

Low-temperature behaviour of the two-dimensional Coulomb gas

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1977 J. Phys. A: Math. Gen. 10 L95

(<http://iopscience.iop.org/0305-4470/10/5/003>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 13:57

Please note that [terms and conditions apply](#).

LETTER TO THE EDITOR

Low-temperature behaviour of the two-dimensional Coulomb gas

C Deutsch

Laboratoire de Physique des Plasmas†, Université de Paris-Sud, Centre d'Orsay, 91405 Orsay, France

Received 23 February 1977

Abstract. The two-dimensional Coulomb gas exhibits a non-zero long-range 'atom-atom' interaction in the $T \rightarrow 0$ limit.

The two-dimensional two-component Coulomb gas of classical point-like particles interacting through the Coulomb potential $\phi(r_{ij}) = -e_i e_j \ln r_{ij}$ (Hauge and Hemmer 1971, Deutsch and Lavaud 1974) experiences a sudden collapse into a nearly perfect gas of neutral pairs of like charges at the critical temperature $T_c = e^2/2k_B$ with $e = |e_{i,j}|$. Such a phenomenon is observed through the diverging trend of the $2N$ canonical partition function in the $T \rightarrow T_c^+$ limit, as well as through the two-body hydrogen-like Slater sum approaching infinity when $T \rightarrow T_c^-$ (Atabek *et al* 1974). The associated change of ionization stage is of a very fundamental significance in view of the numerous isomorphisms of the two-dimensional Coulomb gas with exact solvable models in plasma physics, solid state physics, and constructive quantum field theory (see for instance Fröhlich 1976, for a thorough discussion of this point of view). Also, a recent unification of all the one-component plasma models with respect to the space dimensionality ν (Deutsch 1976) allows for a systematic investigation of the dissociation-recombination catastrophe in the three-dimensional real matter plasma.

These preliminary remarks explain that here we pay special attention to the possibly non-zero residual long-range interaction between neutral pairs when $T < T_c$. This investigation is also necessary to assert the validity of the molecular approximation (MA) as a possible universal low-temperature picture for two-component plasma thermodynamics, valid at all dimensionality.

Therefore, we address ourselves to the two-dimensional extension of the standard derivation of the long-range residual interactions between neutral pairs in their ground states. The classical perturbation function which we are seeking is the mutual potential energy of two neutral molecules with 'nuclei' separated by a distance R , as a series of inverse powers of R . The potential ϕ_P at a point $P(r)$ produced by a positive charge at O and a negative charge at r_1 is $\phi_+ + \phi_-$, and may, if we suppose $r > r_1$, be developed in a Taylor series as

$$\phi_P = e\phi(r) - e\phi(r) + e\left(x_1 \frac{\partial}{\partial x} \phi(r) + y_1 \frac{\partial}{\partial y} \phi(r)\right) - \frac{e}{2}\left(x_1^2 \frac{\partial^2}{\partial x^2} + y_1^2 \frac{\partial^2}{\partial y^2} + 2x_1 y_1 \frac{\partial^2}{\partial x \partial y}\right)\phi(r) \dots \quad (1)$$

† Laboratoire Associé au CNRS.

specialized to $\nu = 2$. If we are not interested in interactions due to poles of higher order than quadrupoles, we need not consider more terms than those written down. Using, for the present, the convention of summing over like indices and putting x^1, x^2, x^3 for x, y, z we may write

$$\phi_P = e \left(x^i \frac{\partial}{\partial x^i} - \frac{x^i x^j}{2} \frac{\partial^2}{\partial x^i \partial x^j} \right) \phi(r) \dots \quad (2)$$

Now placing another 'H atom' with its 'proton' at P and its 'electron' at r_2 relative to P, the mutual interaction of the two becomes, again by a Taylor expansion in which the first three terms are retained,

$$V_2(R) = -e^2 \left[x^i x^k \frac{\partial^2}{\partial x^i \partial x^k} - \frac{1}{2} \left(x^i x^j x^k \frac{\partial^3}{\partial x^i \partial x^j \partial x^k} - x^i x^k x^l \frac{\partial^3}{\partial x^i \partial x^k \partial x^l} \right) - \frac{x^i x^j x^k x^l}{4} \frac{\partial^4}{\partial x^i \partial x^j \partial x^k \partial x^l} \right] \phi(r). \quad (3)$$

