

Two-Dimensional Coulomb Systems: a Larger Class of Solvable Models.

F. CORNU and B. JANCOVICI

*Laboratoire de Physique Théorique et Hautes Energies, Université de Paris-Sud
Bât. 211 - 91405 Orsay, France*

(received 9 October 1987; accepted 28 October 1987)

PACS. 05.20. – Statistical mechanics.

Abstract. – Using new methods, we find that a larger class of two-dimensional Coulomb systems are solvable models, in the framework of equilibrium classical statistical mechanics, for the special value $\Gamma = 2$ of the coupling constant. One-component plasmas with adsorption sites, one-component plasmas in a periodic background, and plasmas made of two components plus a background are discussed.

Matter is made of electrons and nuclei interacting through Coulomb's law; therefore, it is obviously of interest to obtain exact theoretical results about Coulomb systems, and even «toy models» of them. The equilibrium statistical mechanics of several models of classical two-dimensional Coulomb systems has already been exactly worked out [1-5], at the special value $\Gamma = 2$ of the coupling constant $\Gamma = \beta e^2$, where $\pm e$ is the charge of a particle and β is the inverse temperature (the Coulomb interaction potential between two particles of charge e at a distance r from one another is $-e^2 \ln(r/L)$, where L is an arbitrary length scale). In this letter, we describe new methods which allow us to compute explicitly the n -body densities for a larger class of models, besides retrieving known results in a simpler and more systematic way.

For the one-component plasma OCP (a system of particles of charge e embedded in a continuous background of opposite charge), we are now able to deal with a variety of nonuniform backgrounds, and especially a background density having the periodicity of a two-dimensional crystal. At $\Gamma = 2$, the Boltzmann factor for N interacting particles with coordinates $\mathbf{r}_i = (x_i, y_i)$ has the same structure in terms of a Slater determinant as the squared wave function of a system of noninteracting fermions, *i.e.*

$$C |\det \{ \exp[-V(\mathbf{r}_i)] z_i^{j-1} \}_{i,j=1,\dots,N}|^2,$$

where C is a constant, $e^2 V(\mathbf{r}_i)$ is the background potential acting on the i -th particle and $z_i = x_i + iy_i$. For a constant background density ρ_b , $V(\mathbf{r})$ can be chosen as $(1/2)\pi\rho_b r^2$, the functions $\exp[-V(\mathbf{r})]z^j$ are mutually orthogonal; to deal with the Slater determinant is a standard problem, and it is easy to perform the integrals which define the n -particle densities and to take their thermodynamic limits [1]. In the general case of a nonuniform

background, the functions $\exp[-V(\mathbf{r})]z^j$ are no longer orthogonal. However, we can follow the same steps as above in terms of a new basis $\varphi_k(z)$ for the entire functions, chosen in such a way that the functions $\psi_k(\mathbf{r}) = \exp[-V(\mathbf{r})]\varphi_k(z)$ are orthogonal, since the Slater determinant is invariant under such a change of basis. In terms of the projector

$$\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle = \sum_p \psi_k(\mathbf{r}_1) \bar{\psi}_k(\mathbf{r}_2) / \int d\mathbf{r} |\psi_k(\mathbf{r})|^2,$$

the n -particle-truncated densities are

$$\begin{cases} \rho(\mathbf{r}) = \langle \mathbf{r} | P | \mathbf{r} \rangle, \\ \rho_T^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = -|\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle|^2, \\ \rho_T^{(n)}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n) = (-)^{n+1} \sum_{(i_1 i_2 \dots i_n)} \langle \mathbf{r}_{i_1} | P | \mathbf{r}_{i_2} \rangle \dots \langle \mathbf{r}_{i_n} | P | \mathbf{r}_{i_1} \rangle, \end{cases} \quad (1)$$

where the summation runs over all cycles $(i_1 i_2 \dots i_n)$ built with $\{1, 2, \dots, n\}$. Thus, the problem is reduced to computing the projector P on that subspace of Hilbert space which is spanned by the entire functions times $\exp[-V(\mathbf{r})]$; this amounts to diagonalizing the matrix formed by the scalar products $\int d\mathbf{r} \bar{z}^i \exp[-2V(\mathbf{r})] z^j$.

As a first application, we can quickly retrieve all the known results [2] about the case where the background potential depends only on one coordinate: $V(\mathbf{r}) = V(x)$. Since V is translationally invariant along y , it is convenient to choose the functions ψ_k as $\exp[-V(x) + k(x + iy)]$, with $k \in \mathbf{R}$; they are indeed orthogonal because of the plane-wave factor $\exp[iky]$. When the particles are confined to the half-space $x > 0$ by an impenetrable wall, the range of k must be restricted to $k > 0$, as it can be seen by reaching this case through a suitable limiting procedure.

