Comment on "Two-dimensional classical electron gas in a periodic field: Delocalization and dielectric-plasma transition"

A. Alastuey, F. Cornu, and B. Jancovici
Laboratoire de Physique Theórique et Hautes Energies, Université de Paris–Sud, Bâtiment 211, 91405 Orsay, France
(Received 31 March 1988)

For the model of a two-dimensional Coulomb gas made up of finite-size ions fixed on the sites of a lattice, and of classical mobile electrons, the dielectric-plasma (or Kosterlitz-Thouless) transition takes place at a value of the coupling constant which is $\Gamma=4$ in the low-density limit, as for the standard model in which both the ions and the electrons are mobile.

Clérouin, Hansen, and Piller[1] have studied by molecular-dynamics simulations a two-dimensional Coulomb system made up of finite-size ions of charge e, fixed on the sites of a lattice, and of mobile classical point electrons of charge $-e$. This system is a modification of the usual Coulomb gas[2] in which both the ions and the electrons and mobile. In two dimensions, the Coulomb potential between two particles of charge e is $-e^2\ln(r/L)$, where L is some arbitrary length scale which defines the zero of the potential; in the following, we choose $L=1$. The dimensionless coupling constant is $\Gamma=\beta e^2$, where β is the inverse temperature. Both models are expected to exhibit a phase transition between a high-temperature plasma phase and a low-temperature dielectric phase in which oppositely charged particles are bound in pairs in the following sense. According to the linear response theory, the dielectric constant ϵ is given by

$$\epsilon^{-1}=1-2\pi\chi \ , \tag{1}$$

where χ is a "susceptibility" defined in terms of the charge-charge correlation function $S(\mathbf{r})$,

$$\chi=-\frac{\beta}{4}\int d\mathbf{r}\, r^2 S(\mathbf{r}) \ . \tag{2}$$

The transition is not signaled by thermodynamical singularities but by the discontinuity of ϵ^{-1}; in the plasma phase an infinitesimal external charge is perfectly screened by the charges of the system and $\epsilon^{-1}=0$ (the Stillinger-Lovett rule is satisfied), whereas in the dielectric phase $\epsilon^{-1}\neq 0$ and depends on the density. The value of Γ at which the dielectric-plasma transition occurs is a function of the density via ϵ and is predicted to be Γ_c such that $\Gamma_c=4\epsilon$, for the usual symmetric Coulomb gas; in the low-density limit, ϵ approaches 1 in the dielectric phase and $\Gamma_c=4$. On the other hand, the simulations of Clérouin *et al.*[1] suggested that, in the low-density limit, the transition may take place at the coupling value $\Gamma_c=2$, for their fixed-ion model.

In this comment, we argue that the correct value for the fixed-ion model is also $\Gamma_c=4$. Essentially, we show that fixing the ions on a lattice does not alter the large-scale behavior and therefore the location of the Kosterlitz-Thouless transition, which is governed by long-range effects. We use three complementary approaches.

(a) The fixed-ion model is very similar to the symmetric Coulomb gas, when the relevant configurations of the fixed-ion model are such that the proportion of Wigner-Seitz cells containing no electron is small; we can then neglect the probability of having more than two electrons in a cell. Therefore, on a scale large compared to the size of the cell, the model can be viewed as a symmetric Coulomb *lattice* gas, with mostly empty sites (cells containing one ion and one electron), some positive "particles" (cells containing one ion only), and an equal number of negative "particles" (cells containing one ion and two electrons).

A more quantitative correspondence can be obtained. In the fixed-ion model, let σ be the radius of an ion (for simplicity, we assume the ions to be impenetrable) and let a be the ion-disk radius [the definition of a is that the number of ions per unit area is $(\pi a^2)^{-1}$]. We consider here the low-density case $\sigma/a \ll 1$, and assume $\Gamma>2$. In the low-density limit, the Boltzmann factor for an electron near an ion has the independent pair value $C\exp(-\Gamma\ln r)$, where C is a constant and r the ion-electron distance, and the probability that the electron is outside "its" cell is

$$n=\frac{\int_a^\infty r^{-\Gamma} r\, dr}{\int_0^\infty r^{-\Gamma} r\, dr}=\left[\frac{\sigma}{a}\right]^{\Gamma-2} . \tag{3}$$

Therefore, the corresponding symmetric lattice gas will have a density of particles of each sign approximately equal to $n=(\sigma/a)^{\Gamma-2}$.

