\Omega)^{1/3}$ or $\lambda_s=\lambda r_s=6^{1/3}$, where $\Omega=(\frac{4}{3})\pi r_s^3$. It follows that only one particular value of λ_s $(=6^{1/3})$ makes the system neutral as a whole, whereas in their work,[5] MM have used the results based on their model for various values of λ_s (see their graph on p. 2974 of Ref. 5).

(d) While calculating $\phi^{(2)}$, the potential at a lattice point due to the background charge [see their Eq. (15)], MM[5] have used, without any justification, only one term (associated with the above lattice point) in the total background charge density.

(e) In the calculation of the electrostatic energy of the system, MM[5] have ignored the energy of interaction between different parts of the background (perhaps assuming that these are equal for the bcc and the fcc lattices and cancel out when we take the difference), again without any justification. Perhaps it is worthwhile mentioning, in this context, that Hall[6] has also, recently, pointed out that it is the zeros of the difference in Fuchs energy and not the Madelung energy which determines the phase transitions and these zeros are not equal.

In his doctoral thesis, Medeiros e Silva[7] considered a density of background charge as $\rho(r)=(Q\lambda^2/4\pi)\times\exp(-\lambda r)/r$, which together with the screened Coulomb potential $\phi(r)=-Q\exp(-\lambda r)/r$ satisfies the Poisson equation $(\nabla^2\phi=-4\pi\rho)$. But he discarded this solution because, in the limit $\lambda\to 0$, $\rho(r)\to 0$. The correct expression for the density of the background charge $\rho(r)$, as taken by Hall,[6] is

$$\rho(r)=(Q\lambda^2/4\pi)\sum_{\vec\tau}\exp(-\lambda|\vec r-\vec\tau|)/|\vec r-\vec\tau| \ , \quad (3)$$

which is invariant with respect to translation by any lattice vector (as it should be). Now, we consider a new model, the modified screened Wigner-lattice (MSWL) model, in which the point charges $-Q$ at the lattice points interact through pure Coulomb potential and the background charge density is given by Eq. (3). We can show that $\int\rho_1(r)d^3r=Q$, where $\rho_1(r)=(Q\lambda^2/4\pi)\exp(-\lambda r)/r$ is the density of background charge around every lattice point and expression (3) is just the sum of terms of this type. Thus the system, as a whole, is neutral independent of the value of λ or λ_s.

We now find an expression for the potential $\phi_1(r)$ owing to the charge $-Q$ at a lattice point and the background charge density term associated with it, at a point whose distance from the lattice point is r ($\vec r\neq\vec\tau$). Using Coulomb's law,

$$\phi_1(r)=-\frac{Q}{r}+\int_0^r\frac{\rho_1(r')d^3r'}{r}+\int_r^\infty\frac{\rho_1(r')d^3r'}{r'}$$

$$=-Q\exp(-\lambda r)/r \ , \quad (4)$$

and the total potential at this point is given by

$$\phi(r)=-Q\sum_{\vec\tau}\exp(-\lambda|\vec r-\vec\tau|)/|\vec r-\vec\tau| \ . \quad (5)$$

The potential at a lattice point, say the origin, is given by (excluding the contribution of the charge at the lattice point itself)

$$\phi(0)=-Q\sum_{\vec\tau}{}'\exp(-\lambda\tau)/\tau+\int_0^\infty\frac{\rho_1(r')d^3r'}{r'}$$

$$=-Q\sum_{\vec\tau}{}'\exp(-\lambda\tau)/\tau+Q\lambda \ . \quad (6)$$

Thus, we see from Eq. (4) that the screened Coulomb potential emerges, naturally, as a consequence of the distribution of background charge. Of course, in the present case, this potential is not due only to the point charge at a lattice point (it was assumed to be so in the SWL model) but also includes the contribution of the background charge-density term associated with it. Further, we see that Eq. (6) is quite similar to Eq. (14) of MM[5] except for the additional term $Q\lambda$. Also we may point out that Eq. (3) for $\rho(r)$ in addition to the density $-Q\sum_{\vec\tau}\delta(\vec r-\vec\tau)$ due to charges at lattice points and Eq. (5) for $\phi(r)$ of the MSWL model satisfy the Poisson equation, the same statement is not true for Eqs. (1) and (2) of the SWL model. The lattice sum occurring in Eq. (3) can be done by making use of the Poisson summation formula[8] with the result (the details of the calculation will be given elsewhere)

$$\sum_{\vec\tau}\exp(-\lambda|\vec r-\vec\tau|)/|\vec r-\vec\tau|=(4\pi/\Omega\lambda^2)+(\pi\Omega)^{-1}\sum_{\vec\gamma}{}'\exp(-2\pi i\,\vec r\cdot\vec\gamma)/\gamma^2$$
$$-(\lambda^2/\pi\Omega)\sum_{\vec\gamma}{}'\exp(-2\pi i\,\vec r\cdot\vec\gamma)\gamma^{-2}(\lambda^2+4\pi^2\gamma^2)^{-1} \ , \quad (7)$$

where $\{\vec\gamma\}$ is the reciprocal lattice, normalized by the relation $\exp(2\pi i\,\vec\tau\cdot\vec\gamma)=1$. Substituting Eq. (7) in Eq. (3), we get

$$\rho(r)=(Q/\Omega)\left[1+(\lambda^2/4\pi^2)\sum_{\vec\gamma}{}'\exp(-2\pi i\,\vec r\cdot\vec\gamma)/\gamma^2-(\lambda^4/4\pi^2)\sum_{\vec\gamma}{}'\exp(-2\pi i\,\vec r\cdot\vec\gamma)\gamma^{-2}(\lambda^2+4\pi^2\gamma^2)^{-1}\right] \ . \quad (8)$$

We see that, in the limit $\lambda\to0$, $\rho(r)\to Q/\Omega$. Thus we have shown that the WL model is recovered in the limit $\lambda\to0$, the same result was stated (without proof) by Hall.[6]

We have also calculated the electrostatic energy (Fuchs energy) of the the MSWL model by an approach much simpler than that of Hall[6] and arrived at the results which are identical with those obtained by him. We are studying this problem and the related matters in some depth and the results, when ready, will be reported.

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