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On a neutral plasma with quadratic interactions

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Abstract. We calculate the free energy per particle and the correlation functions for a d-dimensional, two-component plasma with quadratic interactions and show that the system's thermodynamics is equivalent to that of a two-component ideal gas mixture. For distinguishable particles this equivalence holds both classically and quantum mechanically.

1. Introduction

A neutral plasma consists of $2N$ particles with charges q_j, $1 \leqslant j \leqslant 2N$, such that

$$\sum_{j=1}^{2N} q_j = 0. \tag{1}$$

We denote the coordinates by $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2N}$, and the momenta by $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_{2N}$, and assume that all particles have the same mass m. The Hamiltonian is taken to be

$$H = \sum_{j=1}^{2N} \frac{1}{2m} |\boldsymbol{p}_j|^2 - \tfrac{1}{2} \sum_{i \neq j} q_i q_j |\boldsymbol{x}_i - \boldsymbol{x}_j|^2, \tag{2}$$

with the understanding that the particles are confined to a d-dimensional volume L^d. Boundary conditions will be specified later. Due to the special form of (2) we can write H as a sum of d independent Hamiltonians, each describing a one-dimensional system. We therefore take $d = 1$. By neutrality

$$H = \sum_{j=1}^{2N} \frac{1}{2m} p_j^2 + \left(\sum_{j=1}^{2N} q_j x_j \right)^2. \tag{3}$$

In this paper we present some simple arguments to show that as $N \to \infty$ and $\rho = 2N/L$ fixed, the thermodynamics of (3) reduces to that of an ideal gas with the same total density. We first turn to the classical case. The quantum case is considered in § 4 and a short discussion of our results is given in § 5.

2. Classical two-component plasma

The thermodynamics of a *classical* neutral plasma is determined by the partition function $(0 < x_j < L)$

$$Z(\beta, 2N, L) = \int_{-\infty}^{+\infty} \mathrm{d}p_1 \ldots \int_{-\infty}^{+\infty} \mathrm{d}p_{2N} \int_0^L \mathrm{d}x_1 \ldots \int_0^L \mathrm{d}x_{2N}\, \mathrm{e}^{-\beta H}. \tag{4}$$

The integration of the momenta gives rise to a factor $(2\pi\beta/m)^N$. The integration over x in (4) is done by using the formula

$$e^{-x^2/2}=\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp(-\tfrac{1}{2}z^2+ixz). \tag{5}$$

We find using (1) once again that (4) may be written

$$(2\pi mL^2/\beta)^N\int_{-\infty}^{+\infty}\frac{dz}{(\pi\beta L^2)^{1/2}}\exp[-z^2/(\beta L^2)]\prod_{j=1}^{2N}\left(\frac{\sin q_jz}{q_jz}\right). \tag{6}$$

From now on we assume a two-component plasma and take $q_1=\ldots=q_N=1$ and $q_{N+1}=\ldots=q_{2N}=-1$ so that the canonical partition function becomes

$$Z(\beta,2N,L)=\left(\frac{L^N}{\lambda^N N!}\right)^2\int_{-\infty}^{+\infty}\frac{dz}{(\pi\beta L^2)^{1/2}}\exp[-z^2/(\beta L^2)]\left(\frac{\sin z}{z}\right)^{2N}. \tag{7}$$

The $(N!)^2$ takes into account the statistics (Huang 1963), while $\lambda=[(2\pi\beta\hbar^2)/m]^{1/2}$ is the thermal wavelength. Since $|\sin z|\leqslant|z|$ we get an upper bound,

$$Z(\beta,2N,L)\leqslant(L^N/\lambda^N N!)^2. \tag{8}$$

Moreover, we have

$$\begin{aligned}Z(\beta,2N,L)&\geqslant\left(\frac{L^N}{\lambda^N N!}\right)^2\frac{2}{(\pi\beta L^2)^{1/2}}\int_0^{\pi}dz\exp[-z^2/(\beta L^2)]\left(\frac{\sin z}{z}\right)^{2N}\\&\geqslant\left(\frac{L^N}{\lambda^N N!}\right)^2\frac{2}{(\pi\beta L^2)^{1/2}}\int_0^{\pi}dz\exp[-z^2/(\beta L^2)]\left(1-\frac{z}{\pi}\right)^{2N}\\&\geqslant\left(\frac{L^N}{\lambda^N N!}\right)^2\frac{2\exp[-\pi^2/(\beta L^2)]}{(\pi\beta L^2)^{1/2}}\frac{\pi}{2N+1}.\end{aligned} \tag{9}$$