Such a low-density lattice gas has its transition near $\Gamma=4$. This well-known result can be obtained, for instance, by using a "spin-block" method. One looks at the lattice of N_a cells of size a, on a larger scale, as a lattice of $N_{a'}=N_a(a/a')^2$ larger cells of size a'. The number of dipoles of size larger than a is nN_a, and, by the same argument as the one which leads to (3), one sees that the number of dipoles of size larger than a' is smaller by a factor $(a/a')^{\Gamma-2}$; this number is $nN_a(a/a')^{\Gamma-2}=nN_{a'}(a/a')^{\Gamma-4}$. If the lattice spacing a' is scaled to infinity, the average number of free electrons per cell, $n(a/a')^{\Gamma-4}$, vanishes when $\Gamma>4$: their renormalized fugacity vanishes, which means that the free energy needed to break a pair becomes infinite, as will be shown in the following paragraphs.

(b) A slightly rephrased version of the original thermodynamical argument by Kosterlitz and Thouless[2] is as follows. We consider a symmetric Coulomb gas in a large box of size R. If there are only bound pairs, the free energy per pair is finite. If one electron-ion pair is broken, and the density is sufficiently small so that $\epsilon \simeq 1$, then its free energy becomes of the order $e^2 \ln R - 2k_B T \ln R^2$ (the interaction Coulomb energy is $e^2 \ln R$, and the entropy is $k_B \ln R^2$ for the free electron and $k_B \ln R^2$ for the free ion). Therefore, it is favorable to break pairs when $e^2 - 4k_B T < 0$, i.e., when $\Gamma < 4$: the first broken pair appears at $\Gamma = 4$, at least in the low-density limit (for a finite density, e^2 must be replaced by e^2/ϵ, where ϵ is the dielectric constant, and this leads to the universal rule[3] that the transition, when approached from the dielectric side, occurs at $\Gamma/4\epsilon = 1$).

The above argument applies as well to the fixed-ion model. The system with one broken pair has again an entropy of order $2k_B \ln R^2$, because that ion which has lost its electron can be chosen on any site, and this gives a contribution $k_B \ln R^2$ to the entropy as if the ions were mobile.

(c) Finally, let us look at some simple dielectric properties in the low-temperature phase. For the symmetric Coulomb gas, the charge-charge correlation function $S(r)$ is expected[3,4] to decay like $r^{-\Gamma/\epsilon}$ (strictly speaking, this has been shown only to the order of a first correction to an independent-pair approximation; this lowest-order correction is equivalent to a mean-field theory). Thus, one might think that the susceptibility χ defined by (2) diverges as Γ/ϵ approaches 4 from the dielectric side. Indeed, this anomaly signals a phase transition at $\Gamma = 4\epsilon$, although χ actually remains finite with only a discontinuity (it is necessary to use renormalization-group techniques to deal correctly with the vicinity of $\Gamma = 4\epsilon$).

Here we present some evidence that the charge-charge correlation function $S(\mathbf{r},\mathbf{r}')$ of the fixed-ion model also decays as $|\mathbf{r}'-\mathbf{r}|^{-\Gamma/\epsilon}$, when we apply a suitable local averaging process. Our derivation has the same kind of limitations as in the symmetric case, namely we work only to first order in the density. For our purpose, it is convenient to consider the system as made of ion-electron pairs, with no loss of generality if the interaction between pairs is taken into account. Thus, in terms of the fixed positions $\mathbf{R}_i$ of the ions and the position variables $\mathbf{r}_i$ of the electrons, we write the potential energy for $|\mathbf{r}_i - \mathbf{R}_j| > \sigma$ as

$$\sum_i e^2 \ln |\mathbf{r}_i - \mathbf{R}_i| + \sum_{i<j} v_{ij} ,$$

where

$$v_{ij} = e^2 (\ln |\mathbf{r}_i - \mathbf{R}_j| + \ln |\mathbf{r}_j - \mathbf{R}_i| - \ln |\mathbf{r}_j - \mathbf{r}_i| - \ln |\mathbf{R}_j - \mathbf{R}_i|) .$$

Because of the presence of the ion lattice, we are bound to use the canonical ensemble (in contrast with the symmetric Coulomb gas which can be studied more easily by a fugacity expansion[5] in the grand-canonical ensemble). The expansion of the two-electron truncated density in powers of $(\sigma/a)^2$ can be built through a cluster expansion with respect to the Mayer functions $f_{ij} = \exp(-\beta v_{ij}) - 1$. However, each cluster integral is itself a series in $(\sigma/a)^2$, and therefore the calculations are more tedious than in the symmetric case.

