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The virial expansion of a classical interacting system

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Abstract

We consider N particles interacting pairwise by an inverse square potential in one dimension (Calogero–Sutherland–Moser model). For a system placed in a harmonic trap, its classical partition function for the repulsive regime is recognised in the literature. We start by presenting a concise re-derivation of this result. The equation of state is then calculated both for the trapped and the homogeneous gas. Finally, the classical limit of Wu’s distribution function for fractional exclusion statistics is obtained and we re-derive the classical virial expansion of the homogeneous gas using this distribution function.

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1. Introduction

We consider a system of identical particles in one dimension interacting via an inverse square pairwise interaction. This is a class of integrable many-body systems known as the Calogero–Sutherland–Moser (CSM) model [1, 2] which is a classic example of an exactly solvable many-body system. For over three decades, the variants of this model have provided a template for analysing disparate problems in high energy and condensed matter physics.

The Hamiltonian of the model in the presence of a harmonic confinement is given by

$$H = \sum_{i=1}^N \left[\frac{1}{2m} p_i^2 + \frac{1}{2} m \omega^2 x_i^2 \right] + \frac{\hbar^2 \lambda}{m} \sum_{1 \leq i < j \leq N} \frac{1}{(x_i - x_j)^2}, \quad (1)$$

where x_i , p_i denote the positions and momenta of the N particles, and λ is a dimensionless coupling constant.

In the absence of a harmonic confinement, the system is classically integrable [2]. Defining $\hbar^2 \lambda = \alpha^2$, the integrals of motion are constructed using the Lax matrix defined as

$$L_{ij} = p_i \delta_{ij} + (1 - \delta_{ij}) \frac{i\alpha}{x_i - x_j}. \quad (2)$$

The integrals of motion are given by

$$I_n = \text{tr}(L^n), \quad \text{for } n = 1, \dots, N. \quad (3)$$

It is straightforward to show that the integrals of motion are in involution, $[I_n, I_m] = 0$, and hence the system is classically integrable.

In this paper we are interested in the classical statistical properties of a system of identical particles whose dynamical behaviour is described by the Hamiltonian in equation (1). The quantum dynamics of such particles has been extensively studied [1, 3], and its exact N -particle quantum canonical partition function is known. By taking its $\hbar \rightarrow 0$ limit, the corresponding classical partition function was derived long ago [4]. More recently, further studies associated with the classical integrals and related Jacobians have been made [5, 6]. In this paper, the emphasis is on the thermodynamic properties of this classical system, particularly in relation to the fractional exclusion statistics (FES) that it obeys in the quantum regime [3, 7]. In section 2, we give a concise derivation of the classical N -particle canonical partition function, and the corresponding equation of state for the trapped gas. The harmonically confined system has a constant density of states, and only the second virial coefficient is found to be non-zero. But our primary interest is obtaining the virial expansion of the *unconfined* gas in the thermodynamic limit. The classical partition function for such a system is divergent. In section 3, we use the harmonic oscillator confinement as a regulator, and obtain the virial expansion for the equation of state in the limit of the oscillator frequency going to zero. In section 4, in the context of FES, we obtain the non-trivial classical distribution function by taking the appropriate limit of Wu's quantum occupancy factor for particles obeying fractional exclusion statistics [7, 8]. Using this, we derive the virial expansion of the homogeneous gas and confirm the results obtained in section 4. We also find the energy of the classical CSM model at zero temperature.

2. Classical limit of the quantum canonical partition function \mathcal{Z}_N

The classical partition function for N identical particles is given by

$$\mathcal{Z}_N(\beta) = \frac{1}{N!(2\pi\hbar)^N} \int d^N x d^N p \exp(-\beta H_N), \quad (4)$$

where the Hamiltonian H_N is given by equation (1). We choose the interaction strength $\hbar^2\lambda = \alpha^2$, with α being real. The interaction is therefore always repulsive. Note the explicit factor of $N!$ in the above expression for identical particles. While it is rather difficult to obtain the classical partition function by direct integration for all N , we may approach the problem as the classical limit of the quantum canonical partition function $\mathcal{Z}_N(\beta)$. This was the route which was originally taken in [4]. We obtain the desired result more directly, however, by using a property of CSM that relates to FES. To this end, we set the interaction strength $\lambda = g(g-1)$, where $g \geq 0$, and recall the known result [9]

$$\mathcal{Z}_N = e^{\hbar\beta\omega(1-g)\frac{N(N-1)}{2}} \mathcal{Z}_N^F, \quad (5)$$

where \mathcal{Z}_N is for an arbitrary g , and \mathcal{Z}_N^F is the N -particle non-interacting fermion partition function (for $g = 1$). Identical results are obtained when the problem is approached from the bosonic representation (for $g = 0$).