On account of the previous equation, the first term in the square brackets describes the dipole-dipole interaction, the second the dipole-quadrupole action and the third the quadrupole-quadrupole action. Putting $x = R$, and then placing the x axis along R , we obtain ($x = R, y = 0$) the desired classical two-dimensional energy expression

$$V_2(R) = \frac{e^2}{R^2} (x_1 x_2 - y_1 y_2) + \frac{e^2}{R^3} [x_1 x_2^2 - x_2 x_1^2 + 2y_1 y_2 (x_1 - x_2)] + \frac{3e^2}{2R^4} (r_1^2 r_2^2 - 3x_1^2 x_2^2 - y_1^2 y_2^2 + 4x_1 x_2 y_1 y_2) \dots \quad (4)$$

The same procedure applied to the one-dimensional interaction $\phi^{(1)}(x) = -q_i q_j |x_{ij}|$ gives zero immediately, thus explaining the striking success of the MA for the one-dimensional Coulomb gas (Lenard 1962, Prager 1963). The above $\nu = 2$ result exhibits a very small long-range residual interaction, in accord with the popular three-dimensional result (Margenau 1931). The MA displayed in this work may be given a quantitative measure by comparing the wave mechanical mutual energy of two 'H atoms' in the ground state (characterized by a subscript 0) with respect to the first excitation energy. Generalizing the standard three-dimensional second-order calculation, which neglects exchange degeneracy and spin, the wavefunction for the unperturbed system may be written $\psi_0(1) \psi_0(2)$ where each ψ_0 is the H wavefunction for the lowest state and the arguments are 'electron' coordinates referred to the separate nuclei as origins. The first-order perturbation energy is the average of V_2 over the space of the electrons, taken with the weighting function $\psi_0^1(1) \psi_0^2(2)$. This clearly vanishes for $\nu = 2$ and 3 on account of the spherical symmetry of the latter and also by cancellation of the remaining terms. In both cases, the required mutual energy may be given the standard second-order form

$$\Delta_2 E = \sum'_{\alpha\beta} \frac{|V_{00,\alpha\beta}|^2}{2E_0 - E_\alpha - E_\beta} \quad (5)$$

where E_α is the energy of one H atom in the state α . Terms with vanishing denominators are excluded from the summation, and $V_{00,\alpha\beta}$ is defined by

$$V_{00,\alpha\beta} = \int \psi_0(1) \psi_0(2) V(1, 2) \psi_\alpha(1) \psi_\beta(2) d\tau_1. \quad (6)$$

The products $\psi_\alpha\psi_\beta$ satisfy the conditions of completeness and orthogonality as do the ψ functions singly. In both cases we have a negative Δ_2E corresponding to the attractive forces $-\partial\Delta_2E/\partial R$ with $\Delta_2E \sim R^{-4}$ and R^{-6} respectively. For $\nu = 3$, this comes out from $E_{\alpha,\beta} > E_0$ with $E_0 < 0$ and $E_{\alpha,\beta} < 0$ (positive $E_{\alpha,\beta}$ are left out), while in two dimensions this arises from the numerical analysis of the 'H atom', yielding $E_0 - E_\alpha - E_\beta < 0$. Nevertheless, considerable differences appear in the quantitative determination of Δ_2E . In two dimensions

$$V_{00,\alpha\beta} = \frac{e^2}{R^2} \left(A_{\alpha\beta} + \frac{B_{\alpha\beta} - B_{\beta\alpha}}{R} + \frac{e^2}{3R^2} C_{\alpha\beta} \right), \quad (7)$$

with

$$A_{\alpha\beta} = x_{0\alpha}x_{0\beta} - y_{0\alpha}y_{0\beta} = A_{\beta\alpha}$$

$$B_{\alpha\beta} = x_{0\alpha}(x^2)_{0\beta} + 2(xy)_{0\alpha}y_{0\beta}$$

$$C_{\alpha\beta} = C_{\beta\alpha} = (r^2)_{0\alpha}(r^2)_{0\beta} - 3(x^2)_{0\alpha}(x^2)_{0\beta} - (y^2)_{0\alpha}(y^2)_{0\beta} + 4(xy)_{0\alpha}(xy)_{0\beta}.$$

