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THERMODYNAMICS OF A ONE-DIMENSIONAL MODEL SYSTEM WITH COULOMB INTERACTION

V. B. MAGALINSKIĬ

Moscow State University

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The occupation number representation is used to investigate the behavior of the partition function for a Gibbs grand canonical distribution. For the case of a one-dimensional one-component system interacting through Coulomb or gravitational forces exact formulae for the free energy and the equation of state are derived and discussed. Possible approximations for the three-dimensional case are discussed.

1\. We consider a system of interacting particles subject to the following conditions: on the one hand, the mean de Broglie wavelength of the particles may be large compared to the mean inter-particle spacing, so that it is necessary to take the type of statistics obeyed by them into account (i.e., to consider statistical correlations); on the other hand, this wavelength is much smaller than the mean scattering amplitude, which makes it legitimate to describe the interaction classically (i.e., to neglect quantum dynamical correlations).

We use the index s to denote the set of variables which describe the individual state of a single particle (for instance, the coordinate **q** and momentum **p**). We shall divide the space of individual states (the μ-space) into cells of equal and sufficiently small volume ω (in the case of quantum statistics, $\omega = (2\pi\hbar)^3$, while in the case of classical statistics, as is well known, the precise value of ω is unimportant), and denote by n_s the number of particles occupying the cell which includes the state s. Then the microscopic state of the system is specified by the set of occupation numbers n_s, which we shall denote by n. We also write ϵ_s for the additive part of the energy of the particles in the state s (e.g., the kinetic energy and the energy in an external field) and $w_{ss'} = w_{s's}$ for the absolute magnitude of the interaction energy of two particles in states s and s′ (we assume a pair interaction).

The energy of the system is:

$$H(n) = \sum_s \varepsilon_s n_s - \frac{\nu^2}{2} \sum_{ss'} w_{ss'} n_s n_{s'}, \tag{1}$$

where ν^2 is 1 for a negative interaction energy and -1 for a positive one (the interaction potential is assumed to have a definite sign). The total particle number is:

$$N(n) = \sum_s n_s. \tag{2}$$

If we exclude from consideration the other additive constants of the motion (viz., the total momentum and angular momentum), and assume a distribution which is canonical with respect to energy and microcanonical with respect to particle number, then the probability of a given microscopic state (n) of the system is given by the Gibbs canonical distribution in the occupation number representation:

$$w(n) = Z_N^{-1} e^{-H(n)/\Theta} \delta[N - N(n)] \prod_s \gamma(n_s), \tag{3}$$

where Θ is the modulus of the distribution and the statistical weighting factor γ (s) is introduced to take account of the statistics and is given by:

$$\gamma(n_s) = \begin{cases} 1, n_s = 0, 1 \text{ (Fermi-Dirac statistics)} \\ 1, n_s = 0, 1, 2 \ldots \text{ (Bose-Einstein statistics)} \\ (n_s!)^{-1} \quad \text{(Boltzmann statistics)} \end{cases}$$

All information on the thermodynamics of the system is contained in the partition function

$$Z_N = \sum_{(n)} e^{-H(n)/\Theta} \delta[N - N(n)] \prod_s \gamma(n_s), \tag{4}$$

which, as is well known, can be written in the form

$$Z_N = (-1)^N \left[\frac{\partial^N}{\partial \xi^N} \Xi(\xi) \right]_{\xi=0}, \tag{5}$$

where $\Xi(\xi)$ is the partition function for a grand canonical distribution, which in our case is:

$$\Xi(\xi) = \sum_{(n)} \exp\left\{ \frac{\nu^2}{2\Theta} \sum_{ss'} w_{ss'} n_s n_{s'} \right\} \prod_s (-\xi e^{-\varepsilon_s/\Theta})^{n_s} \gamma(n_s). \tag{4'}$$