We are now in a position to take the classical limit. We define the classical limit as one in which the parameters m, ω, β, α are held fixed and we take the limit $\hbar \rightarrow 0$. Assuming this, we proceed as follows. Note that we have set

$$\alpha^2 = \hbar^2\lambda = \hbar^2 g(g-1), \quad (6)$$

where the classical interaction strength α is independent of \hbar . Both α and g are positive definite and are related by

$$g\hbar = \frac{\hbar}{2} + \sqrt{\alpha^2 + \hbar^2/4}. \tag{7}$$

Now taking the limit $\hbar \rightarrow 0$ while keeping α fixed implies $g \rightarrow \infty$ and

$$g\hbar \rightarrow \alpha. \tag{8}$$

This defines the approach to the classical limit. Taking this limit in equation (5) we obtain

$$\lim_{\hbar \rightarrow 0} Z_N = e^{-\alpha\beta\omega \frac{N(N-1)}{2}} \lim_{\hbar \rightarrow 0} [Z_N^F]. \tag{9}$$

The non-interacting fermion partition function is given by the well-known expansion, namely,

$$\begin{aligned} Z_N^F &= (-1)^N \sum_{\mathcal{P}} \prod_l \frac{1}{n_l!} \left[-\frac{Z_1(l\beta)}{l} \right]^{n_l} \\ &= \frac{1}{N!} \left[Z_1^N(\beta) - \frac{N(N-1)}{2} Z_1(2\beta) Z_1^{N-2}(\beta) + \dots \right], \end{aligned} \tag{10}$$

where the sum over \mathcal{P} is given by the number of partitions of N such that $\sum_{l=1}^N n_l l = N$ for n_l and l positive integers and

$$Z_1(\beta) = \frac{1}{2 \sinh(\hbar\beta\omega/2)}. \tag{11}$$

Now, taking the limit $\hbar \rightarrow 0$, we obtain the desired result

$$\hbar^N Z_N = e^{-\alpha\beta\omega \frac{N(N-1)}{2}} \frac{1}{N!(\beta\omega)^N}. \tag{12}$$

This is the same result obtained in [4] using a different but longer method.

2.1. Equation of state of the trapped classical gas

We can easily calculate the thermodynamic properties of the trapped gas from $Z_N(\beta)$ given in equation (12). The free energy is given by $F_N = -\tau \ln Z_N$, where $\tau = 1/\beta$. Since the density of states is constant for a harmonic confinement, it is like a two-dimensional gas, and the pressure is given by

$$P = - \left(\frac{\partial F_N}{\partial A} \right)_{\tau}, \tag{13}$$

where $A = l^2 = \hbar/m\omega$, l being the oscillator length. Writing

$$\left(\frac{\partial F_N}{\partial A} \right)_{\tau} = \left(\frac{\partial F_N}{\partial \omega} \right)_{\tau} \left(\frac{d\omega}{dA} \right), \tag{14}$$

and $\rho = N/A$, we obtain the equation of state

$$\beta P = \rho + \frac{\alpha \hbar \beta}{2} \rho^2, \tag{15}$$

where P is the pressure. Note that the virial coefficients of order 3 and higher are zero.

3. Classical equation of state for the homogeneous gas ($\omega \rightarrow 0$)

We now consider the virial expansion of the *unconfined* gas in the thermodynamic limit. The classical partition function for such a system is divergent. However, we use the harmonic oscillator confinement as a regulator to calculate the partition function as before and obtain the virial expansion for the equation of state in the limit of the oscillator frequency going to zero.

