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Two-Dimensional Electron Fluid at High Temperature

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The two-dimensional and one-component plasma (OCP) model with r^{-1} interactions is investigated in the high-temperature limit, where the thermal wavelength gets larger than the classical distance of closest approach. Nonnegligible diffraction effects are rigorously taken care of (up to e^2) through a temperature-dependent effective interaction. Debye thermodynamics, analyzed in terms of a classical plasma parameter Λ, is shown to diverge as $\Lambda \ln h$, when $\hbar \to 0$. There is no classical limit. A result at variance with the corresponding one in three dimensions.

KEY WORDS: Two dimensions; Coulomb system; quantums corrections at high temperature; classical limit.

1. INTRODUCTION

The statistical mechanics of the two-dimensional electron fluid is of a considerable practical significance.(1) Usually, it is approached through a one-component plasma (OCP) model of pointlike charges interacting via a three-dimensional Coulomb potential r^{-1}, in the presence of a rigid and continuous neutralizing background.

The OCP thermodynamics is thus analyzed in terms of a dimensionless plasma parameter $\Lambda = \beta e^2/\lambda_D$, when λ_D denotes the usual screening length, and $\beta = (k_B T)^{-1}$.

The weakly coupled regime ($\Lambda \ll 1$) has been examined several times(2-4) within a mean field (Debye–Hückel) framework. The system is then taken as dilute and classical, with $k_B T \leqslant 1$ Ry $= me^4/2\hbar^2$, binding energy of a pair of unlike charges in two dimensions.

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A salient feature of all these studies is a first order thermodynamics proportional to

$$\int_{\beta e^2}^{\lambda_D} \frac{dr}{r} = \ln \frac{1}{\Lambda}$$

a phenomenon usually interpreted as a poor performance of the mean field approximation (MFA), which fails to account properly for the short-ranged correlations. In an attempt to restore finite values for these nonanalytic quantities, Fetter[2] proposed to replace the classical distance of closest approach βe^2 by the thermal wavelength $\hbar/(2mk_B T)^{1/2} \equiv \lambda$ while keeping $\hbar \neq 0$.

However, such a ad hoc replacement appears difficult to legitimate in the usual temperature range of interest ($T \ll 1$ Ry) for condensed matter physics.[2-4]

This explains that we pay a special attention to the opposite high-temperature domain ($\lambda \geqslant \beta e^2$, $T \geqslant 1$ Ry) where the above proposal is obviously a plausible one.

Technically speaking, we have to work out a new situation where particles are so dilute that we neglect the Pauli repulsion $[(\pi\pi)^{-1/2} \gg \lambda]$, while diffraction corrections are expected to delocalize the point charges through the uncertainty principle.

A similar problem has already been investigated at length in three dimensions.[5]

The corresponding adaptation of the OCP model consists essentially in encapsulating the $\hbar \neq 0$ diffraction effects in a suitably modified two-body Coulomb interaction. A step taken up in Section 2.

Then, the potential energy is computed in Section 3. It allows a most economical derivation of the canonical thermodynamics, in Section 4. This way, we circumvent a tedious calculation of the Debye pair distribution, postponed to a latter work.

The results are finally contrasted to the corresponding three-dimensional one.

2. HIGH-TEMPERATURE QUANTUM OCP (DIFFRACTION)

We extend the usual classical MFA (Debye) expansion in Λ, to a domain defined by the parameters

$$e^2/k_B T \leqslant \lambda < \lambda_D, \qquad \Lambda \leqslant 1$$

through a double expansion in Λ and $a = \lambda / \lambda_D$.

We expect to locate the main diffraction modifications of the previous classical OCP' expansions[2-4] in the short-distance domain $0 \leqslant r \lesssim \lambda$. The

Λ-expansion will be adapted in the easiest and most transparent way, if we succeed in modifying the bare Coulomb potential r^{-1} itself to include the diffraction effects. Schematically, we are searching for a temperature-dependent effective interaction potential decreasing in a Coulomb-like fashion at large distances and remaining finite for $r \leqslant \lambda$. This program may be easily implemented through a standard trick which consists in approximating the two-body high-temperature quantum Slater sum by the classical Gibbs expression, with the ansatz

$$\exp(-\beta H_0 - \beta H_1) = \exp(-\beta H_1)\exp(-\beta H_0)G \tag{1}$$

where

$$H_0 = \sum_{i=1}^{N} \frac{p_i^2}{2m_e} \quad \text{and} \quad H_1 = \sum_{1 \leqslant i<j<N} e^2 \frac{1}{|r_i - r_j|}$$