From the theory of Gaussian integrals we have the equation:

$$\exp\left\{\frac{\nu^2}{2\Theta}\sum_{ss'} w_{ss'}n_s n_{s'}\right\}$$

$$= \int_{-\infty}^{+\infty} \exp\left\{\nu\sum_s n_s\varphi_s - \frac{\Theta}{2}\sum_{ss'} w_{ss'}^{-1}\varphi_s\varphi_{s'}\right\}D\varphi, \qquad (6)$$

where $D\varphi = B\prod_S d\varphi_S$, B is a normalization constant which has no effect on the thermodynamics of the system, and w^{-1} is the matrix reciprocal to the interaction matrix w (i.e. $\Sigma_{ss'} w^{-1}_{ss''} w_{s''s'} = \delta_{ss'}$). Substituting (6) in (4) and interchanging the processes of taking the product over cells and summation over occupation numbers, we obtain

$$\Xi(\xi) = \int \exp\left(-\frac{\Theta}{2}\sum_{ss'} w_{ss'}^{-1}\varphi_s\varphi_{s'}\right)$$

$$\times \prod_s \sum_{n_s} (-\xi e^{-\varepsilon_s/\Theta+\nu\varphi_s})^{n_s}\gamma(n_s)D\varphi$$

$$= \int \exp\left(-\frac{\Theta}{2}\sum_{ss'} w_{ss'}^{-1}\varphi_s\varphi_{s'}\right)\Xi_0(\xi|\varphi)D\varphi, \qquad (7)$$

where

$$\Xi_0(\xi|\varphi) = \exp\left\{\delta\sum_s \ln(1-\delta\xi e^{-\varepsilon_s/\Theta+\nu\varphi_s})\right\} \qquad (8)$$

is the grand partition function of an ideal quantum gas in the presence of an additional external field $u_S = -\Theta\nu\varphi_S$. Thus we can write

$$\Xi(\xi) = \langle\Xi_0(\xi|\varphi)\rangle_w, \qquad (7')$$

where the pointed brackets denote an average taken with weight

$$\exp\left(-\frac{\Theta}{2}\sum_{ss'} w_{ss'}^{-1}\varphi_s\varphi_{s'}\right).$$

The significance of the average in (7′) will become clear from what follows. In the case $w_{ss'} = w_{qq'} = w(|q - q'|)$ the index s takes a continuous set of values within the volume V available to the system; so in this case the reciprocal matrix $w^{-1}_{ss'}$, must be taken as an operator:

$$w^{-1}_{qq'} = \delta_{qq'}L_{q'}, \qquad (9)$$

where $\hat{L}_q$ is an operator such that the interaction potential $w_{qq'}$ constitutes the corresponding Green function.

Consider in particular the case of an interaction propagated by a scalar field; in this case

$$(\Delta_{q'} - \varkappa^2)w_{qq'} = -4\pi g^2\delta_{qq'}, \qquad (10)$$

so that

$$\hat{L}_{q'} = -\frac{1}{4\pi g^2}(\Delta_{q'} - \varkappa^2). \qquad (10')$$

where g is the coupling constant and κ^{-1} the interaction radius. Formulae (10) and (10′) are the well-known equations describing a screened Coulomb or gravitational potential (depending on the sign of ν^2 in (1), (8)). Using (9) and (10′), replacing the sums by integrals and integrating by parts, we get

$$\sum_{ss'} w_{ss'}{}^{-1}\varphi_s\varphi_{s'} = \frac{1}{4\pi g^2}\int [(\nabla\varphi)^2 + \varkappa^2\varphi^2]\,d\mathbf{q}. \qquad (11)$$

Consequently we can write Eqs. (7) and (7′) in a more explicit form:

$$\Xi(\xi) = \int e^{-U(\psi)/\Theta}\,\Xi_0(\xi\,|\,\psi)D\psi(\mathbf{q}), \qquad (12)$$

where

$$U(\psi) = \frac{1}{8\pi}\int [(\nabla\psi)^2 + \varkappa^2\psi^2]\,d\mathbf{q}$$

is the potential energy of the scalar field, and

$$\Xi_0(\xi\,|\,\psi)$$

$$= \exp\left\{\int\frac{d\mathbf{p}\,d\mathbf{q}}{\omega}\,\delta\ln[1 - \delta\xi e^{-[\varepsilon(\mathbf{q},\,\mathbf{p})+\nu g\psi(\mathbf{q})]/\Theta}]\right\}. \qquad (8')$$

Thus (12) is a Gibbsian average, over all possible configurations of the field propagating the interaction of the partition function of an ideal gas situated in this field. In the special case of a pure Coulomb interaction ($\kappa = 0$) and Boltzmann statistics ($\delta \rightarrow 0$) formula (12) has previously been obtained by Edwards[1], starting from the configuration representation for a canonical ensemble. In subsequent work[2,3], Edwards and Lenard considered an electrically neutral multi-component one-dimensional system of electrically interacting particles (or, more precisely, charge densities) and showed that in this case the continuous integral (12) reduces to a Wiener integral and the calculation of $\Xi(\xi)$ to the solution of a differential equation of the Schrödinger type in a periodic potential. However, these authors were prevented by the complexity of their chosen model system from obtaining any detailed results by this method.