In the dilute limit, the equation of state is given by

$$\beta P = \sum_{l=1}^{\infty} b_l z^l, \quad (16)$$

where $z = e^{\beta\mu}$, and b_l are the cluster expansion coefficients [10, 11] which appear in the fugacity expansion as above. They can be expressed in terms of the canonical partition functions

$$b_l = (Z_1)^{l-1} \sum_{\{m_i\}} (-1)^{(\sum_i m_i - 1)} \left(\sum_i m_i - 1 \right)! \prod_i \left[\frac{Z_i}{Z_1} \right]^{m_i} \frac{1}{m_i!}. \quad (17)$$

Note that a cluster coefficient of order l involves all the partition functions up to Z_l . The summation over m_i is constrained by the number of partitions of l , that is $\sum_{i=1}^l i m_i = l$.

Using the expansion for the density in terms of the cluster coefficients, namely,

$$\rho = \sum_{l=1}^{\infty} l b_l z^l, \quad (18)$$

along with equation (16), the virial expansion coefficients are defined by

$$\beta P = \rho \left[1 + \sum_{n=2}^{\infty} a_n (\lambda_T \rho)^{n-1} \right], \quad (19)$$

where $\lambda_T = \sqrt{2\pi\hbar^2\beta/m}$ is the thermal wavelength. The a_k are the virial coefficients of the system. Note that $b_1 = a_1 = 1$.

Consider the limit in which the confinement is removed. We do this by taking the limit $\omega \rightarrow 0$ as follows. The cluster coefficients are given by

$$\begin{aligned} b_2 &= \lim_{\omega \rightarrow 0} \frac{Z_1}{\sqrt{2}} \left[\frac{2Z_2}{Z_1^2} - 1 \right], \\ b_3 &= \lim_{\omega \rightarrow 0} \frac{Z_1^2}{\sqrt{3}} \left[\frac{3Z_3}{Z_1^3} - \frac{3Z_2}{Z_1^2} + 1 \right]. \end{aligned} \quad (20)$$

Note that the numerical pre-factors in these expressions for the harmonic regularization $\omega \rightarrow 0$ are different from the box regularization $L \rightarrow \infty$. In d dimensions ($d = 1$ in our case), the expressions for b_n in the simple harmonic regularization must be taken to be larger by a factor of $n^{d/2}$, where n is the order of the virial coefficient, than for the box regularization. This ensures that they give the same result as $\omega \rightarrow 0$ and $L \rightarrow \infty$, respectively [12].

Then the first two virial coefficients are given by

$$a_2 = -b_2, \quad a_3 = 4b_2^2 - 2b_3. \quad (21)$$

For the quantum gas, we find that

$$\begin{aligned} b_2 &= \frac{1}{\sqrt{2}} \left(\frac{1}{2} - g \right), \\ b_3 &= \frac{\sqrt{3}}{2} g(g-1) + \frac{1}{3\sqrt{3}}, \end{aligned} \quad (22)$$

and therefore,

$$\begin{aligned} a_2 &= \frac{1}{\sqrt{2}}(g - 1/2), \\ a_3 &= (2 - \sqrt{3})g(g - 1) + \frac{1}{2} - \frac{2}{3\sqrt{3}}. \end{aligned} \tag{23}$$

For $g = 0$ (1), we recover the virial coefficients for a one-dimensional gas of non-interacting bosons (fermions). If we take the limit $\hbar \rightarrow 0$ and $g \rightarrow \infty$ keeping α fixed as before, we get the virial expansion for the classical gas

$$\beta P = \rho \left[1 + \frac{1}{\sqrt{2}} \sqrt{\frac{2\pi\beta}{m}} \alpha \rho + (2 - \sqrt{3}) \frac{2\pi\beta}{m} \alpha^2 \rho^2 + \dots \right]. \tag{24}$$

4. Classical distribution function

An interacting system of particles described by a CSM model may be mapped on to an *ideal* gas obeying fractional exclusion statistics (FES) [3, 7]. In this section, we derive the classical virial expansion of the homogeneous gas from this starting point and confirm that we obtain the same results as in section 3. It is also shown that the energy per unit length at zero temperature may be consistently obtained from our classical description by taking the limit $\hbar \rightarrow 0$.

The definition of the statistical parameter in FES, denoted by $g (>0)$, is based on the rate at which the number of available states in a system of fixed size decreases as more and more particles are added to it. The statistical parameter g assumes the values 0 and 1 for bosons and fermions respectively, because the addition of one particle reduces the number of available states by g . The application of the finite temperature distribution function [8] then enables us to calculate the temperature-dependent quantities of the system.