G is thus a measure of the noncommutativity of H_0 and H_1 in the small β range. It is obtained as a solution to the Bloch-like equation

$$\partial G/\partial\beta = \exp(\beta H_0)[H_0 - \exp(\beta H_1)H_0\exp(-\beta H_1)]\exp(-\beta H_0)G \tag{2}$$

Expanding the bracket with respect to β, we get a series which terminates exactly after the second-order terms, i.e.,

$$\frac{\partial G}{\partial\beta} = -\exp(\beta H_0)\left\{\beta[H_1, H_0] + \frac{\beta^2}{2!}[H_1, [H_1, H_0]]\right\}\exp(-\beta H_0)G \tag{3}$$

The equation is solved to order H_1

$$G = 1 + \int_0^\beta d\beta_1\, \beta_1 \frac{d}{d\beta_1}[\exp(\beta_1 H_0)H_1\exp(-\beta_1 H_0)] \tag{4}$$

which allows the density operator $\rho = \exp[\beta(F - H)]$ to be given as

$$\rho e^{-\beta F} = e^{-\beta H} = e^{-\beta H_1}e^{-H_0} + e^{-\beta H_1}\int_0^\beta d\beta_1\, \beta_1 \frac{d}{d\beta_1} \times\left[e^{(\beta_1-\beta)H_0}H_1 e^{-(\beta_1-\beta)H_0}\right]e^{-\beta H_0} \tag{5}$$

where F is the canonical free energy and $H = H_0 + H_1$. The above expression is further simplified, with $\beta' = \beta_1 - \beta$, by virtue of

$$e^{\beta' H_0}H_1 e^{-\beta' H_0} = \frac{1}{2}\sum_{i \neq j} e^{\beta' H_0}(2\pi)^{-2}\int d^2\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r}_{ij})\frac{2\pi e^2}{k}e^{-\beta' H_0} \tag{6}$$

Together with

$$e^{\beta' H_0}\exp(i\mathbf{k}\cdot\mathbf{r}_{ij})e^{-\beta' H_0} = \exp(i\mathbf{k}\cdot\mathbf{r}_{ij})\exp\left(\frac{\beta'\pi}{m_e}\mathbf{k}\cdot\mathbf{p}_{ij}\right)\exp\left(\frac{\beta'\hbar^2k^2}{m_e}\right) \tag{7}$$

The result is ($2\pi e^2/k$ is the two-dimensional transform of e^2/r)

$$e^{-\beta H} = e^{-\beta H_1} e^{-\beta H_0} + \frac{1}{2(2\pi)^2} \sum_{i \neq j} e^{-\beta H_1} \int_0^\beta d\beta' \int d^2\mathbf{k}$$
$$\times \left\{ \frac{2\pi e^2}{k} \exp(i\mathbf{k} \cdot \mathbf{r}_{ij}) \beta' \frac{d}{d\beta'} \right.$$
$$\left. \times \left[\exp\left(- \frac{\beta' \hbar \mathbf{k} \cdot \mathbf{p}_{ij}}{m_e} \right) \exp\left(- \frac{\beta' \hbar^2 k^2}{m_e} \right) \right] e^{-\beta H_0} \right\} \tag{8}$$

where $p_{ij} = p_j - p_i$. The corresponding canonical partition function $Z = Tre^{-\beta H}$ is explained as

$$\langle r_1, \ldots, r_N | e^{-\beta H} | r_1, \ldots, r_N \rangle$$
$$= \left(\frac{2m_e}{\beta \hbar^2} \right)^N \exp\left(- \frac{\beta}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} \right)$$
$$\times \left\{ 1 + \frac{1}{2(\pi)^2} \sum_{i \neq j} \int_0^\beta d\beta' \, \beta' \frac{d}{d\beta'} \int d^2\mathbf{k} \, \frac{2\pi e^2}{k} \exp(i\mathbf{k} \cdot \mathbf{r}_{ij}) \right.$$
$$\left. \times \exp\left[\frac{h^2 k^2}{m_e} \left(-\beta' + \frac{\beta'^2}{\beta} \right) \right] \right\} \tag{9}$$