In this work we shall consider only a one-component system, with a view to subsequent application of the results to the case of most physical interest, namely a system with gravitational interactions. It will turn out that the problem can be solved exactly for a model one-dimensional gravitational system, and the results used for an approximate investigation of real (three-dimensional) systems.

In the one-dimensional case we have only one spatial variable, which we denote by t; t satisfies the restriction $0 \leq t \leq V$, where V is the "volume" (i.e., length) of the system. Then we have

$$\Xi(\xi) = \int \exp\left\{-\frac{1}{4D}\int_0^V \dot{x}^2(t)\,dt - \int_0^V \Gamma[x(t)]\,dt\right\}Dx(t), \qquad (12')$$

$$D = \frac{2\pi g^2}{\Theta},$$

$$\Gamma(x) = \frac{\varkappa^2}{4D}x^2 - \frac{\delta}{\omega}\int_{-\infty}^{+\infty} dp \ln[1 - \delta\xi e^{-p^2/2m\Theta + \nu x}] \quad (13)$$

The continuous integral (12′) is a Wiener integral (cf., e.g.,[4]). It follows from the theory of Wiener integrals that

$$\Xi = \int_{-\infty}^{+\infty} G(x, V)\,dx, \quad (14)$$

where G(x, t) is the Green function of the equation:

$$\frac{\partial G}{\partial t} = D\frac{\partial^2 G}{\partial x^2} - \Gamma(x)G, \quad (15)$$

which satisfies the boundary condition corresponding to a source at t = 0:

$$G(x, 0) = \delta(x). \quad (16)$$

Formally, Eq. (15) describes diffusion in a medium with a constant diffusion coefficient D and an absorption coefficient Γ(x) whose spatial variation is described by (13).

It is probably not possible to obtain an analytic expression for the Green function in the general case (δ and κ arbitrary). We shall consider the simplest case, which is at the same time the most interesting for our purposes: the case of a classical system ($\delta \to 0$) without screening ($\kappa \to 0$). Let us first single out the case where the interaction energy is negative, i.e., $\nu = 1$. For a one-dimensional system this corresponds to particles occupying a flat "slab" of thickness V and interacting by the Coulomb repulsion. In this case

$$\Gamma(x) = \zeta_0\xi e^x, \quad \zeta_0 = \sqrt{2\pi m\Theta}/\omega. \quad (13')$$

Then the eigenfunctions of (15) are the Bessel functions of the second kind (i.e., with imaginary argument) of imaginary order, $K_{i\lambda}(z)$, where

$$z = z_0 e^{x/2}, \quad z_0 = (4\xi\zeta_0/D)^{1/2}. \quad (17)$$

Using these functions we can express the Green function for (13′) (with (15) and (16)) as a Kontorovich-Lebedev integral (cf., e.g.,[5])

$$G(x, t) = \frac{1}{\pi^2}\int e^{-Dt\lambda^2/4} K_{i\lambda}(z) K_{i\lambda}(z_0)\lambda \operatorname{sh}\pi\lambda\, d\lambda. \quad (18)^*$$

Using the integral representation

$$K_{i\lambda}(z) = \int_0^\infty e^{-z\operatorname{ch}y}\cos\lambda y\,dy, \quad (19)^\dagger$$

we first integrate (18) over x, according to (14). This gives:

$$\Xi = \frac{2}{\pi}\int_0^\infty e^{-Dt\lambda^2/4} K_{i\lambda}(z_0)\operatorname{ch}\frac{\pi\lambda}{2}\,d\lambda. \quad (20)$$

Moreover, using the integral representation

$$\operatorname{ch}\frac{\pi\lambda}{2}K_{i\lambda}(z) = \int_0^\infty \cos(z \operatorname{sh} y)\cos\lambda y\,dy \quad (19')$$

and putting t = V as required by (14), we can write (20) in the form

$$\Xi = \frac{2}{\sqrt{\pi DV}}\int_0^\infty \cos(z_0 \operatorname{sh} y)e^{-y^2/DV}\,dy. \quad (21)$$