As is well known, the Haldane–Wu statistics is realized by the CSM model in one dimension [3], with the statistical parameter g in the FES being identical to the interaction strength in the CSM model as noted earlier. The potential and kinetic energies scale in the same way in this model, and both the energy densities scale as ρ^3 . The distribution function or average occupancy for FES particles has been derived by Wu [8] and is given by

$$n_p = \frac{1}{w_p + g}, \tag{25}$$

where p denotes the momentum, and the dispersion relation is given by $\epsilon_p = p^2/2m$. The parameter g is called the statistical parameter of FES since the occupancy of a given momentum state depends on g . It has been shown that the statistical parameter of FES is also the interaction coupling in the CSM model as used in the previous section. The function w_p satisfies the equation

$$w_p^g (1 + w_p)^{1-g} = e^{\beta(\epsilon_p - \mu)}. \tag{26}$$

We now ask the question: *what is the classical limit of the distribution function or, equivalently, how do we take the limit $g \rightarrow \infty$?* Let us assume that

$$w_p = g/\gamma_p \quad \text{and} \quad e^{-\beta\mu} = g e^{-\beta\mu_c}, \tag{27}$$

where γ_p depends on the momentum p , and μ_c is a renormalized chemical potential relevant to the classical limit. They also depend on other variables like temperature and density as will become clear below.

Using the above, we can write equation (26) in the following form:

$$w_p \left[\frac{w_p}{1 + w_p} \right]^{g-1} = g e^{\beta(\epsilon_p - \mu_c)}. \tag{28}$$

If we now take the limit $g \rightarrow \infty$ keeping all other variables $\beta, \gamma_p, \epsilon_p, \mu_c$ fixed, we find that

$$\frac{e^{-\gamma_p}}{\gamma_p} = e^{\beta(\epsilon_p - \mu_c)}, \quad (29)$$

where we have made use of the identity $\lim_{g \rightarrow \infty} (1 - \gamma_p/g)^g = e^{-\gamma_p}$. Note that equation (29) uniquely fixes γ_p in terms of the momentum p , temperature and the chemical potential since the function $\frac{e^{-\gamma_p}}{\gamma_p}$ monotonically goes from ∞ to 0 as a function of γ_p for $0 < \gamma_p < \infty$. Furthermore, using equations (25) and (27) we see that

$$n_p = \frac{1}{g} \frac{\gamma_p}{1 + \gamma_p}, \quad (30)$$

which is now the analogous classical distribution function for CSM particles.

There is yet another way of obtaining the above result from the grand partition function corresponding to FES, namely,

$$\ln Z_G = \sum_p \ln \left(1 + \frac{1}{w_p} \right) = \sum_p \frac{\gamma_p}{g} \quad (31)$$

in the limit $g \rightarrow \infty$. We immediately find that

$$n_p = -\frac{1}{\beta} \frac{\partial \ln Z_G}{\partial \epsilon_p} = \frac{1}{g} \frac{\gamma_p}{1 + \gamma_p}, \quad (32)$$

as desired.

We can now obtain the classical limit by setting $g\hbar = \alpha$. In a system with length L , the free energy $F = -(1/\beta) \ln Z_G$ follows from equation (31):

$$F = -\frac{L}{\beta} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{\gamma_p}{g} = -\frac{L}{\beta} \int_{-\infty}^{\infty} \frac{dp}{2\pi\alpha} \gamma_p. \quad (33)$$

Since the pressure is given by $P = -(\partial F/\partial L)_\beta$, we see that

$$\beta P = \int_{-\infty}^{\infty} \frac{dp}{2\pi\alpha} \gamma_p. \quad (34)$$

The density (i.e. the number of particles per unit length) is given by

$$\rho = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} n_p = \int_{-\infty}^{\infty} \frac{dp}{2\pi\alpha} \frac{\gamma_p}{1 + \gamma_p}, \quad (35)$$

while the energy per unit length is

$$E = \int_{-\infty}^{\infty} \frac{dp}{2\pi\alpha} \frac{\gamma_p}{1 + \gamma_p} \frac{p^2}{2m}. \quad (36)$$

