Journal of Statistical Physics, Vol. 34, Nos. 1/2, 1984

A Refined Mermin Argument for the Two-Dimensional Jellium

F. Martinelli[1] and D. Merlini[1]

Received April 5, 1983

We consider the two-dimensional classical jellium with periodic boundary conditions and with translation invariance broken by an external periodic localizing one-body potential. Using a refinement of Mermin's argument, we show that a symmetry breakdown of translation invariance (appearance of a crystalline phase with positional long-range order) does not occur, if the correlation function $h(\mathbf{r})$ decays faster than $1/r^2$ as $r \to \infty$.

KEY WORDS: Two-dimensional one-component plasma; Mermin argument; crystalline order, fluid.

1. INTRODUCTION

In recent papers,[2,3] the origin Mermin argument[1] has been redefined and adapted to investigate the problem of absence of long-range crystalline order in the ν-dimensional one-component plasma (jellium with long-range Coulomb interaction. In a first refined formulation of Mermin's idea, it was shown by Baus[2] that Mermin's argument is inconclusive for the ν-dimensional genuine one-component plasma (with ν-dimensional Coulomb potential) and for the two-dimensional surface plasma (two-dimensional model with $1/r$ potential). For the latter system Alastuey and Jancovici,[3] using a modification of Mermin's argument, proved that the positional order may be destroyed by the transversal phonons. In this note we combine these methods and get a result concerning the absence of long-range positional order in the genuine two-dimensional jellium with long-range two-dimensional logarithmic Coulomb potential. For this model and for the two-dimensional surface plasma, recent computer experiments[4,5]

[1] Mathematisches Institut, Ruhr-Universität Bochum, 4630 Bochum, Federal Republic of Germany.

indicate that there may exist a "fluid–solid" transition at sufficiently low temperature (i.e., in the range $\gamma \geqslant e^2/kT \sim 130$–$140$). This situation is analogous to the one discussed earlier through computer experiments in the three-dimensional case. In this region the radial correlation function seems to decay much slower than in the fluid phase and shows a typical solidlike structure, with peak positions corresponding to characteristic distances of the triangular lattice.

In investigating the region of absence of a crystalline order, attention should be payed to the breaking of translation invariance of the Hamiltonian at finite volume due to the various relevant boundary conditions. The situation is here analogous to the Ising model on a lattice, where in order to prove or disprove a symmetry breakdown of the state at low temperature (existence of a spontaneous magnetization), the Hamiltonian should be broken either by imposing some boundary conditions outside a finite box Λ ($+$ or $-$ boundary conditions corresponding to the two pure phases) or either by introducing a small external magnetic field $h \geqslant 0$ at every lattice point, computing the magnetization, and removing the field afterwards.

For the two-dimensional jellium, a natural boundary condition, called a Dobrushin boundary condition for the jellium, is given by putting a fixed crystalline configuration of charges with background, outside the vessel $\Lambda \subset \mathbb{R}^2$; this was introduced recently in the investigation of the uniqueness of the free energy density;[6] as mentioned above, another way to break the translation invariance consists in introducing an external localizing one body potential $\alpha\varphi_{\text{ext}}(x)$, $\alpha < 0$, with peaks at the sides of a given lattice and letting $\alpha \to 0$ afterwards. Here we confine ourselves to this second alternative and show in Section 2 that for the two-dimensional jellium if the net pair correlation function $h(\mathbf{r})$ decays faster than or at equal speed as $1/r^2$, as $r \to \infty$, then no positional long-range order will persist in the system.

2. THE MODEL

Let $(\mathbf{a}_1, \mathbf{a}_2)$ be the generators of a Bravais lattice $\mathbb{L}^2$ and let $\Lambda = \{x \in \mathbb{R}^2;\ \mathbf{x} = Lx_1\mathbf{a}_1 + Lx_2\mathbf{a}_2\ 0 \leqslant x_1 \leqslant 1,\ 0 \leqslant x_2 \leqslant 1\}$. Let us consider in Λ a system of N classical point particles of charge $+e$ and a neutralizing background described by a uniform charge density $\rho = -(N/|\Lambda|)e$, interacting through a two-body potential $\varphi_\Lambda(\mathbf{x}, \mathbf{y})$. The Hamiltonian of the system (the jellium) is then given by

$$H_\Lambda(\mathbf{x}_1, \ldots, \mathbf{x}_N) = e^2 \sum_{i<j} \varphi_\Lambda(\mathbf{x}_j, \mathbf{x}_i) - e\rho \sum_{i=1}^{N} \int_\Lambda d\mathbf{y}\, \varphi_\Lambda(\mathbf{x}_i, \mathbf{y}) + \frac{1}{2}\rho^2 \int_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y}\, \varphi_\Lambda(\mathbf{x}, \mathbf{y}) \tag{1}$$