When the background potential is periodic along y , with a period b , we can start with the same φ -functions $\exp[k(x + iy)]$, writing $k = 2\pi(\zeta + n)/b$, $\zeta \in [0, 1]$, n integer; the scalar-product matrix is of the form

$$\int d\mathbf{r} \exp[2\pi(\zeta + n)(\bar{z}/b) - 2V(\mathbf{r}) + 2\pi(\zeta' + n)(z/b)] = \delta(\zeta - \zeta') A_\zeta(n, n').$$

Thus, as a second application, we are able to revisit a model for localized adsorption, which has been previously studied [3] by a *tour de force* of expansion resummations; we now obtain more general results in an easier way. The model is a line of equidistant adsorption sites located along the y -axis, creating a potential V_{ads} of the Baxter type, *i.e.* such that $\exp[-\beta V_{\text{ads}}] = 1 + \lambda \delta(x) \sum_m \delta(y - mb)$. The continuous background density $\rho_b(x)$ is assumed to depend only on x , creating a potential chosen as $V_0(x)$. Thus $e^2 V(\mathbf{r}) = e^2 V_0(x) + V_{\text{ads}}$. This is, for instance, a model for an electrode with adsorption sites. The matrix $A_\zeta(n, n')$ is found to be, up to a multiplicative constant, of the form $\delta_{nn'} + f_\zeta(n) f_\zeta(n')$; thus, the diagonalization can be easily completed. We find

$$\begin{aligned} \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle = \exp[-V(\mathbf{r}_1) - V(\mathbf{r}_2)] \int_0^1 d\zeta \sum_{nm} S(\zeta + n) \exp[2\pi(\zeta + n)z_1/b] \cdot \\ \cdot \left\{ \delta_{nm} - \frac{\lambda \exp[-2V_0(0)] S(\zeta + m)}{1 + \lambda \exp[2V_0(0)] \sum_l S(\zeta + l)} \right\} \exp[2\pi(\zeta + m)\bar{z}_2/b], \end{aligned}$$

where S is a normalization factor:

$$S(\zeta + n) = \left\{ b \int dx \exp[4\pi(\zeta + n)x/b] \exp[-2V_0(x)] \right\}^{-1}.$$

The summations on n, m , are on \mathbf{Z} if the system occupies the whole plane, on \mathbf{N} if the system is confined to the half-plane $x > 0$.

Lastly, we can deal with a background density having the double periodicity of a two-dimensional crystal. This model can be understood as made of mobile «electrons» interacting between themselves and with a lattice of extended fixed «ions»; this classical caricature of a metal (or perhaps of an ionic superconductor) has already been studied by computer simulation [6]. The background potential is of the form $e^2V(\mathbf{r}) = e^2[V_0(x) + \phi(x, y)]$, where the potential $e^2V_0(x)$ created by the average background density ρ_0 can be taken such that $V_0(x) = \pi\rho_0 x^2$ and $e^2\phi(x, y)$ is a doubly periodical potential: $\phi(x + na, y + mb) = \phi(x, y)$; since there is one ion per lattice cell, $\rho_0 = (ab)^{-1}$. As a consequence of the symmetries of $V(\mathbf{r})$, an orthogonal basis is formed by the Bloch-type functions

$$\psi_{\zeta\tau}(\mathbf{r}) = \sum_n \exp[2\pi i\tau n] [S(\zeta + n)]^{1/2} \exp[-V(\mathbf{r}) + 2\pi(\zeta + n)z/b],$$

with $\zeta, \tau \in [0, 1]$. The two-body correlation function is found to obey the Stillinger-Lovett sum rule [7] which characterizes a conducting phase. The detail will be published elsewhere; triangular lattices are also tractable. Here, we only quote a result for the simplest choice: a square lattice with $a = b = 1$, and $\exp[-2\phi] = 1 + \lambda(\cos 2\pi x + \cos 2\pi y)$. Then, the one-particle density is

$$\rho(\mathbf{r}) = \rho_0 \sqrt{2} \exp[-2\varphi] \int_{-\infty}^{\infty} d\zeta \int_{-\infty}^{\infty} d\tau \frac{\exp[-\pi(x - \zeta)^2 - \pi(y - \tau)^2 - 2i\pi(x - \zeta)(y - \tau)]}{1 + \lambda \exp[-\pi/2](\cos 2\pi\zeta + \cos 2\pi\tau)}.$$

