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Partition Function for a Two Dimensional Plasma in the Random Phase Approximation*

by

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ABSTRACT

The partition function for a two-dimensional plasma is evaluated within the random phase approximation. The periodic boundary conditions are fully taken into account by including the periodic image interactions. In the guiding-center limit, the "negative temperature" threshold energy is evaluated, and a value different from previous calculations results. When an identical random phase evaluation is applied to the finite gyroradius plasma, the Salzberg-Prager-May equation of state is recovered.

Considerable interest has arisen lately in the equilibrium statistical mechanics of two-dimensional plasmas, both in the "guiding center" and finite gyroradius limits.[1-8] The "guiding center" model is particularly interesting because its total phase volume is finite, so that above a critical energy $\mathcal{E}_m$, the temperature is formally negative.[9] Here we evaluate the partition function for both systems within the random phase approximation, and so arrive at the threshold energy $\mathcal{E}_m$.

In the random phase approximation, periodic boundary conditions are implicit, which means that in calculating the total energy we must include the interactions of all the charges with the images of all the others. Until now this fact has not been appreciated. We use the two-body non-central Ewald potential to calculate the energy of the system, which includes the image interactions and leads to a volume dependent term. For the finite gyroradius case, the Salzberg-Prager-May equation of state is recovered, and for the guiding center model a new value of $\mathcal{E}_m$ results.

We proceed from the canonical ensemble, which apparently has not been done directly for the guiding center model. (For energies near $\mathcal{E}_m$, the usual steepest-descent evaluation of the partition function may not be assumed to imply the equivalence of the canonical and microcanonical ensembles.) All our evaluations of thermodynamic quantities derive explicitly from the partition function.

The total energy for N positive and N negative charges in a box of volume V may be written as $\mathcal{E} = \sum_{i=1}^{2N} (\underset{\sim}{p}_i^2/2m_i) + \sum_{i<j} \Psi(\underset{\sim}{x}_{ij}) + \mathcal{E}_o$. $\mathcal{E}_o$ is a constant which will be specified below. $\Psi(\underset{\sim}{x}_{ij})$ is the Ewald potential which includes the periodic images, and is $\Psi(\underset{\sim}{x}_{ij}) = (4\pi e_i e_j/\ell V) \sum_{\underset{\sim}{k}}' k^{-2} \exp(i\underset{\sim}{k}\cdot\underset{\sim}{x}_{ij})$. $\underset{\sim}{k} = 2\pi\underset{\sim}{n}/V^{1/2}$, $\underset{\sim}{n}$ is a vector with integer components, V is the volume of the system, and the prime on the summation means to omit $\underset{\sim}{k} = 0$. The ith charge is a very long rod of length ℓ and charge e_i. Following Brush, Sahlin, and Teller,[10] and Nijboer and DeWette,[11] we may put $\Psi(\underset{\sim}{x}_{ij})$ into a form convenient for numerical evaluation,

$$\Psi(\underset{\sim}{\xi}_{ij}) = \frac{e_i e_j}{\ell} \left\{ E_1(\pi\xi_{ij}^2) - 1 + \sum_{\underset{\sim}{n}\neq 0} \left[\frac{\exp\left(-\pi n^2 + 2\pi i \underset{\sim}{n}\cdot\underset{\sim}{\xi}_{ij}\right)}{\pi n^2} \right.\right.$$

$$\left.\left. + E_1(\pi|\underset{\sim}{n} - \underset{\sim}{\xi}_{ij}|^2) \right] \right\} , \qquad (1)$$

where $\underset{\sim}{\xi}_{ij} = \underset{\sim}{x}_{ij}/V^{1/2}$, and $E_1(x)$ is the exponential integral. The constant $\mathcal{E}_o$ is $\mathcal{E}_o = N \lim_{x\to 0} \left[\Psi(x/V^{1/2}) - \phi(x) \right]$, where $\phi(x) = -(2e^2/\ell) \ln x$ is the two-body Coulomb interaction. The numerical value of $\mathcal{E}_o$ turns out to be $\mathcal{E}_o = -2.672(Ne^2/\ell) + (Ne^2/\ell) \ln V$.

The partition function for the finite gyroradius case is $Z = (V^{2N}/(N!)^2 h^{4N}) \cdot \int d\underset{\sim}{p}^{2N} d\underset{\sim}{\xi}^{2N} \exp(-\mathcal{E}/\theta)$, where $\theta = k_B T$ is the temperature in energy units. The momentum space part is trivial, and the configuration space part becomes

$$Z_{\text{config.}} = \int d\underset{\sim}{\xi}^{2N} \exp\left\{ \left[\mathcal{E}_o + \sum_{i<j} \Psi(\underset{\sim}{\xi}_{ij}) \right] /\theta \right\} .$$