$|V_{00,\alpha\beta}|^2$ can be computed very simply if we remember that the sum over differences like $A_{\alpha\beta}B_{\alpha\beta} - A_{\alpha\beta}B_{\beta\alpha}$ and $B_{\alpha\beta}C_{\alpha\beta} - B_{\beta\alpha}C_{\alpha\beta}$ is zero. We may interchange at liberty indices of summation in each term, so we get ($G_{\alpha\beta} = \frac{1}{2}(B_{\alpha\beta}^2 + B_{\beta\alpha}^2)$)

$$\Delta_2E = \frac{e^2}{R^4} \sum'_{\alpha\beta} \frac{1}{2E_0 - E_\alpha - E_\beta} \left(A_{\alpha\beta}^2 + \frac{2}{R^2} (G_{\alpha\beta} - B_{\beta\alpha}B_{\alpha\beta}) + \frac{9}{4R^4} C_{\alpha\beta}^2 \right), \quad \dots \quad (8)$$

Every wavefunction occurring here may be written

$$\psi_\alpha = \left(\frac{\epsilon_m}{2\pi} \right)^{1/2} r^{-1/2} \chi_{m,n}(r) \begin{cases} \cos m\theta \\ \sin m\theta, \end{cases} \quad \epsilon_0 = 1, \epsilon_1 = \epsilon_2 = \dots = 2. \quad (9)$$

A matrix element such as $(x^2)_{0\alpha}$ has

$$(x^2)_{0\alpha} = \int_0^\infty dr \int_0^{2\pi} d\theta \chi_{00}(r) \chi_{n_\alpha, m_\alpha}(r) \frac{r^2 \cos^2 \theta}{\sqrt{(2\pi)}} \begin{cases} \sin m_\alpha \theta \\ \cos m_\alpha \theta. \end{cases}$$

A good approximation to equation (8) may be obtained by retaining the first excited state terms ($E_{\alpha,\beta}$ increases steadily up to ∞), i.e.

$$\Delta_2E \sim \frac{e^2}{R^4} \left(\frac{G_{01} + G_{10}}{E_0 - E_1} + \frac{G_{11}}{2E_0 - 2E_1} + \dots \right)$$

where 0 and 1 respectively denote the ground state (0, 0) and the superposition $((0, 1) + (1, 0) + (1, 1) + (0, 2) + \dots + (0, n))$ of excited states with nearly equal energy. Performing the θ -average in the required matrix element shows that $A_{0P} = A_{P0} = 0$, all P. Also $C_{01} = C_{10} = A_{11} = B_{11} = C_{11} = A_{12} = A_{21} = 0$. Hence $G_{01} = G_{11} = 0$, while $G_{10} = B_{01}^2/2R^2$, so that $\Delta_2E \sim 10^3/R^6$ in two-dimensional units.

Therefore the residual correction to the MA is relatively much smaller in two dimensions, when compared to the ordinary Van der Waals interaction for $\nu = 3$ ($\sim R^{-6}$ relative to R in place of $\ln R$). So, we may risk the very reasonable conjecture that the given corrections to the MA increase steadily with dimensionality. The above results show that the MA, although a very accurate zero-order approximation, is not rigorously exact in the small- T range. The very small 'atom-atom' interactions remain completely negligible with respect to the diverging 'electron-proton' Slater sum in the vicinity of T_c .

The hospitality of the Research Laboratory of Electronics of the Massachusetts Institute of Technology, where part of this work was completed, is gratefully acknowledged.

References

- Atabek O, Deutsch C and Lavaud M 1974 *Phys. Rev. A* **9** 2617–24
Deutsch C 1976 *J. Math. Phys.* **17** 1404–13
Deutsch C and Lavaud M 1974 *Phys. Rev. A* **9** 2598–616
Fröhlich J 1976 *Commun. Math. Phys.* **47** 233–68
Hauge E H and Hemmer P C 1971 *Physica Norv.* **5** 209–23
Lenard A 1962 *J. Math. Phys.* **2** 682–93
Margenau H 1931 *Phys. Rev.* **38** 747–56
Prager S 1963 *Adv. Chem. Phys.* **4** 210–24