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

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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 $\exp[-V(\boldsymbol{r})]\,z^j$ 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 $\psi_k(\boldsymbol{r}) = \exp[-V(\boldsymbol{r})]\,\varphi_k(z)$ are orthogonal, since the Slater determinant is invariant under such a change of basis. In terms of the projector

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

the n-particle–truncated densities are

$$\begin{cases} \rho(\boldsymbol{r}) = \langle \boldsymbol{r}|P|\boldsymbol{r}\rangle\,, \\ \rho_T^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = -\,|\langle \boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle|^2\,, \\ \rho_T^{(n)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n) = (-)^{n+1} \sum\limits_{(i_1 i_2 \ldots i_n)} \langle \boldsymbol{r}_{i_1}|P|\boldsymbol{r}_{i_2}\rangle \ldots \langle \boldsymbol{r}_{i_n}|P|\boldsymbol{r}_{i_1}\rangle\,, \end{cases} \tag{1}$$

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

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: $V(\boldsymbol{r}) = V(x)$. Since V is translationally invariant along y, it is convenient to choose the functions ψ_k as $\exp[-V(x) + k(x+iy)]$, with $k \in \boldsymbol{R}$; 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

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

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 $\exp[-\beta V_{\mathrm{ads}}] = 1 + \lambda\delta(x)\sum_m \delta(y - mb)$. The continuous background density $\rho_{\mathrm{b}}(x)$ is assumed to depend only on x, creating a potential chosen as $V_0(x)$. Thus $e^2V(\boldsymbol{r}) = e^2V_0(x) + V_{\mathrm{ads}}$. 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

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

where S is a normalization factor:

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

The summations on n, m, are on $\boldsymbol{Z}$ if the system occupies the whole plane, on $\boldsymbol{N}$ 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 a ionic superconductor) has already been studied by computer simulation [6]. The background potential is of the form $e^2V(\boldsymbol{r})=e^2[V_0(x)+\phi(x,y)]$, where the potential $e^2V_0(x)$ created by the average background density ρ_0 can be taken such that $V_0(x)=\pi\rho_0x^2$ 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 $V(\boldsymbol{r})$, an orthogonal basis is formed by the Bloch-type functions

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

with $\zeta,\eta\in[0,1]$. 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

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

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 $m_s(\boldsymbol{r})=m_s\exp[2sV(\boldsymbol{r})]$, where $s=+1(-1)$ if the particle at $\boldsymbol{r}$ is positive (negative). The n-particle densities are again of the form (1), where now $\langle\boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle$ is a 2×2 matrix in charge space (its s_1s_2 element corresponds to a particle of charge $s_1e(s_2e)$ at $\boldsymbol{r}_1(\boldsymbol{r}_2)$); this matrix is no longer a projector but the Green function

$$\langle\boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle_{s_1s_2}=[m_{s_1}(\boldsymbol{r}_1)]^{1/2}\langle\boldsymbol{r}_1|\left[\sigma_x\partial_x+\sigma_y\partial_y+\sum_{s=\pm1}m_s(\boldsymbol{r})\frac{1+s\sigma_z}{2}\right]^{-1}|\boldsymbol{r}_2\rangle_{s_1s_2}[m_{s_2}(\boldsymbol{r}_2)]^{1/2},$$

where σ_x, σ_y, σ_z are the Pauli matrices. These matrix elements can be re-expressed in terms of the isoscalar operators $A=\partial_x+i\partial_y+\partial_xV+i\partial_yV$ and $A^+=-\partial_x+i\partial_y+\partial_xV-i\partial_yV$ as

$$\begin{cases}\langle\boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle_{--}=\langle\boldsymbol{r}_1|m^2[m^2+A^+A]^{-1}|\boldsymbol{r}_2\rangle\,,\\ \langle\boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle_{++}=\langle\boldsymbol{r}_1|m^2[m^2+AA^+]^{-1}|\boldsymbol{r}_2\rangle\,,\\ \langle\boldsymbol{r}_1|P|\boldsymbol{r}_2\rangle_{+-}=-\overline{\langle\boldsymbol{r}_2|P|\boldsymbol{r}_1\rangle}_{-+}=-\langle\boldsymbol{r}_1|mA[m^2+A^+A]^{-1}|\boldsymbol{r}_2\rangle\,,\end{cases}\tag{2}$$

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

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

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

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

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

In the limit $\rho \to 0$, we recover the usual TCP without a background. In the limit $m_+ \to 0$, 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.

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