Aix*Marseille université

Homework 3 – Statistical Physics

Physics Master 2020

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Abstract

The goal of this assignment is to study, using the virial cumulant expansion, the Debye-Hückel theory of an electron plasma.

1. Electron plasma Debye-Hückel screening theory

A simple diluted plasma is a neutral gas of electrostatically interacting electrons in a background of ions. The electron mass and charge are noted m and $-e$, respectively; the system hamiltonian is

$$H_N = H_0(\boldsymbol{P}) + W(\boldsymbol{X}) = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \sum_{nm=1}^{N} w(|\boldsymbol{x}_n - \boldsymbol{x}_m|) \tag{1}$$

where the first term H_0 is the kinetic energy of N electrons, and the second term W, the interaction energy, contains the two particles coulomb potential

$$w(r) = \frac{\alpha}{r} - w_0\,, \quad \alpha = \frac{e^2}{4\pi\varepsilon_0} \tag{2}$$

where $r = |\boldsymbol{x}|$ is the distance between the two electrons, and we added a constant w_0 which takes into account the neutralizing ion background. It ensures that the integral

$$\int_0^\infty 4\pi r^2 \, \mathrm{d}r \, w(r) = 0\,, \tag{3}$$

vanishes; we also defined the phase space coordinates $\boldsymbol{X} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)$ and $\boldsymbol{P} = (\boldsymbol{p}_1, \dots, \boldsymbol{p}_N)$.

1.1. Cumulant expansion

The partition function,

$$Z(T,V,N) = \frac{1}{N!} \int_{\mathbb{R}^N} \frac{\mathrm{d}\boldsymbol{P}}{(2\pi\hbar)^{3N}} \int_{V^N} \mathrm{d}\boldsymbol{X} \mathrm{e}^{-H_0(\boldsymbol{P})/T} \mathrm{e}^{-W(\boldsymbol{X})/T} \tag{4}$$

where V is the system's volume.

1. Show that

$$Z = Z_0 \langle \mathrm{e}^{-W(\boldsymbol{x})/T} \rangle \,, \quad \langle \cdots \rangle = \int_{\mathbb{R}^N} \frac{\mathrm{d}\boldsymbol{p}}{(2\pi\hbar)^{3N}} \frac{\mathrm{e}^{-H_0(\boldsymbol{p})/T}}{Z_0} (\cdots) \tag{5}$$

with Z_0 the ideal gas partition function ($W = 0$):

$$Z_0 = \frac{1}{N!} \left(\frac{V}{\lambda} \right)^{3N} \,, \quad \lambda = \sqrt{\frac{2\pi\hbar^2}{mT}} \,. \tag{6}$$

The brackets $\langle \cdots \rangle$ are for the mean over the non-interacting system probability distribution.

The cumulant expansion of the canonical partition function is defined by the power series,

$$\ln Z = \ln Z_0 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\langle\!\langle W^n \rangle\!\rangle}{T^n} \tag{7}$$

where the cumulant of the interaction energy $\langle\!\langle W^n \rangle\!\rangle$ contains all the terms of order n in the expansion of the logarithm:

$$\langle\!\langle W \rangle\!\rangle = \langle W \rangle = \bullet = \frac{N(N-1)}{2V} \int_0^{\infty} 4\pi r^2 \, \mathrm{d}r \, w(r) \tag{8}$$

is the first order term ; the second order one is,

$$\langle\!\langle W^2 \rangle\!\rangle = \bullet\!\!-\!\!\bullet = \langle W^2 \rangle - \langle W \rangle^2 \,, \tag{9}$$