Now, let us simplify the β'-quadrature with the new variable $\alpha = \beta'/\beta$ and $-\beta' + \beta'^2/\beta = \beta\alpha(\alpha - 1)$ and approximate the high-order quantum corrections, by virtue of the exponential expansion, which read as

$$\langle r_1, \ldots, r_N | e^{-\beta H} | r_1, \ldots, r_N \rangle = \left[\pi \left(\frac{2m_e}{\beta h^2} \right) \right]^N \exp\left[- \frac{\beta}{2} \sum_{i \neq j} W(r_{ij}) \right] \tag{10}$$

where $W(r_{ij})$ is the temperature-dependent effective potential of interaction introduced as

$$W(r_{ij}) = \frac{1}{(2\pi)^2} \int d^2k \exp(i\mathbf{k} \cdot \mathbf{r}_{ij}) \frac{2\pi e^2}{k} \left\{ \int_0^1 d\alpha \exp\left[-\beta \hbar^2 k^2 \alpha (1 - \alpha)/m_e \right] \right\} \tag{11}$$

the Fourier-transform of which is readily obtained as

$$w(k) = \frac{2\pi e^2}{k} \, {}_1F_1(1; \tfrac{3}{2}; -k^2 \lambda^2/4) \tag{12}$$

3. MEAN POTENTIAL ENERGY

Avoiding a direct attack on the Debye pair distribution $g(r)$, the corresponding thermodynamics is approach in the easiest way by[5] (n = number density)

$$U_{\text{pot}} = \frac{n^2V}{2}\int d^2r\,\frac{e^2}{r}\,[g(r)-1]$$
$$\cong \frac{n^2V}{2}\int \frac{d^2\mathbf{k}}{(2\pi)^2}\cdot\frac{2\pi e^2}{k}\cdot\left[\frac{-\beta w(k)}{1+\rho\beta w(k)}\right]$$
$$= \frac{-Nk_BT\Lambda}{2}\cdot\int_0^\infty dK\cdot\frac{{}_1F_1\left(1;\tfrac{3}{2};(-\lambda^2/4\lambda_D)K^2\right)}{K+{}_1F_1\left(1;\tfrac{3}{2};(-\lambda^2/4\lambda_D^2)K^2\right)} \tag{13}$$

with $\lambda_D = k_BT/2\pi ne^2$.

In the present high dilution domain, the linearization of $g(r)-1$ is mostly appropriate. Moreover, as in three dimensions a very accurate estimate of the resulting dimensionless quadrature is achieved by retaining only the first term in the expansion

$$\frac{{}_1F_1\left(1;\tfrac{3}{2};(-\lambda^2K^2/4\lambda_D^2)\right)}{K+1}\cdot(1-X+X^2+\cdots),\qquad |X|\ll 1 \tag{14}$$

where

$$X = \frac{{}_1F_1\left(1;\tfrac{3}{2};(-\lambda^2K^2/4\lambda_D^2)\right)-1}{K+1}$$

So, we get ($a = \lambda/\lambda_D$)

$$U_{\text{pot}} \cong \frac{Nk_BT}{2}\Lambda\left(\frac{C}{2}+\ln a-1.1470\right) \tag{15}$$

where $C = 0.577215$. The derivation of Eq. (15) is detailed in the Appendix.

4. THERMODYNAMICS

The canonical thermodynamics is then straightforwardly deduced from the excess free energy, taken as a expectation value of the potential energy for coupling strength λe^2, in the form[6]

$$F^{\text{exc}} = \int_0^1 \frac{d\lambda}{\lambda}\,U_{\text{pot}}(\lambda e^2) = \frac{Nk_BT}{4}\,[\ln a - 1.3484] \tag{16}$$

from which follow the other usual quantities

$$E^{\text{exc}} = \frac{\partial}{\partial \beta}(\beta F^{\text{exc}}) = \frac{Nk_B T}{2}\Lambda(\ln a - 0.5984) \tag{17}$$

$$\frac{C_V^{\text{exc}}}{N} = k_B \beta^2 \frac{\partial E^{\text{exc}}}{\partial \beta} = -\frac{k_B \Lambda}{2}(\ln a + 0.9016) \tag{18}$$

$$\frac{S^{\text{exc}}}{N} = \beta^2 \frac{\partial F^{\text{exc}}}{\partial \beta} = \frac{k_B \Lambda}{4}(\ln a + 0.1516) \tag{19}$$

$$\beta P^{\text{exc}} = -\left.\frac{\partial \beta F}{\beta V}\right|_\beta = \frac{\Lambda n}{4}(\ln a - 0.3484) \tag{20}$$

and the compressibility

$$\left.\frac{\partial \beta P}{\partial n}\right|_\beta = \frac{\Lambda}{2}(\ln a + 0.1516) \tag{21}$$

in a characteristic form

$$\Lambda\left(\ln \frac{\lambda}{\lambda_D} + \text{const}\right) \tag{22}$$

which makes obvious the nonexistence of a classical limit ($\hbar \to 0$) at high temperature.

