

E5969: 2D Coulomb gas

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The problem:

N ions of positive charge q and N ions of negative charge $-q$ are constrained to move in a two dimensional square of side L and area $A = L^2$. The interaction energy of charge q_i at position r_i with another charge q_j at position r_j is $-q_i q_j \ln[|r_i - r_j|/a]$, where $q_i, q_j = \pm q$ and a is a microscopic length scale. The mass of the ions is m .

- (a) By rescaling space variables to $r_i := r_i/L$, the partition function can be written as $Z(L) = CL^\alpha$, where C does not depend on L . Find α . Hint: $\sum_{ij} q_i q_j$ has a very simple dependence on N .
- (b) Calculate the pressure, and show that for $T < T_c$ the system is unstable. Determine what is T_c . Comment on the reason for this instability.
- (c) Determine what is C if the dimensionless dr integral is approximated by unity. In particular verify that your expression is strictly correct if $q = 0$.
- (d) Find the chemical potential $\mu(T, N, L)$, and solve for $N(\mu, T, L)$, using C of the previous item.

The solution:

- (a) The system Hamiltonian is given by:

$$H = \sum_{i=1}^{2N} \frac{\mathbf{p}_i^2}{2m} + \sum_{\langle ij \rangle} u(\mathbf{r}_i - \mathbf{r}_j) \quad (1)$$

Where the sum $\sum_{\langle ij \rangle}$ is over distinct pairs. Thus the canonical partition function is given by:

$$Z_{2N}(\beta, V) = Z_{\text{kin}} \int_0^L d^2 r_1 \dots d^2 r_{2N} \exp \left[\beta \sum_{\langle ij \rangle} q_i q_j \ln (|\mathbf{r}_i - \mathbf{r}_j|/a) \right] \quad (2)$$

Where Z_{kin} is the kinetic part of the partition function, including the Gibbs factor. Defining $r_i := \tilde{r}_i L$, Eq(2) can be rewritten as:

$$Z_{2N}(\beta, V) = Z_{\text{kin}} \cdot L^{4N} \int_0^1 d^2 \tilde{r}_1 \dots d^2 \tilde{r}_{2N} \exp \left[\beta \sum_{\langle ij \rangle} q_i q_j \ln \left(\frac{L}{a} |\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j| \right) \right] \quad (3)$$

We now need to calculate the sum $\sum_{\langle ij \rangle} q_i q_j$. There are $\frac{1}{2}N(N-1)$ of each $(+q)(+q)$ and $(-q)(-q)$ product pairs and N^2 mixed pairs. Altogether:

$$\sum_{\langle ij \rangle} q_i q_j = q^2(N_{++} + N_{--} - N_{+-}) = q^2[N(N-1) - N^2] = -q^2 N \quad (4)$$

Substituting into Eq(3) we get:

$$Z_{2N}(\beta, V) = Z_{\text{kin}} \cdot L^{4N} \cdot \left(\frac{L}{a} \right)^{-\beta q^2 N} \int_0^1 d^2 \tilde{r}_1 \dots d^2 \tilde{r}_{2N} \prod_{\langle ij \rangle} |\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|^{\beta q_i q_j} \equiv CL^\alpha \quad (5)$$

So:

$$\alpha = N(4 - \beta q^2). \quad (6)$$

(b) Since C does not depend on L calculating the pressure is straightforward:

$$P = T \frac{\partial \ln Z}{\partial A} = T \frac{\partial}{\partial A} \ln \left(C A^{\alpha/2} \right) = \frac{\alpha T}{2A} \quad (A \equiv L^2) \quad (7)$$

It is apparent from Eq(6) that there is a region in which $\alpha < 0$ and in turn, from Eq(7), $P < 0$. This implies an unstable system when:

$$T < \frac{q^2}{4} \equiv T_c. \quad (8)$$

Disregarding entropy, it is favorable for opposite charged ions to bunch together and for similarly charged ions to stay apart. Given a limited confining area A , The $T=0$ ground state configuration will consist of positive and negative ions pairing up and collapsing into one another. Possibly (although not described by this model) they will "combine" to form neutral molecules.

(c) Approximating the dimensionless $d^{4N} \tilde{r}$ integral in Eq(5) by unity, the factor C simplifies to:

$$C = Z_{\text{kin}} \cdot \left(\frac{1}{a} \right)^{-\beta q^2 N} = \left(\frac{1}{N!} \right)^2 \left(\frac{1}{\lambda_T^2} \right)^{2N} \cdot \left(\frac{1}{a} \right)^{-\beta q^2 N} \quad (9)$$

Z_{kin} in the equation above consists of the standard kinetic factor for a system with $2N$ particles $\left(\frac{1}{\lambda_T^2} \right)^{2N}$ and a Gibbs factor of $\left(\frac{1}{N!} \right)^2$. The reasoning behind the Gibbs factor above as apposed to $\frac{1}{(2N)!}$ is that the particles are only exchangeable amongst their equally charged peers. And in fact, for $q = 0$ and C from Eq(9), Eq(5) simplifies to:

$$Z_{2N}(\beta, V) = \left[\frac{1}{N!} \left(\frac{A}{\lambda_T^2} \right)^N \right]^2 \quad (10)$$

Meaning the problem is reduced to the 2D ideal gas case where the partition function can be factored into two partition functions of N identical particles which in turn factorize to single particle partition functions.

(d) The partition function in full, using C of the previous item, is:

$$Z_{2N}(\beta, V) = \frac{1}{N!^2} \left(\frac{A}{\lambda_T^2} \right)^{2N} \left(\frac{L}{a} \right)^{-\beta q^2 N} \quad (11)$$

And the chemical potential, of either the positive or the negative ions, is:

$$\mu_{\pm}(T, N, L) = T \frac{\partial \ln Z}{\partial N} = -T \frac{\partial}{\partial N} \ln \left[\frac{1}{N!^2} \cdot \left(\frac{A}{\lambda_T^2} \right)^{2N} \cdot \left(\frac{a^2}{A} \right)^{2N \frac{T_c}{T}} \right] \quad (12)$$

Where we substituted T_c from Eq(8). From the equation above we recognize the contribution of twice the standard N particle ideal 2D gas $\mu_N^{2D} = T \ln \left(\frac{N\lambda_T^2}{A} \right)$. The remaining term accounts for the interaction, all together:

$$\mu_{\pm}(T, N, L) = 2 \left[T \ln \left(\frac{N\lambda_T^2}{A} \right) + T_c \ln \left(\frac{A}{a^2} \right) \right] \quad (13)$$

Reversing the formula to get $N(\mu, \tau, L)$ yields :

$$N(\mu, \tau, L) = \frac{A}{\lambda_T^2} \cdot e^{\frac{\mu/2}{T}} \cdot \left(\frac{a^2}{A} \right)^{\frac{T_c}{T}} . \quad (14)$$

The the equation above shows that for $T < T_c$ and constant chemical potential μ we have $N \rightarrow \infty$ as $A \rightarrow \infty$ which hints of the instability.