Hence, from (5),

$$Z_N = \frac{2}{(2N-1)!!}\left(\frac{2\zeta_0}{D}\right)^N \frac{1}{\sqrt{\pi DV}}\int_0^\infty e^{-y^2/DV}\operatorname{sh}^{2N} y\,dy. \quad (22)$$

Since the number of particles N is very large, we may calculate the integral (22) by the method of steepest descents. As a result we get the following expression for the free energy $\Psi = -\Theta \ln Z_N$

$$\Psi = \Psi_0 + N\Theta A(\eta), \quad (23)$$

where $\Psi_0 = -N\Theta \ln (V\sqrt{2\pi m\Theta}$ is the free energy of an ideal gas, and

$$A(\eta) = f(\eta) + \ln f(\eta) + \eta - 1, \quad (24)$$

$$f(\eta) = s^2/\eta - \eta = \eta/\operatorname{sh}^2 s. \quad (25)$$

In (25), $s = s(\eta)$ denotes the saddle-point of the integrand in (22), which is determined as the root of the transcendental equation

$$s = \eta \operatorname{th} s. \quad (26)^*$$

Let us clarify the physical meaning of the parameter $\eta = NDV = 2\pi g^2 NV/\Theta$ which measures the departure from ideality. The interaction energy of the system under consideration, if we assume the particles to be uniformly distributed with density N/V, is equal (in absolute magnitude) to $U_0 = 2\pi g^2 N^2 V/3$, so that

$$\eta = 3U_0/2E_0, \quad (27)$$

where $E_0 = \Theta N/2$ is the mean kinetic energy. In the one-dimensional case the ratio (27) of the mean potential energy to the mean kinetic energy increases both with increasing particle number and with increasing volume, so that in this sense the system considered is clearly "non-additive."

The equation of state derived from (23)—(27) has the form

$$p = p_0[1 - \eta A'(\eta)], \quad (28)$$

where $p_0 = N\Theta/V$ is the pressure of an ideal gas.

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*sh = sinh.

†ch = cosh.

*th = tanh.

The mean energy is equal to

$$E = E_0[1 + 2\eta A'(\eta)]. \tag{29}$$

Here, in view of (24)–(26),

$$\eta A'(\eta) = 1 - s^2(\eta) / \eta. \tag{30}$$

Using the approximate expressions for the root s of the transcendental equation (26) in the limits of small and large η, we get

$$\eta A'(\eta) = \begin{cases} -\frac{1}{3}\eta - \frac{4}{45}\eta^2, & \eta \ll 1; \\ 1 - \eta - 4\eta e^{-2\eta}, & \eta \gg 1. \end{cases} \tag{31}$$

Hence for small η (high temperatures)

$$p = p_0 + \frac{1}{3} p_\infty + \frac{4}{45} p_\infty \eta, \tag{28'}$$

$$E = E_0 - U_0 - \frac{4}{45} U_0 \eta, \tag{29'}$$

while for large η (low temperatures)

$$p = p_\infty(1 + 4e^{-2\eta}), \tag{28''}$$

$$E = 3(E_0 - U_0) - 12U_0 e^{-2\eta}. \tag{29''}$$

Here $p_\infty = 2\pi g^2 N^2$ denotes the value of the pressure in the limit as $\eta \to \infty$.

For $(\partial p/\partial V)_T$ we get from (28)

$$\frac{\partial p}{\partial V} = \left(\frac{\partial p}{\partial V}\right)_0 [1 + \eta^2 A''(\eta)], \tag{32}$$

or, using (24)–(26),

$$\frac{\partial p}{\partial V} = \left(\frac{\partial p}{\partial V}\right)_0 \frac{s^2(\eta)}{\eta} \frac{2f(\eta)}{1 + f(\eta)}. \tag{32'}$$

Since $f(\eta)$ is everywhere positive, $(\partial p/\partial V)_T < 0$ everywhere, although, as is obvious from (28''), it tends to zero very rapidly (in fact exponentially) with increasing interaction energy ($\eta \to \infty$):

$$\left(\frac{\partial p}{\partial V}\right)_{\eta\to\infty} \longrightarrow \left(\frac{\partial p}{\partial V}\right)_0 8\eta^2 e^{-2\eta} = -8(2\pi g^2)\frac{N^3}{\Theta} e^{-2\eta}. \tag{33}$$

This result illustrates the general thermodynamic proposition that no phase transition is possible in a one-dimensional system (cf., e.g.,[6]) for the particular example of a system with long-range forces.