To order zero in the density, we can replace each f_{ij} by 1, and we obtain for the charge-charge correlation function (which depends on two electron coordinates $\mathbf{r}$ and $\mathbf{r}'$) the independent-dipole approximation

$$S(\mathbf{r},\mathbf{r}') = -e^2 \left[\frac{(\Gamma-2)\sigma^{\Gamma-2}}{2\pi} \right]^2 \times \sum_i \frac{1}{|\mathbf{r}-\mathbf{R}_i|^{\Gamma} |\mathbf{r}'-\mathbf{R}_i|^{\Gamma}}, \quad \mathbf{r} \neq \mathbf{r}' . \tag{4}$$

On the other hand, to order zero in the density, $\epsilon = 1$ and $S(\mathbf{r},\mathbf{r}')$ indeed decays as $|\mathbf{r}-\mathbf{r}'|^{-\Gamma}$ [this is easily seen by noting that the sum in (4) is dominated by the terms in which $\mathbf{R}_i$ is close either to $\mathbf{r}$ or to $\mathbf{r}'$].

To obtain the first correction to the independent-pair approximation, it is enough to expand the Boltzmann factor to first order in f_{ij}. Then two kinds of terms appear in the large distance behavior of the charge-charge correlation function $S(\mathbf{r},\mathbf{r}')$. The first contribution has the bare decay $|\mathbf{r}-\mathbf{r}'|^{-\Gamma}$ with a logarithmic correction, to the order of interest

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|^{\Gamma}} \left[1 + \Gamma^2 \left[\frac{\Gamma-2}{\Gamma-4} \right] \left[\frac{\sigma}{a} \right]^2 \ln |\mathbf{r}-\mathbf{r}'| \right] \tag{5}$$

(this logarithmic correction comes from the interaction with another dipole). The second contribution comes from multipolar expansions and is peculiar to the microscopic structure of the ion-lattice model. For instance, there is a dipole-dipole interaction term proportional to

$$\frac{1}{|t|^{\Gamma}} \frac{1}{|t'|^{\Gamma}} t_\alpha t'_\beta \left[\frac{\delta_{\alpha\beta}}{|\mathbf{R}-\mathbf{R}'|^2} - 2 \frac{(\mathbf{R}-\mathbf{R}')_\alpha (\mathbf{R}-\mathbf{R}')_\beta}{|\mathbf{R}-\mathbf{R}'|^4} \right],$$

where $\mathbf{t} = \mathbf{r} - \mathbf{R}$ with $\mathbf{R}$ the lattice site which is nearest to $\mathbf{r}$ (the induces α and β stand for Cartesian components). However, when we average over the cells to which $\mathbf{r}$ and $\mathbf{r}'$ belong, the multipolar contributions disappear to the order of our calculation; in the same way they do not contribute to the value of

$$\epsilon^{-1} = 1 + \frac{\beta}{2} \frac{1}{a^2} \int_{\text{cell}} d\mathbf{r} \int d\mathbf{r}' S(\mathbf{r},\mathbf{r}') |\mathbf{r}-\mathbf{r}'|^2 .$$

Thus, to the same order of approximation, ϵ is given by the independent-pair approximation (as expected), with the result

$$\epsilon^{-1} = 1 - \Gamma \left[\frac{\Gamma-2}{\Gamma-4} \right] \left[\frac{\sigma}{a} \right]^2 .$$

In the low-density limit, (5) can be reexponentiated into $|\mathbf{r}-\mathbf{r}'|^{-\Gamma/\epsilon}$, and we find that the suitably averaged $S(\mathbf{r},\mathbf{r}')$ decays like the charge-charge correlation function of the symmetric Coulomb gas.

From the above, we believe that it can be safely concluded that the fixed-ion model has a Kosterlitz-Thouless transition at a value of Γ which approaches 4 in the low-density limit, as the symmetric Coulomb gas. This conclusion is in agreement with exact results about the symmetric Coulomb gas[6] and the fixed-ion model[7] which were both shown to be in their plasma phase at $\Gamma=2$. Near $\Gamma=2$, there is no phase transition, as long as the density is finite. However, for small densities, most pairs are tightly bound for $\Gamma>2$; the fixed-ion model has a number of delocalized electrons which becomes very small for $\Gamma>2$ [see Eq. (3)], and these electrons cannot be seen in a computer simulation,[1] which attempts to characterize the transition by dynamical diagnostics.

We are indebted to the authors of Ref. 1 for stimulating discussions. Laboratoire de Physique Théorique et Hauts Energies is a "Laboratoire associé au Centre National de la Recherche Scientifique."

[1]J. Clérouin, J. P. Hansen, and B. Piller, Phys. Rev. A **36**, 2793 (1987).

[2]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[3]See, e.g., P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987).

[4]J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).

[5]E. R. Speer, J. Stat. Phys. **42**, 895 (1986).

[6]F. Cornu and B. Jancovici, J. Stat. Phys. **49**, 33 (1987).

[7]F. Cornu and B. Jancovici, Europhys. Lett. **5**, 125 (1988); F. Cornu, B. Jancovici, and L. Blum, J. Stat. Phys. **50**, 1221 (1988).