This two-dimensional behavior may be given more perspective by revisiting the three-dimensional one, where[5]

$$U_{\text{pot}} = -Nk_B T \frac{\Lambda}{\pi} \int_0^\infty d(K) \frac{{}_1F_1\left(1, \frac{3}{2}; -K^2\lambda^2/\lambda_D^2 4\right)}{(K)^2 + {}_1F_1\left(1, \frac{3}{2}; -k^2\lambda^2/\lambda_D^2 4\right)} \tag{23}$$

and

$$w(k) = \frac{4\pi e^2}{k^2}\, {}_1F_1\left(1, \tfrac{3}{2}; -k^2\lambda^2/4\lambda_D^2\right) \tag{24}$$

Expansion of the denominator of Eq. (23) then gives

$$\begin{gathered} \left\{ U_{\text{pot}} = -\tfrac{1}{2} N k_B T \Lambda \left[1 - \tfrac{1}{4}(\pi\lambda)^{1/2}/\lambda_D + \cdots \right] \right\} \\ F - F_0 = -\frac{N\Lambda}{3}\left(1 - \frac{3\sqrt{\pi}}{16}\frac{\lambda}{\lambda_D} + \cdots\right) \end{gathered} \tag{25}$$

in quantitative agreement with the exact $\hbar$-correction already obtained[7] from an independent many-body formalism. Higher-order terms in $\hbar^2$ would certainly require at least the next exact e^4-correction to $w(k)$, in view of the fact that the higher-order contributions obtained from the h-expansion of Eq. (23) are systematically smaller than the few available exact results.[7]

The corresponding $\hbar \to 0$ limit is therefore well-defined in three dimensions and at order Λ.

Please note, again, that the singularity as $\hbar \to 0$ is derived under the condition

$$\lambda \geqslant \beta e^2$$

when $\beta \to 0$.

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APPENDIX

We compute the quadrature

$$I_1 \equiv \int_0^\infty dK \frac{{}_1F_1\left(1; \frac{3}{2}; -K^2\lambda^2/4\lambda_D^2\right)}{K+1} \tag{A.1}$$

in the right-hand side of Eq. (13). Let us introduce the Hankel representation

$${}_1F_1\left(1; \frac{3}{2}; -\frac{\lambda^2 K^2}{4\lambda_D^2}\right) = \frac{\lambda_D^2}{\lambda^2} \cdot \left(\frac{2\pi}{K}\right)^{1/2} \int_0^\infty J_{1/2}(Kt) e^{-\lambda_D^2/\lambda^2} t^{1/2}\, dt$$

so that

$$I_1 = \frac{2\lambda_D^2}{\lambda^2} \cdot \left\{ \frac{\pi^{3/2}}{4} \cdot \frac{\lambda}{\lambda_D} - \int_0^\infty dt\, e^{-(\lambda_D^2/\lambda^2)t^2} \left[\mathrm{Ci}(t)\sin t - \mathrm{Si}(t)\cos t \right] \right\} \tag{A.2}$$

where

$$-\mathrm{Si}(au) = \int_a^\infty \frac{dt \sin tu}{t}, \qquad -\mathrm{Ci}(au) = \int_a^\infty \frac{dt \cos tu}{t}$$

is rewritten as ($a = \lambda/\lambda_D$)

$$I_1 = \frac{2\lambda_D}{\lambda}\left[\frac{\pi^{3/2}}{4} - \int_a^\infty \frac{dt}{2t}(t-a)\,{}_1F_1\left(1; \frac{3}{2}; -\frac{(t-a)^2}{4}\right)\right] \tag{A.3}$$

Making use of

$$\int_a^\infty dt\, {}_1F_1\left(1; \frac{3}{2}; -\frac{(t-a)^2}{4}\right) = \frac{\pi^{3/2}}{4} \tag{A.4}$$

and ($C = 0.577215$)

$$\int_a^\infty du\, u \ln u \; {}_1F_1\left(2; \frac{5}{2}; -\frac{(4-a)^2}{4}\right)$$
$$\cong -\frac{3}{4\sqrt{2}}\left[2^{3/2}(C - 3\ln 2) + \frac{\pi}{2}(1 - 2\ln 2)\right] \qquad \text{(A.5)}$$

one finally obtains

$$I_1 \cong -\ln a - \frac{1}{4\sqrt{2}}\left[2^{3/2}(C - 3\ln 2) + \frac{\pi}{2}(1 - 2\ln 2)\right] + O(a) \qquad \text{(A.6)}$$

yielding back Eq. (15).

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