The virial expansion at high temperature can be obtained using equations (29), (34) and (35) as follows. We find that as $\beta \rightarrow 0$, we must take $e^{\beta\mu_c} \rightarrow 0$ so that $e^{-\beta(\epsilon_p - \mu_c)} \ll 1$ for all values of p . Using equation (29), we can expand γ_p as a power series in $e^{-\beta(\epsilon_p - \mu_c)}$. To go up to the third virial coefficient, we find that

$$\gamma_p = e^{-\beta(\epsilon_p - \mu_c)} - e^{-2\beta(\epsilon_p - \mu_c)} + \frac{3}{2} e^{-3\beta(\epsilon_p - \mu_c)} + \dots \quad (37)$$

Equation (35) then gives

$$\rho = \frac{1}{\alpha} \sqrt{\frac{m}{2\pi\beta}} \left(e^{\beta\mu_c} - \sqrt{2} e^{2\beta\mu_c} + \frac{3\sqrt{3}}{2} e^{3\beta\mu_c} + \dots \right). \quad (38)$$

This equation can be inverted to give

$$e^{\beta\mu_c} = \sqrt{\frac{2\pi\beta}{m}}\alpha\rho + \sqrt{2}\left(\sqrt{\frac{2\pi\beta}{m}}\alpha\rho\right)^2 + \left(4 - \frac{3\sqrt{3}}{2}\right)\left(\sqrt{\frac{2\pi\beta}{m}}\alpha\rho\right)^3 + \dots \quad (39)$$

Equations (34) and (37) now give

$$\beta P = \frac{1}{\alpha}\sqrt{\frac{m}{2\pi\beta}}\left(e^{\beta\mu_c} - \frac{1}{\sqrt{2}}e^{2\beta\mu_c} + \frac{\sqrt{3}}{2}e^{3\beta\mu_c} + \dots\right). \quad (40)$$

Substituting equation (39) into (40), we obtain the expression in equation (24).

Finally, let us consider the zero temperature limit. Note that as $\beta \rightarrow \infty$, $\gamma_p = 0$ if $\epsilon_p > \mu_c$, and $\gamma_p = \infty$ if $\epsilon_p < \mu_c$; thus, $\gamma_p/(1 + \gamma_p)$ is 0 or 1 in these two cases. This is very similar to the Fermi distribution function at zero temperature. Using this fact in equation (25), we find that there exists a Fermi momentum $p_F = \sqrt{2m\mu_c}$ which is related to the density through $\rho = p_F/(\pi\alpha)$. Equation (36) then shows that the energy per unit length is given by $E = \pi^2\alpha^2\rho^3/(6m)$. Let us now show directly that this is the expected value of the classical energy at zero temperature. At $T = 0$, the particles are at rest; hence, the kinetic energy is zero. The repulsive two-body interactions in equation (1) (where we have taken $\hbar^2\lambda = \alpha^2$ as usual and also set $\omega = 0$) will be minimized if the particles are equally spaced on a line, with the nearest neighbour spacing being equal to $1/\rho$. If the particles are ordered such that $x_i < x_{i+1}$ for all i , we will have $x_{i+n} - x_i = n/\rho$. The interaction energy per particle is then given by

$$\frac{\alpha^2}{m}\sum_{n=1}^{\infty}\frac{1}{(n/\rho)^2} = \frac{\pi^2\alpha^2\rho^2}{6m}. \quad (41)$$

Thus, the energy per unit length is given by $\pi^2\alpha^2\rho^3/(6m)$.

5. Summary

In this paper, we have used the exact solvability of the energy spectrum of the quantum CSM model for any value of the interaction parameter g to study the classical limit; this limit is obtained by taking $\hbar \rightarrow 0$ and $g \rightarrow \infty$ keeping $g\hbar = \alpha$ fixed. Our derivation of $Z_N(\beta)$ is more concise than previous derivations. We have computed the virial expansions for the classical CSM model with or without a harmonic confining potential (i.e. for a homogeneous system). Finally, we have found the classical limit of the Wu distribution function for FES and used this to show consistency between the virial expansions of the homogeneous CSM model obtained from $Z_N(\beta)$ and from FES up to the third virial coefficient.

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