Let us now go on to consider a one-dimensional model with positive interaction energy, which corresponds to attractive forces (i.e., a one-dimensional gravitational system). As indicated above, the transition to this case is effected by making the replacement $\xi\zeta_0 e^x \to \xi\zeta_0 e^{ix}$ in (13'), which in the last analysis leads to the replacement of sinh y by sin y in the final formula (22) for the partition function Z_N. Thus for a one-dimensional system with attractive forces,

$$Z_N = \frac{2}{(2N-1)!!}\left(\frac{2\zeta_0}{D}\right)^N \frac{1}{\sqrt{\pi D V}} \int_0^\infty e^{-y^2/DV} \sin^{2N} y\, dy. \tag{22'}$$

The fundamental thermodynamic functions follow from the formulae:

$$\Psi = \Psi_0 + N\Theta B(\eta), \tag{23'}$$

$$B(\eta) = \varphi(\eta) + \ln\varphi(\eta) - \eta - 1, \tag{24'}$$

$$\varphi(\eta) = \sigma^2/\eta + \eta = \eta/\sin^2\sigma, \tag{25'}$$

where $\sigma(\eta)$ is defined by the equation

$$\sigma = \eta \cot\sigma, \tag{26'}$$

Thus,

$$p = p_0 - \frac{1}{3} p_\infty + \frac{4}{45} p_\infty \eta, \quad \eta \ll 1; \tag{34}$$

$$E = E_0 + U_0 - \frac{4}{45} U_0 \eta, \quad \eta \ll 1. \tag{35}$$

For large interaction energies ($\eta \gg 1$)

$$p = p_0 \pi^2/4\eta = \pi^2 p_\infty/4\eta^2 \to 0. \tag{35'}$$

The vanishing of the pressure at the walls obviously points to a contraction of systems with strong attractive forces. As before, $(\partial p/\partial V)_T < 0$.

It is of considerable interest to investigate the thermodynamic properties of real (three-dimensional) gravitational systems in the non-relativistic approximation. It is well known that at sufficiently large values of the interaction the long range of the gravitational force means that the thermodynamic functions of such a system are no longer additive functions of the particle number (for constant mean particle density). To guarantee the existence of an equilibrium state, we must first set not only an upper limit to the volume (to avoid the escape of the particles to infinity) but also a lower limit, to avoid their collapse to a single point; this can be done by introducing a short-range repulsion or equivalently by assigning a characteristic volume to the particles of the system. Once this is done, it is possible to investigate the behavior of the thermodynamic functions of such a system for interaction energies comparable to the thermal energy, as functions of parameters such as the temperature and mean density.

Since a rigorous examination of this problem is mathematically difficult, it is of interest to develop various approximation methods not based on perturbation theory. To conclude this paper we shall briefly consider one such possibility. For simplicity we consider a system of gravitationally interacting particles, whose equilibrium state is described by a spherically symmetric density distribution. We shall estimate for such a system the contribution to the partition function (12) from spherically symmetric distributions of the field only: $\psi = \psi(r)$ ("quasi-one-dimensional approximation"). The contribution of any one distribution of this type to the field energy is

$$\frac{1}{8\pi}\int_{r_0}^{R}\left(\frac{d\psi}{dr}\right)^2 4\pi r^2 dr = \frac{1}{8\pi}\int_{v_0}^{V}\left(\frac{d\psi}{dt}\right)^2 S^2(t)\,dt, \qquad (36)$$

where $v_0 \ll V$ is the characteristic volume of the particles, t is the volume variable, and $S(t) = (36\pi)^{1/3}t^{2/3}$ is the area of the surface of the sphere of volume t.

Thus the evaluation of Ξ, according to (14)—(16), reduces to the solution of a diffusion equation of the type (15) with the same form of $\Gamma(x)$ as before, but now with a variable diffusion coefficient

$$D(t) = D / S^2(t) = D / (36\pi)^{2/3} t^{4/3}. \qquad (37)$$

Obviously the corresponding thermodynamic formulae will now contain a value of the "non-ideality" parameter η which is lower than the true value. Further improvement of the results may be achieved by choosing η on the basis of a comparison, in the limit $\eta \rightarrow 0$, of the formulae obtained in the quasi-one-dimensional approximation with the corresponding results of perturbation theory for the exact expression (12).

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