Following Taylor, we invoke the random phase approximation to convert the integral over the ξ's to one over density variables $r_{\underset{\sim}{k}}^2 = \sum_{i,j} (e_i e_j/\ell^2 V^2) \exp i\underset{\sim}{k}\cdot(\underset{\sim}{x}_i - \underset{\sim}{x}_j)$, with corresponding Jacobian $J = \prod'_{\underset{\sim}{k}} (V^2\ell^2/2Ne^2) \exp\left\{-(V^2\ell^2/2Ne^2) r_{\underset{\sim}{k}}^2\right\}$. This gives

$$Z_{\text{config.}} = \int_0^\infty \prod'_{\underset{\sim}{k}} (V^2\ell^2/2Ne^2) \exp\Big[-(V^2\ell^2/2Ne^2) r_{\underset{\sim}{k}}^2 - (\mathcal{E}_0 + 2\pi V r_{\underset{\sim}{k}}^2/k^2)/\theta + (4\pi Ne^2/\ell\theta V k^2)\Big]\, d\, r_{\underset{\sim}{k}}^2 \quad . \tag{2}$$

The integrations over $r_{\underset{\sim}{k}}^2$ are easily done and give $Z_{\text{config.}} = \prod'_{\underset{\sim}{k}} (1 + k_D^2/k^2)^{-1} \exp\left[k_D^2/k^2 - \mathcal{E}_0/\theta\right]$, where $k_D^2 \equiv 4\pi Ne^2/\ell V\theta$, which may be represented as an integral over k, to give ($m_\pm$ are the masses of the rods):

$$\begin{aligned} Z &= \frac{V^{2N}}{(N!)^2} \left(\frac{2\pi m_+\theta}{h^2}\right)^N \left(\frac{2\pi m_-\theta}{h^2}\right)^N \exp\left\{-\frac{\mathcal{E}_0}{\theta} - \frac{V}{2\pi}\int_{\sqrt{4\pi/V}}^\infty k\, dk \left[\ln\left(1 + \frac{k_D^2}{k^2}\right) - \frac{k_D^2}{k^2}\right]\right\} \\ &= \frac{V^{2N}}{(N!)^2} \left(\frac{2\pi m_+\theta}{h^2}\right)^N \left(\frac{2\pi m_-\theta}{h^2}\right)^N \exp\left\{-\frac{\mathcal{E}_0}{\theta} - \frac{Ne^2}{\ell\theta} + \left(1 + \frac{Ne^2}{\ell\theta}\right) \ln\left(1 + \frac{Ne^2}{\ell\theta}\right)\right\} \quad . \end{aligned} \tag{3}$$

The various thermodynamic functions may be computed from Eq. (3). The pressure is $P = -\theta\partial(\ln Z)/\partial V = 2(N/V)\theta\,(1 - e^2/2\ell\theta)$, which is the Salzberg-Prager-May equation of state.[7,8] The internal energy is $\langle\mathcal{E}\rangle = \theta^2\,\partial(\ln Z)/\partial\theta = 2N\theta + \mathcal{E}_o - (Ne^2/\ell)\ln(1 + Ne^2/\ell\theta)$. The entropy is $S = k_B[\theta\,\partial(\ln Z)/\partial\theta + \ln Z] = 2Nk_B[\ln(2\pi\sqrt{m_+m_-}\,\theta V/h^2N) + 2] + k_B[\ln(1 + Ne^2/\ell\theta) - Ne^2/\ell\theta]$.

Results for the "guiding center" model may be obtained by ignoring the momentum-space contribution to Z. Thus we find for the energy and entropy

$$\langle\mathcal{E}\rangle_{g.c.} = \mathcal{E}_o - (Ne^2/\ell)\ln(1 + Ne^2/\ell\theta) \tag{4}$$

and

$$S_{g.c.} = k_B\left\{\ln\left[1 + \frac{Ne^2}{\ell\theta}\right] - \frac{Ne^2}{\ell\theta}\right\} \quad . \tag{5}$$

We may eliminate θ in favor of energy to obtain

$$S_{g.c.} = k_B\left[1 - \frac{\langle\mathcal{E}\rangle_{g.c.} - \mathcal{E}_o}{Ne^2/\ell} - \exp\left[-(\langle\mathcal{E}\rangle_{g.c.} - \mathcal{E}_o)/(Ne^2/\ell)\right]\right] \quad . \tag{6}$$

The temperature is given by $T^{-1} = \partial S/\partial \langle \mathcal{E} \rangle_{g.c.}$ Eqs. (4), (5), (6) hold for $\theta = k_B T > 0$. Therefore, the threshold value of $\langle \mathcal{E} \rangle_{g.c.}$ may be obtained by letting $T \rightarrow +\infty$, and gives the threshold energy $\mathcal{E}_m$

$$\mathcal{E}_m = \mathcal{E}_o = -\,2.672(Ne^2/\ell) + (Ne^2/\ell)\ell n N \quad , \tag{7}$$

which differs from previous results.[5,8]

Previous evaluations of $\mathcal{E}_m$ have assumed an equivalence between the sum of the pairwise potentials and $\int \vec{E}^2\, d\vec{x}/8\pi - \int \vec{E}^2_{self}\, d\vec{x}/8\pi$, where $\vec{E}$ is the electric field expressed as a Fourier series, and $\int \vec{E}^2_{self}\, d\vec{x}/8\pi$ is the infinite Coulomb self-energy of the charges. The Fourier representation of the $\vec{E}$, however, assumes periodic boundary conditions. Therefore, the two energies are equal only if the image charges are included in the sums of the pairwise interactions. The expression in Eq. (7) can be interpreted as the sum of the energies of the interaction of each of the charges with its own images. Thus the threshold distribution is still the random distribution, as previously determined. A different conclusion was reached in Ref. (8).

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