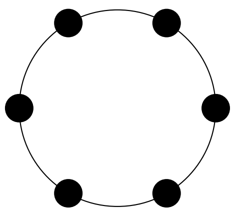
or explicitly,

$$\langle\!\langle W^2 \rangle\!\rangle = \overline{\sum_{1234}} \left[\langle w(\boldsymbol{x}_1 - \boldsymbol{x}_2) w(\boldsymbol{x}_3 - \boldsymbol{x}_4) \rangle - \langle w(\boldsymbol{x}_1 - \boldsymbol{x}_2) \rangle \langle w(\boldsymbol{x}_3 - \boldsymbol{x}_4) \rangle \right] \tag{10}$$

where the barred sum takes only over the connected closed paths (represented by the diagrams), in the case of two particles it corresponds to $1 \to 2 \to 1$ (or for instance, $1 = 4$ and $2 = 3$), leading to

$$\langle\!\langle W^2 \rangle\!\rangle = \frac{N(N-1)}{2} \left[\int_0^{\infty} 4\pi r^2 \frac{\mathrm{d}r}{V} \, w(r)^2 - \left(\int_0^{\infty} 4\pi r^2 \frac{\mathrm{d}r}{V} \, w(r) \right)^2 \right] . \tag{11}$$

A typical graph contributing to the partition function is the ring,



$= \langle w(12) w(23) \ldots w(61) \rangle$

1.2. Ring graph cumulant

In the case of the coulomb interaction, because of its long range, the usual cumulant expansion breaks down. We need to compute terms with arbitrary powers of the density. We focus here on the ring graphs, which give, as we will demonstrate, a physically interesting picture of the diluted plasma high temperature plasma.

Therefore, we calculate now the contribution of these ring graphs to the logarithm of the partition function, neglecting the other possible graphs. This corresponds to the diluted limit.

2. Compute the fourier transform of the coulombian two particles interaction $w(\boldsymbol{k})$, where $\boldsymbol{k}$ is the wavenumber, conjugate to $\boldsymbol{x}$. The neutrality condition ensures $w(0) = 0$. Show that for $\boldsymbol{k} \neq 0$,

$$w(\boldsymbol{k}) = \frac{4\pi\alpha}{k^2} \tag{12}$$

3. Compute, using the convolution theorem, the ring graph of order $n \geq 2$:

$$R_n = \int_{V^n} \prod_{i=1}^{n} \frac{\mathrm{d}\boldsymbol{x}_i}{V} w(\boldsymbol{x}_1 - \boldsymbol{x}_2) w(\boldsymbol{x}_2 - \boldsymbol{x}_3) \dots w(\boldsymbol{x}_n - \boldsymbol{x}_1) \,. \tag{13}$$

   Show that the result of this integration is

$$R_n = \frac{1}{V^{n-1}} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} w(\boldsymbol{k})^n \,. \tag{14}$$

1.2.1. Convolutions

Consider the integral

$$I = \int \mathrm{d}x_1 \,\mathrm{d}x_2 \,\mathrm{d}x_3 f(x_1 - x_2) f(x_2 - x_3) f(x_3 - x_1)$$

the change of variables $x_{12} = x_1 - x_2$, $x_{23} = x_2 - x_3$, gives

$$I = \int \mathrm{d}x_{12} \,\mathrm{d}x_{23} \,\mathrm{d}x_3 f(x_{12}) f(x_{23}) f(-x_{12} - x_{23}) \,,$$

we observe that the integral do not depend on x_3, then

$$I = V \int \mathrm{d}x_{12} \,\mathrm{d}x_{23} f(x_{12}) f(x_{23}) f(-x_{12} - x_{23}) \,,$$

where V results form the integration over x_3. Now we use the fourier transform

$$f(x) = \int \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}kx} f(k)$$

to transform the integral into,

$$I = V \int \mathrm{d}x_{12} \,\mathrm{d}x_{23} \int \frac{\mathrm{d}k_1}{2\pi} \frac{\mathrm{d}k_2}{2\pi} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}k_1 x_{12}} \mathrm{e}^{\mathrm{i}k_2 x_{23}} \mathrm{e}^{-\mathrm{i}k(x_{12} + x_{23})} f(k_1) f(k_2) f(k).$$

Using the fourier representation of the Dirac delta,

$$\int \mathrm{d}x \mathrm{e}^{\mathrm{i}kx} = 2\pi\delta(k)$$

we easily obtain

$$I = V \int \frac{\mathrm{d}k}{2\pi} f(k)^3 \,.$$

1.2.2. The logarithm of the partition function

4. Explain the formula

$$N_R(n) = \frac{N!}{(N-n)!} \times (n-1)! \times \frac{1}{2} \tag{15}$$

of the number of ring graphs with n points (the coordinates appearing in the binary interaction factors). Use the stirling formula to show that

$$N_R(n) = \frac{(n-1)!}{2} N^n \tag{16}$$

5. The rings contribution to $\ln Z$ is

$$\ln Z_R = \ln Z_0 + \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} N_R(n) \frac{R_n}{T^n} \tag{17}$$