We now choose $\varphi_\Lambda(\mathbf{x},\mathbf{y})$ to be the kernel of the inverse of $-\Delta$ on $\tilde{L}^2(\Lambda)$ with periodic boundary conditions, where $\tilde{L}^2(\Lambda)$ is the orthogonal complement in $L^2(\Lambda)$ of the constant functions. In Fourier representation

$$\varphi_\Lambda(\mathbf{x},\mathbf{y}) = \frac{1}{|\Lambda|} \sum_{\substack{\mathbf{k}\neq 0 \\ \mathbf{k}=(2\pi/L)(\mathbb{L}^2)^*}} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{k^2} \tag{2}$$

where $(\mathbb{L}^2)^*$ is the reciprocal lattice.

With this choice of $\varphi_\Lambda(\mathbf{x},\mathbf{y})$, H_Λ becomes

$$H_\Lambda(\mathbf{x}_1, \ldots, \mathbf{x}_N) = e^2 \sum_{i<j} \varphi_\Lambda(\mathbf{x}_i, \mathbf{x}_j) \tag{3}$$

We want to consider perturbations of H_Λ by means of an external localizing field $\alpha\varphi_{\text{ext}}(\mathbf{x})$, $\mathbf{x}\in\mathbb{R}^2$.

Then

$$H_\Lambda^\alpha(\mathbf{x}_1, \ldots, \mathbf{x}_N) = e^2 \sum_{i<j} \varphi_\Lambda(\mathbf{x}_i \cdot \mathbf{x}_j) + \alpha \sum_{i=1}^{N} \varphi_{\text{ext}}(\mathbf{x}_i) \tag{4}$$

Here φ_{ext} is assumed to be a smooth positive function invariant under translations of the lattice $\mathbb{L}^2$ and well localized around the sites in $\mathbb{L}^2$, where it obtains its maximum; α is an arbitrary negative constant. Following Alastuey and Jancovici[3] we now define for an arbitrary fixed vector

$$\mathbf{e}_t \in \mathbb{R}^2, \quad |\mathbf{e}_t| = 1 \quad \text{and} \quad \mathbf{k}\in(2\pi/L)(\mathbb{L}^2)^*; \quad \mathbf{K}\in 2\pi(\mathbb{L}^2)^*$$

$$\begin{aligned} A(\mathbf{x}_1, \ldots, \mathbf{x}_N) &= \sum_{i=1}^{N} \psi(\mathbf{x}_i), \qquad \psi(\mathbf{x}) = e^{i(\mathbf{K}+\mathbf{k})\mathbf{x}} - \delta_{\mathbf{K}+\mathbf{k}} \\ \delta_{\mathbf{K}'} &= 1 \qquad \text{if} \quad \mathbf{K}' = 0 \\ \delta_{\mathbf{K}'} &= 0 \qquad \text{otherwise} \end{aligned} \tag{5}$$

and

$$\begin{aligned} B(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{i=1}^{N} &\exp\left[\,\beta H_\Lambda^\alpha(\mathbf{x}_1, \ldots, \mathbf{x}_N)\right] \\ &\times \left(\nabla_{t_i}\{\varphi(\mathbf{x}_i)\exp\left[-\beta H_\Lambda^\alpha(\mathbf{x}_1, \ldots, \mathbf{x}_N)\right]\}\right) \\ \varphi(\mathbf{x}) &= e^{i\mathbf{k}\mathbf{x}} \end{aligned} \tag{6}$$

Here ∇_{t_i} denotes the gradient $\mathbf{e}_t \cdot \nabla_{\mathbf{x}_i}$ with respect to $\mathbf{x}_i$ in the direction $\mathbf{e}_t$. The Schwarz inequality with respect to the Gibbs measure $\langle f\rangle_\alpha = \int_\Lambda (e^{-\beta H_\Lambda^\alpha}/Z_\Lambda^\alpha) f\, d\mathbf{x}_1, \ldots, d\mathbf{x}_N$ gives

$$\langle |A|^2\rangle_\alpha \geqslant \frac{|\langle A^* B\rangle_\alpha^2}{\langle |B|^2\rangle_\alpha} \tag{7}$$