Combining (8) and (9) we obtain for the free energy per particle in the thermodynamic limit ($N\to\infty$, $L\to\infty$, $2N/L=\rho$)

$$f(\rho,\beta)=\lim_{N\to\infty}\frac{-1}{2N\beta}\log Z(\beta,2N,2N/\rho)=\frac{1}{\beta}\log\frac{\rho\lambda}{e}. \tag{10}$$

So the thermodynamic functions of the model (3) are those of a two-component ideal gas mixture with the same total density. Apparently for 'most' particle configurations $\{x_1,\ldots,x_{2N}\}$ we have $\Sigma_{j=1}^N(x_j-x_{j+N})\approx0$, which implies that the centre of mass of the particles with positive charge coincides 'on the average' with the centre of mass of the particles with negative charge. Similar results were obtained earlier by van den Berg (1981). However, the use of (5) simplifies e.g. the derivation of (10) considerably. In particular, we are now able to calculate all the correlation functions.

3. Correlation functions

In this section we show also that the correlation functions of the classical plasma converge in the thermodynamic limit to those of a two-component ideal gas mixture.

As an example we calculate the $+-$ pair correlation function $g_L(s; r)$:

$$
\begin{aligned}
g_L(s; r) &:= N^2\langle\delta(x_1-s)\delta(x_{N+1}-r)\rangle_L \\
&= \frac{N}{Z(\beta, 2N, L)}\frac{N^2}{(N!)^2\lambda^{2N}}\int_0^L \mathrm{d}x_1 \dots \int_0^L \mathrm{d}x_{2N}\,\delta(x_1-s)\delta(x_{N+1}-r) \\
&\quad\times \exp\left[-\beta\left(\sum_i (x_i - x_{i+N})\right)^2\right] \\
&= \frac{N^2}{L^2}\frac{\int_{-\infty}^{+\infty}\mathrm{d}z\,\exp[-z^2/(\beta L^2)]\cos(2z(s-r)/L)(\sin z/z)^{2N-2}}{\int_{-\infty}^{+\infty}\mathrm{d}z\,\exp[-z^2/(\beta L^2)](\sin z/z)^{2N}},
\end{aligned}
\tag{11}
$$

where we have used (5) and (7). From (11) we conclude that $g_L(s; r) \leqslant (\rho/2)^2$. On the other hand,

$$
\begin{aligned}
g_L(s; r) &\geqslant \left(\frac{\rho}{2}\right)^2 \frac{\int_0^\infty \mathrm{d}z\,(\sin z/z)^{2N-2}[1-(z^2/\beta L^2)-(2z^2(s-r)^2/L^2)]}{\int_0^\infty \mathrm{d}z\,(\sin z/z)^{2N}} \\
&\geqslant \left(\frac{\rho}{2}\right)^2\left[1-\frac{1}{L^2}\left(\frac{1}{\beta}+2(s-r)^2\frac{J(2N-4)}{J(2N)}\right)\right]
\end{aligned}
\tag{12}
$$

where

$$
J(N) = \int_0^\infty \left(\frac{\sin z}{z}\right)^N \mathrm{d}z. \tag{13}
$$

Since

$$
J(N) \sim (3\pi/2N)^{1/2} + \mathrm{O}(1/N) \qquad N\to\infty \tag{14}
$$

we find that the right-hand side of (12) converges to $(\rho/2)^2$. Hence

$$
\lim_{L\to\infty} g_L(s; r) = (\rho/2)^2. \tag{15}
$$

In a similar vein, one finds for the $k+$, $l-$ correlation function

$$
\begin{aligned}
&\lim_{L\to\infty} g_L(s_1, \dots, s_k; r_1, \dots, r_l) \\
&\quad := \lim_{L\to\infty}\binom{N}{k}\binom{N}{l}\langle\delta(x_1-s_1)\dots\delta(x_k-s_k)\,\delta(x_{N+1}-r_1)\dots\delta(x_{N+L}-r_l)\rangle_L \\
&\quad = \frac{1}{k!\,l!}\left(\frac{\rho}{2}\right)^{k+l}.
\end{aligned}
\tag{16}
$$

Taking into account the proper statistics (1) one can easily generalise the arguments of §§ 2 and 3 to a $2m$-component plasma.