We are also able to generalize known results [5, 8-10] about the two-component plasma TCP (a system of positive and negative particles of charges $\pm e$). At $\Gamma = 2$, the TCP is equivalent to a free-fermion field. The system is unstable against collapse, unless some short-distance cut-off is introduced; however, if the cut-off is removed at constant *fugacity*, although the one-particle densities diverge, the n -particle-truncated densities ($n \geq 2$) have well-defined limits. We are able to consider a generalized TCP, made of positive particles, negative particles and a charged positive background. The background potential can be taken into account by introducing position-dependent fugacities $m_s(\mathbf{r}) = m_s \exp[2sV(\mathbf{r})]$, where $s = +1(-1)$ if the particle at \mathbf{r} is positive (negative). The n -particle densities are again of the form (1), where now $\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle$ is a 2×2 matrix in charge space (its $s_1 s_2$ element corresponds to a particle of charge $s_1 e(s_2 e)$ at $\mathbf{r}_1(\mathbf{r}_2)$); this matrix is no longer a projector but the Green function

$$\langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle_{s_1 s_2} = [m_{s_1}(\mathbf{r}_1)]^{1/2} \langle \mathbf{r}_1 | \left[\sigma_x \partial_x + \sigma_y \partial_y + \sum_{s=\pm 1} m_s(\mathbf{r}) \frac{1 + s\sigma_z}{2} \right]^{-1} | \mathbf{r}_2 \rangle_{s_1 s_2} [m_{s_2}(\mathbf{r}_2)]^{1/2},$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices. These matrix elements can be re-expressed in terms of the isoscalar operators $A = \partial_x + i\partial_y + \partial_x V + i\partial_y V$ and $A^+ = -\partial_x + i\partial_y + \partial_x V - i\partial_y V$ as

$$\begin{cases} \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle_{--} = \langle \mathbf{r}_1 | m^2 [m^2 + A^+ A]^{-1} | \mathbf{r}_2 \rangle, \\ \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle_{++} = \langle \mathbf{r}_1 | m^2 [m^2 + A A^+]^{-1} | \mathbf{r}_2 \rangle, \\ \langle \mathbf{r}_1 | P | \mathbf{r}_2 \rangle_{+-} = -\overline{\langle \mathbf{r}_2 | P | \mathbf{r}_1 \rangle_{-+}} = -\langle \mathbf{r}_1 | mA [m^2 + A^+ A]^{-1} | \mathbf{r}_2 \rangle, \end{cases} \quad (2)$$

where $m^2 = m_+ m_-$.

In the case of a uniform background of charge density $e\varphi$, we can choose $V(\mathbf{r}) = (1/2)\pi\varphi r^2$. The inversion of $m^2 + A^+A$ and $m^2 + AA^+$ is easily done by solving a simple differential equation if we take \mathbf{r}_2 at the origin; this is enough for computing $\rho_T^{(2)}$ which depends only on $r = |\mathbf{r}_1 - \mathbf{r}_2|$. We find

$$\langle \mathbf{r} | P | 0 \rangle_{--} = \rho \Gamma(\alpha + 1) (\pi\varphi r^2)^{-1/2} W_{(1/2) - \alpha, 0}(\pi\varphi r^2),$$

$$\langle \mathbf{r} | P | 0 \rangle_{++} = \rho \alpha \Gamma(\alpha + 1) (\pi\varphi r^2)^{-1/2} W_{-(1/2) - \alpha, 0}(\pi\varphi r^2),$$

where $\alpha = m^2/4\pi\varphi$ and W is a Whittaker function; the $(+ -)$ and $(- +)$ matrix elements can be obtained by acting with the operator A .

In the limit $\varphi \rightarrow 0$, we recover the usual TCP without a background. In the limit $m_+ \rightarrow 0$, the positive particles disappear and we are left with an OCP of negative particles in a positive background. In this limit, (2) becomes the projector on the solutions ψ of $A\psi = 0$, and these solutions are indeed of the form of an entire function of $z = x + iy$ times $\exp[-V]$. Thus, the OCP appears as a limiting case of our generalized TCP.

* * *

We are indebted to A. ALASTUEY and L. BLUM for stimulating discussions. The Laboratoire de Physique Théorique et Hautes Energies is a Laboratoire Associé au Centre National de la Recherche Scientifique.

REFERENCES

- [1] JANCOVICI B., *Phys. Rev. Lett.*, **46** (1981) 386.
- [2] ALASTUEY A. and LEBOWITZ J. L., *J. Phys. (Paris)*, **45** (1984) 1859, and references quoted therein.
- [3] ROSINBERG M. L., LEBOWITZ J. L. and BLUM L., *J. Stat. Phys.*, **44** (1986) 153.
- [4] GAUDIN M., *J. Phys. (Paris)*, **46** (1985) 1027.
- [5] CORNU F. and JANCOVICI B., *J. Stat. Phys.*, **49** (1987) 33.
- [6] CLÉROUIN J. and HANSEN J. P., *Phys. Rev. Lett.*, **54** (1985) 2277; CLÉROUIN J., HANSEN J. P. and PILLER B., *Phys. Rev. A* (to be published).
- [7] STILLINGER F. H. and LOVETT R., *J. Chem. Phys.*, **49** (1968) 1991.
- [8] COLEMAN S., *Phys. Rev. D*, **11** (1975) 2088.
- [9] MANDELSTAM S., *Phys. Rev. D*, **11** (1975) 3026.
- [10] SAMUEL S., *Phys. Rev. D*, **18** (1978) 1916.