Replacing the previous expression (14) and (16) demonstrate the relation

$$\ln Z_R = \ln Z_0 + \frac{V}{12\pi}\kappa^2, \quad \kappa = \sqrt{\frac{4\pi\alpha n}{T}} \tag{18}$$

where κ^{-1} is the Debye length and n the density.
Useful formulas:

$$\ln(1+x) = \sum_{n=1}^{\infty} \frac{(-x)^n}{n}$$

$$\int_0^{\infty} \mathrm{d}x \, \frac{1}{1+x^2} = \frac{\pi}{2}$$

6. Compute the equation of state:

$$P = T\frac{\partial}{\partial V} \ln Z_R \tag{19}$$

and show that,

$$P = P_0 - \frac{T}{24\pi}\kappa^3 \,. \tag{20}$$

Discuss the pressure behavior as a function of the temperature. What happens when $\kappa n^{1/3} > 1$? (dense state limit).

1.3. Debye effective potential

The previous discussion shows that the collective effect of the coulomb interaction modifies the pressure, introducing a *negative* correction of the order $\kappa n^{1/3}$. This is related to the long range of the coulomb potential. We ask now what is the effective interaction of two charges, in the same approximation (related to the ring graphs).

We define the effective potential by

$$\overline{w}(\boldsymbol{x}-\boldsymbol{y}) = w(\boldsymbol{x}-\boldsymbol{y}) + \sum_{n=1}^{\infty} \left(\frac{-N}{TV}\right)^n \int_{V^N} \mathrm{d}\boldsymbol{x}_1 \dots \mathrm{d}\boldsymbol{x}_n w(\boldsymbol{x}-\boldsymbol{x}_1) \dots w(\boldsymbol{x}_n - \boldsymbol{y}) \tag{21}$$

which leads to the screened Debye potential:

$$\overline{w}(\boldsymbol{x}) = \alpha \frac{\mathrm{e}^{-\kappa|\boldsymbol{x}|}}{|\boldsymbol{x}|} \,. \tag{22}$$

This formula takes into account the paths form $\boldsymbol{x}$ to $\boldsymbol{y}$ without loops; identifying the extreme points gives the ring graph.

7. To demonstrate this formula, show that the second order term (in w^2), can be written as,

$$\overline{w}_2(\boldsymbol{x}-\boldsymbol{y}) = w(\boldsymbol{x}-\boldsymbol{y}) - \frac{N}{VT}\int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} w(\boldsymbol{k})^2 \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \tag{23}$$

8. The generalization of (23) is straightforward:

$$\overline{w}(\boldsymbol{x}) = w(\boldsymbol{x}-\boldsymbol{y}) + \sum_{n=1}^{\infty}\left(\frac{N}{VT}\right)^n \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} w(\boldsymbol{k})^{n+1} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \tag{24}$$

   Compute the integral via the residue theorem to obtain the Debye potential (22).
   Hint. Use spherical coordinates $\mathrm{d}\boldsymbol{k} = 2\pi\sin(\theta)k^2\,\mathrm{d}k\,\mathrm{d}\theta$, and integrate the angle θ. You get the integral

$$\overline{w}(\boldsymbol{x}) = \frac{\alpha}{\pi}\int_{-\infty}^{\infty} \mathrm{d}k\,\frac{\sin(kx)}{kx}\sum_{n=0}^{\infty}(-1)^n\left(\frac{\kappa}{k}\right)^{2n}$$

   that, after summation of the power series, can be computed using residues.
9. (Optional question) Use the Poisson formula for the electrostatic potential, and consider the electrons distributed according to the Boltzmann distribution in a uniform ion background, to find the Debye length and the Debye potential.

The Debye-Hückel theory is discussed in the book by Kardar [1] (problems section of chapter 5).

References

[1] M. Kardar. *Statistical Physics of Particles*. Cambridge University Press, 2007.