Using the definition of ψ and φ and the periodic boundary conditions on $\varphi_\Lambda(\mathbf{x},\mathbf{y})$, the above inequality reads (see for details Ref. 3)

$$S(\mathbf{K}+\mathbf{k}) \geqslant \frac{\left[(\mathbf{K}+\mathbf{k})\cdot\mathbf{e}_t\right]^2 \cdot |\rho_{\mathbf{K}}|^2}{(\mathbf{k}\cdot\mathbf{e}_t)^2 + D_{tt}(\mathbf{k})} \tag{8}$$

where

$$S(\mathbf{K}+\mathbf{k}) = \frac{1}{N}\left\langle \left| \sum_{j=1}^{N} \left(e^{i(\mathbf{K}+\mathbf{k})\mathbf{x}}{}_j - \delta_{\mathbf{K}+\mathbf{k}}\right)\right|^2 \right\rangle_\alpha$$

is the structure factor,

$$\rho_{\mathbf{K}} = \left\langle \frac{1}{N} \sum_{j=1}^{N} e^{i\mathbf{K}\cdot\mathbf{x}_j} \right\rangle_\alpha$$

the Fourier transform of the one particle density and

$$D_{tt}(\mathbf{k}) = \frac{1}{N}\left\langle \sum_{i,j} e^{i\mathbf{k}(\mathbf{x}_i-\mathbf{x}_j)} \nabla_{t_i}\nabla_{t_j} H_\Lambda \right\rangle_\alpha + \alpha\langle \nabla_t \nabla_t \varphi_{\exp}\rangle_\alpha = I_{1,\Lambda}(\mathbf{k}) + I_{2,\Lambda}(\mathbf{k})$$

It is clear that $\alpha I_2,(\mathbf{k})$ vanishes if we take the limit $\Lambda\uparrow\mathbb{R}^2$ and $\alpha\to 0$ in the stated order. As for the first term $I_{1,\Lambda}(\mathbf{k})$ we rewrite it as follows:

$$\begin{aligned} I_{1,\Lambda}(\mathbf{k}) &= \frac{1}{N}\left\langle \sum_{i,j} e^{i\mathbf{k}(\mathbf{x}_i-\mathbf{x}_j)} \nabla_{t_i}\nabla_{t_j} H_\Lambda \right\rangle_\alpha \\ &= \frac{1}{N}\left\langle \sum_{\mathbf{p}\neq 0} \frac{(\mathbf{p}\cdot\mathbf{e}_t)^2}{p^2}\left[\sum_{i,j} e^{i(\mathbf{p}-\mathbf{k})(\mathbf{x}_i-\mathbf{x}_j)} - e^{i\mathbf{p}(\mathbf{x}_i-\mathbf{x}_j)}\right]\right\rangle_\alpha \end{aligned}$$

Since $S(\mathbf{p}) = 1/N\langle|\sum_i(e^{i\mathbf{p}\mathbf{x}_j} - \delta_{\mathbf{p}})|^2\rangle_\alpha$, we obtain

$$\begin{aligned} I_{1,\Lambda}(\mathbf{k}) &= \frac{\beta}{\Lambda}\sum_{p\neq 0}\frac{(\mathbf{p}\cdot\mathbf{e}_t)^2}{p^2}\left[(S(\mathbf{p}-\mathbf{k})-1) - (S(\mathbf{p})-1)\right] \\ &\quad + \beta\sum_{p\neq 0}\frac{(\mathbf{p}\cdot\mathbf{e}_t)^2}{p^2}\cdot\left[\delta_{\mathbf{p}-\mathbf{k}} - \delta_{\mathbf{p}}\right] = \bar{I}_{1,\Lambda}(\mathbf{k}) + \bar{\bar{I}}_{1,\Lambda}(\mathbf{k}) \end{aligned}$$

We now choose $\mathbf{e}_t$ such that $\mathbf{e}_t\cdot\mathbf{k} = 0$. Thus $\forall\mathbf{k}\in(2\pi/L)(\mathbb{L}^2)^*$

$$I_{1,\Lambda}(\mathbf{k}) = \bar{I}_{1,\Lambda}(\mathbf{k}) = \beta\rho\int_\Lambda d^2r\, h(\mathbf{r})(1-\cos\mathbf{kr})\nabla_t^2\varphi_\Lambda(\mathbf{r}) \tag{9}$$

where $\rho h(\mathbf{r}) = \tilde{F}(h(\mathbf{p}) = S(\mathbf{p}) - 1)$ and $h(\mathbf{p}=0) = -1$.

As noted in (2) Eq. (9) differs from the corresponding quantity considered by Mermin because of the appearance of $h(\mathbf{r})$ in it instead of the total correlation function $g(\mathbf{r}) = 1 + h(\mathbf{r})$.