4. Two-component quantum plasma with quadratic interactions

In this section we calculate bounds on the canonical partition function for a two-component *quantum* plasma (Boltzmann statistics) with quadratic interactions and show that the free energy of this system converges in the thermodynamic limit to the classical one. In the quantum case we replace in (3) $p_j^2 \to -\hbar^2 \, \mathrm{d}^2/\mathrm{d}x^2$ with Dirichlet boundary conditions on $x=0$, $x=L$. Using the Feynman–Kac formula we write the quantum partition function

$$Z_q(\beta, 2N, L) = \frac{1}{(N!)^2}\left(\frac{m}{2\pi\beta\hbar^2}\right)^N \times \int_{\boldsymbol{x}\in\square_L} \mathrm{d}\boldsymbol{x}\, \mathbb{E}\left\{\exp\left[-\int_0^\beta \left(\sum_{j=1}^N (x_j(\tau)-x_{j+N}(\tau))\right)^2 \mathrm{d}\tau\right], \boldsymbol{x}(\tau)\in\square_L, 0\leq\tau\leq\beta \,|\, \boldsymbol{x}(0)=\boldsymbol{x}(\beta)=x\right\} \tag{17}$$

where $\boldsymbol{x}=(x_1,\ldots,x_{2N})$ and $\square_L=\{\boldsymbol{x}: 0\leq x_j\leq L, j=1,\ldots,2N\}$. Moreover, $\mathbb{E}\{\exp\{-\int_0^\beta V(\boldsymbol{x}(\tau))\,\mathrm{d}\tau\}|\boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}\}$ denotes the average of $\exp\{-\int_0^\beta V(\boldsymbol{x}(\tau))\,\mathrm{d}\tau\}$ for all paths $\boldsymbol{x}(\cdot)$ of a Wiener process on $\mathbb{R}^{2N}$ satisfying $\boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}$ (see Kac 1951). Because of the Dirichlet boundary conditions on the boundary $\partial\square_L$ only paths contained in $\square_L$ $(0\leq\tau\leq\beta)$ give a non-zero contribution. Expression (17) enables us to calculate bounds on $Z_q(\beta, 2N, L)$. The upper bound on $Z_q(\beta, 2N, L)$ is trivial,

$$Z_q(\beta, 2N, L) \leq \frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{\boldsymbol{x}\in\square_L} \mathrm{d}\boldsymbol{x}\, \mathbb{E}\{\mathbb{1}, \boldsymbol{x}(\tau)\in\square_L, 0\leq\tau\leq\beta\,|\,\boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}\}$$

$$\leq \frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{x\in\square_L} \mathbb{1}\,\mathrm{d}\boldsymbol{x} = \left(\frac{L^N}{\lambda^N N!}\right)^2.$$

For the lower bound we obtain

$$\begin{aligned} Z_q(\beta, 2N, L) \geq{}& \frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{\boldsymbol{x}\in\square_{L-\varepsilon}} \mathrm{d}\boldsymbol{x}\, \mathbb{E}\left\{\exp\left[-\int_0^\beta\left(\sum_{i=1}^N (x_j(\tau)-x_{j+N}(\tau))\right)^2 \mathrm{d}\tau\right], \boldsymbol{x}(\tau)\in\square_L, 0\leq\tau\leq\beta\,|\,\boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}\right\} \\ \geq{}& \frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{\boldsymbol{x}\in\square_{L-\varepsilon}} \times\mathbb{E}\left\{\exp\left[-\int_0^\beta\left(\sum_j (x_j(\tau)-x_{j+N}(\tau))\right)^2\mathrm{d}\tau\right], \boldsymbol{x}(\tau)\in\mathbb{R}^{2N}, 0\leq\tau\leq\beta\,\middle|\,\boldsymbol{x}(0) = \boldsymbol{x}(\beta)=\boldsymbol{x}\right\} \\ &- \frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{\boldsymbol{x}\in\square_{L-\varepsilon}} \times\mathrm{d}\boldsymbol{x}\,\mathbb{E}\left\{\mathbb{1}, \sup_{j,0\leq\tau\leq\beta} |\tfrac{1}{2}L-x_j(\tau)|>\tfrac{1}{2}L\,|\,\boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}\right\}. \end{aligned} \tag{18}$$

The absolute value of the second term in (18) can be estimated from above by means of lemma 2 of Ray (1954). It is smaller than

$$[(L-2\varepsilon)^N/N!\lambda^N]^2 4N \exp[-\varepsilon^2/(2\beta)]. \tag{19}$$

