

E5969: 2D Coulomb gas

Submitted by: Yair Margalit

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 $-q_i q_j \ln|r_i - r_j|$, where $q_i, q_j = \pm q$. 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: $\sum_{\langle ij \rangle} q_i q_j$ 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 interaction can be neglected. Handle the Gibbs factor correctly.
- (d) Find the chemical potential $\mu(T, N, L)$, and solve for $N(\mu, T, L)$. In particular write what is N for a fixed μ in the limit $L \rightarrow \infty$ for both $T > T_c$ and $T < T_c$.

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 $\sum_{\langle ij \rangle}^{2N}$ is only over distinct pairs. Thus the canonical partition function is given by:

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

Where Z_{kin} is the kinetic part of the partition function, including the Gibbs factor. Using rescaling such that $r_i = \tilde{r}_i L$, $dr_i = d\tilde{r}_i L$ we obtain:

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

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

We now need to calculate the sum $\sum_{\langle ij \rangle} q_i q_j$. Observing that there are in total $N(N-1)$ positive product pairs and N^2 negative product pairs, by subtracting we get:

$$\sum_{\langle ij \rangle} q_i q_j = q^2(N_{pos} - N_{neg}) = q^2[N(N-1) - N^2] = -q^2 N \quad (5)$$

Substituting into eq. 4 we get:

$$Z_{2N}(\beta, V) = Z_{kin} L^{4N - \beta q^2 N} \int_0^1 d^2 \tilde{r}_1 \dots d^2 \tilde{r}_{2N} \exp[\beta \sum_{\langle ij \rangle} q_i q_j \ln(L|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|)] \equiv CL^\alpha \quad (6)$$

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

$$P = - \left(\frac{\partial F}{\partial A} \right)_{\tau, N} = \tau \frac{\partial}{\partial A} \ln(CA^{\alpha/2}) = \frac{\tau \alpha}{2A} \quad (7)$$

The system will become unstable in the region where $\frac{\partial P}{\partial A} > 0$:

$$\frac{\partial P}{\partial A} = - \frac{\tau \alpha}{2A^2} = \frac{N}{2A^2} (q^2 - 4\tau) > 0 \quad (8)$$

$$\Rightarrow T < \frac{q^2}{4k_B} \equiv T_c \quad (9)$$

This unphysical positive slope in which the pressure increases as the area is increased indicates a phase transition (similar to the Van Der Waals gas case) due to positive - negative ion pairing, and in this regime both phases (ion pairs and free ions) coexist.

(c) If the interaction can be neglected then the partition function takes the form:

$$Z_{2N}(\beta, V) = \frac{1}{(N!)^2} \left(\frac{1}{\lambda_T^2} \right)^{2N} \int_0^L d^2 r_1 \dots d^2 r_{2N} \quad (10)$$

$$= \frac{1}{(N!)^2} \left(\frac{L^2}{\lambda_T^2} \right)^{2N} \equiv CL^{4N} = \frac{(Z_1^{2D})^{2N}}{(N!)^2} \quad (11)$$

Meaning the problem is reduced to the 2D ideal gas case where the partition function can be factorized to single particle partition functions. The only difference is the reduction of the Gibbs factor which is due to the fact that we have two distinct groups of N ions each.

(d) In order to find the chemical potential we will explicitly write the partition function, including the kinetic part:

$$Z_{2N}(\beta, V) = \frac{L^{4N - \beta q^2 N}}{(N!)^2 \lambda_T^{4N}} \int_0^1 d^2 \tilde{r}_1 \dots d^2 \tilde{r}_{2N} \exp[\beta \sum_{\langle ij \rangle} q_i q_j \ln(L|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|)] \quad (12)$$

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

$$\mu_{\pm}(\tau, N, L) = \left(\frac{\partial F}{\partial N_{\pm}} \right)_{\tau, A} \quad (13)$$

$$= -\tau \frac{\partial}{\partial N} \ln \left[\frac{L^{4N - \beta q^2 N}}{(N!)^2 \lambda_T^{4N}} \int_0^1 d^2 \tilde{r}_1 \dots d^2 \tilde{r}_{2N} \exp[\beta \sum_{\langle ij \rangle} q_i q_j \ln(L|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j|)] \right] \quad (14)$$

$$= 2\tau \ln(N \lambda_T^2) - (4\tau - q^2) \ln(L) \quad (15)$$

Where the integral disappears being independent of N . In order to get $N(\mu, \tau, L)$ we simply reverse the formula:

$$N(\mu, \tau, L) = \frac{e^{\frac{\beta\mu}{2}}}{\lambda_T^2} L^{2 - \frac{\beta q^2}{2}} \quad (16)$$

The limit of $L \rightarrow \infty$:

For $T < T_c$ L 's exponent is negative, we get $N(\mu, \tau, L) \rightarrow 0$ indicating that the number of ions in the system goes to zero due to pair creation and all the particles that remain are neutral.

For $T > T_c$ L 's exponent is positive and we get $N(\mu, \tau, L) \rightarrow \infty$ which is the same as the classical result, meaning interactions becomes negligible compared to the temperature and we return to the ideal gas case as in (c).