It is easy to see now that for r fixed independent of Λ,

$$|\nabla_t^2 \varphi_\Lambda(\mathbf{r})| = \left| \frac{1}{L^2} \nabla_t^2 \varphi_{V=C_0}\left(\frac{\mathbf{r}}{L}\right) \right| \leqslant \frac{C_3}{r^2} + \frac{C_4}{L^2}$$

for positive constants C_3 and C_4 independent of L, where C_0 is the unit cell of $(\mathbb{L}^2)$. The first equality follows from the definition of $\varphi_\Lambda(\mathbf{r})$ and the inequality from the fact that $\varphi_{\Lambda=C_0}(\mathbf{r}) - \ln|\mathbf{r}|$ is a harmonic function in C_0.

We now make the following assumption: there exists positive constants r_0, C_1, C_2, independent of L, for L sufficiently large, such that

$$|h_\Lambda(\mathbf{r})| \leqslant C_1 \forall |\mathbf{r}| \leqslant r_0, \qquad |h_\Lambda(\mathbf{r})| \leqslant \frac{C_2}{r^2} \forall |\mathbf{r}| > r_0 \tag{10}$$

Using this assumption we can now easily estimate $\text{limit}_{\Lambda\uparrow\mathbb{R}^2} I_{1,\Lambda}(\mathbf{k})$ by

$$\lim_{\Lambda\uparrow\mathbb{R}^2} I_{1,\Lambda}(k) \leqslant -C_5 k^2 \ln k$$

for $|\mathbf{k}|$ sufficiently small, $C_5 > 0$. Then with (8) we have $\forall \mathbf{k} \in (2\pi/L)(\mathbb{L}^2)^*$ that

$$S(\mathbf{K}+\mathbf{k}) \geqslant \frac{(\mathbf{K}\cdot\mathbf{e}_t)^2 |\rho_\mathbf{K}|^2}{-\beta C_5 k^2 \ln k} \tag{11}$$

In (11) we have already taken the limit $\alpha \to 0$. The final step follows the line of the original argument given by Mermin. Both sides of (11) are multiplied by a positive Gaussian function $f(|\mathbf{K}+\mathbf{k}|)$, divided by the volume $|\Lambda|$ of the box and summed on all $\mathbf{k} \in (2\pi/L)(\mathbb{L}^2)^*$. Taking the thermodynamic limit $\Lambda\uparrow\mathbb{R}^2$ we get

$$F(0) = \rho \int (h(r)+1) F(r)\, dr \geqslant \int d^2k \frac{|\mathbf{K}\cdot\mathbf{e}_t(\mathbf{k})|^2 |\rho_\mathbf{K}|^2 f(|\mathbf{K}+\mathbf{k}|)}{-\beta C_5 k^2 \ln k} \tag{12}$$

where $F(r)$ is the Fourier transform of f.

By restricting the region of integration on the right-hand side of (12) to the values of $\mathbf{k}$ such that $|\mathbf{K}\cdot\mathbf{e}_t(k)| \geqslant \delta > 0$ and using the divergence of $\int d^2k/-k^2 \ln K$, we get that $\rho_\mathbf{K} = 0\ \forall \mathbf{K} \neq \mathbf{0}$, $\mathbf{K} \in 2\pi(\mathbb{L}^2)^*$.

We remark here that using our assumptions on $h(\mathbf{r})$ the left-hand side of (12) is finite.

For the special two-dimensional case we have treated here, our result is similar to the one given recently,[7] where it was found with a more general approach using the BBGKY hierarchy that if the truncated two-point function [different from our $h(\mathbf{r})$] has a clustering of the type $|\rho^T(\mathbf{x}_1, \mathbf{x}_1 + \mathbf{r})| < (1/r^3) \forall \mathbf{x}_1$, then a crystalline order in the two-dimensional jellium is not possible.

ACKNOWLEDGMENTS

The authors have the pleasure to thank Professor S. Albeverio and Dr. D. Dürr for reading the manuscript and making interesting remarks. They also thank the "Deutsche Forschungsgemeinschaft" for financial support.

REFERENCES

1. N. D. Mermin, *Phys. Rev.* **176**:250 (1968); *Phys. Rev.* **176**:20 (1968).
2. M. Baus, *J. Stat. Phys.* **22**:111 (1980).
3. A. Alastuey and B. Jancovici, *J. Stat. Phys.* **24**:443 (1981).
4. J. W. Perram and S. W. De Leew, *Physica* **113A**:546 (1982).
5. J. M. Caillol, D. Levesque, J. J. Weiss, and J. P. Hansen, *J. Stat. Phys.* **28**:324 (1982).
6. S. Albeverio, D. Dürr, and D. Merlini, *J. Stat. Phys.* **31**:389 (1983).
7. Ch. Gruber, Ph. A. Martin, and Ch. Oguey, *Commun. Math. Phys.* **84**:55 (1982); see also Ch. Gruber and Ph. A. Martin, *Phys. Rev. Lett.* **45**:853 (1980).