The first term in (18) is bounded from below by

$$\begin{aligned}
&\frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{x\in\square_{L-\varepsilon}} \mathrm{d}x \exp\left[-3\beta\left(\sum_{j=1}^{N}(x_j-x_{j+N})\right)^2\right] \\
&\quad\times\mathbb{E}\left\{\exp\left[-3\int_0^\beta \mathrm{d}\tau\left(\sum_{j=1}^{N}(x_j-x_i(\tau))\right)^2\right.\right. \\
&\quad\left.\left.-3\int_0^\beta \mathrm{d}\tau\left(\sum_{i=N+1}^{2N}(x_j-x_j(\tau))\right)^2\right]\middle|\, \boldsymbol{x}(0)=\boldsymbol{x}(\beta)=\boldsymbol{x}\right\} \\
&=\frac{1}{(N!)^2}\frac{1}{\lambda^{2N}}\int_{\boldsymbol{x}\in\square_{L-\varepsilon}} \mathrm{d}\boldsymbol{x} \exp\left[-3\beta\left(\sum_{j=1}^{N}(x_j-x_{j+N})\right)^2\right] \\
&\quad\times\left[\!\!\left[\mathbb{E}\left\{\exp\left[-3\int_0^\beta \mathrm{d}\tau\left(\sum_{j=1}^{N}x_j(\tau)\right)^2\right]\middle|\, x_j(0)=x_j(\beta)=0, j=1,\dots,N\right\}\right]\!\!\right]^2 \\
&=3^N Z(3\beta,2N,L-2\varepsilon) \\
&\quad\times\left[\mathbb{E}\left\{\exp\left(-3\int_0^{\beta\sqrt{N}} \mathrm{d}\tau\, x^2(\tau)\right)\middle|\, x(0)=x(\beta\sqrt{N})=0\right\}\right]^2 \\
&=3^N Z(3\beta,2N,L-2\varepsilon)(6\beta\sqrt{N}/\sinh\{6\beta\sqrt{N}\}),
\end{aligned} \tag{20}$$

where we have used (6.23) of Kac (1951). If we set $\varepsilon=L^{+1/2}$ we arrive at

$$Z_q(\beta,2N,L)\geqslant 3^N\,\mathrm{e}^{-6\beta\sqrt{N}}\,Z(3\beta,2N,L-2L^{1/2})-\frac{(L-2L^{1/2})^{2N}}{(N!)^2\lambda^{2N}}4N\,\mathrm{e}^{-L/(2\beta)}. \tag{21}$$

The second term in (21) becomes in the limit $N\to\infty$, $L\to\infty$, $2N/L=\rho$, much smaller than the first. Combining (21) and (17) we have proved that

$$f_q(\rho;\beta)\equiv\lim_{N\to\infty}\frac{-1}{2N_\beta}\log Z_q\left(\beta,2N,\frac{2N}{\rho}\right)=\frac{1}{\beta}\log\frac{\rho\lambda}{e}=f(\rho,\beta), \tag{22}$$

i.e., the quantum plasma with Boltzmann statistics behaves thermodynamically like a classical plasma with the same density and temperature.

5. Discussion

Apparently the quadratic interaction becomes irrelevant as $N\to\infty$, at least for Boltzmann statistics. It is an open question whether the same behaviour persists for Bose–Einstein statistics. For distinguishable particles, the physical mechanism is clear. The quadratic interaction,

$$\left(\sum_{j=1}^{N}x_j-\sum_{j=1}^{N}x_{j+N}\right)^2, \tag{23}$$

only favours those configurations where the centre of mass of the particles with positive charges more or less coincides with the centre of mass of the particles with negative charge. There is also a second, more formal, argument which ‘explains’ the irrelevance of the quadratic interaction (23) as $N \to \infty$. Let A be a $2N \times 2N$ *orthogonal* matrix such that $\boldsymbol{y} = A\boldsymbol{x}$ and

$$y_1 = \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} (x_j - x_{j+N}). \tag{24}$$

There are many orthogonal matrices satisfying the requirements (24). Since the mapping A is linear and orthogonal it gives rise to a *canonical* transformation which maps the original Hamiltonian onto a much simpler one, namely

$$H^1 = \left\{ \frac{1}{2m} p_1^2 + 2Ny_1^2 \right\} + \sum_{j=2}^{2N} \frac{1}{2m} p_j^2. \tag{25}$$

Except for one degree of freedom, this is the Hamiltonian of an ideal gas. However, the hypercube $[0, L]^{2N}$ is rotated as well, and specifying its boundaries in terms of the y coordinates is by no means easy. Apparently, most of its volume corresponds to the $(2N-1)$-dimensional hyperplane $y_1 = 0$ or more precisely (see the previous argument), to a family of hyperplanes with $y_1 \approx 0$. Indeed, this is just what we have shown.

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