

Thermodynamics of trapped interacting bosons in one dimension

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On the basis of Bethe ansatz solution of bosons with δ -function interaction in a one-dimensional potential well, the thermodynamics equilibrium of the system in finite temperature is studied by using the strategy of Yang and Yang. The thermodynamics quantities, such as specific heat, etc., are obtained for the cases of the strong coupling and weak coupling limits respectively. © 2001 American Institute of Physics. [DOI: 10.1063/1.1331562]

I. INTRODUCTION

There has been much interest recently in the study of strongly correlated electronic systems in one dimension. This is because not only various nonperturbative methods¹⁻¹⁰ are applicable to models in one dimension but also several photoemission experiments for one-dimensional compounds of alkali-metal copper oxides¹¹⁻¹³ are carried out. Bosons with δ -function interaction in one dimension is a simple but interesting model. It was solved in Ref. 14 under the periodic boundary condition, in Refs. 15 and 16 under the boundary condition of potential well of infinite depth, and in Ref. 17 under that of potential well of finite depth. A strategy for studying the thermodynamics of exactly solvable models was proposed in Ref. 18 when discussing the solution of Ref. 14. In the present paper, using the strategy of Ref. 18 we study the thermodynamics on the basis of the Bethe-ansatz solution of Ref. 17. After we recall the model Hamiltonian and the Bethe-ansatz equation we study the thermal equilibrium in Sec. II. The formal expressions of free energy and pressure are obtained. In Sec. III we consider the strong coupling limit and obtain the quasimomentum distribution and specific heat explicitly. In Sec. IV the case of weak coupling limit is discussed extensively.

II. THERMAL EQUILIBRIUM AT FINITE TEMPERATURE

The Hamiltonian of bosons in a one-dimensional potential well of finite depth with δ interaction reads

$$H = - \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + \sum_{i=1}^N V(x_i) + 2c \sum_{i>j=1}^N \delta(x_i - x_j), \quad (1)$$

where

$$V(x_i) = \begin{cases} 0 & |x| < L/2, \\ V_0^2 & |x| > L/2. \end{cases} \quad (2)$$

Eq. (1) is the first quantization version of the Gross–Pitaevski¹⁹ equation, which was widely used to study the Bose–Einstein condensation²⁰ in recent years. The model Hamiltonian (1) was solved by means of Bethe-ansatz method.¹⁷ The logarithm of the Bethe-ansatz equation reads

$$\frac{2\pi}{L} I_j = k_j + \frac{2}{L} \sin^{-1} \left(\frac{k_j}{V_0} \right) + \frac{1}{L} \sum_{l \neq j} \left[\tan^{-1} \left(\frac{k_j + k_l}{c} \right) + \tan^{-1} \left(\frac{k_j - k_l}{c} \right) \right], \quad (3)$$

where the integers I_j play the role of the quantum numbers. Equation (3) is the secular equation to determine the spectrum. Moreover the transcendental equation (3) is difficult to solve directly. Now, we consider the problem in the thermodynamic limit: $N \gg 1$ and $L \gg 1$ with a fixed concentration $D = N/L$ by introducing a “smooth” positive-defined density $\bar{\rho}(k)$ describing the distribution of roots and holes²¹

$$\bar{\rho}(k) = \frac{1}{L} \frac{dI(k)}{dk}.$$

Treating k_j as a continuous variable k and differentiating Eq. (3) with respect to k , we get an integral equation

$$\begin{aligned} 2\pi\bar{\rho}(k) = 1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + \int dk' \bar{\rho}(k') \left[\frac{c}{c^2 + (k - k')^2} + \frac{c}{c^2 + (k + k')^2} \right] \\ - \frac{1}{L} \sum_m \left[\frac{c}{c^2 + (k - h_m)^2} + \frac{c}{c^2 + (k + h_m)^2} \right], \end{aligned} \quad (4)$$

where we have used the replacement

$$\lim_{N, L \rightarrow \infty} \frac{1}{L} \sum_{l \neq j} f(k_l) = \int \bar{\rho}(k) f(k) dk - \frac{1}{L} \sum_m f(h_m),$$

in the thermodynamics limit. The summation in the right-hand side runs over “holes” (including k_j) which can be written formally as an integral $\int \rho_h(k) f(k) dk$ with $\rho_h(k) = (1/L) \sum_m \delta(k - h_m)$. Furthermore, Eq. (4) is written as an integral equation for the density of holes $\rho_h(k)$ and the density of roots $\rho(k) = \bar{\rho}(k) - \rho_h(k)$,

$$2\pi(\rho + \rho_h) = 1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + \int dk' \rho(k') \left[\frac{c}{c^2 + (k - k')^2} + \frac{c}{c^2 + (k + k')^2} \right]. \quad (5)$$

The Bethe-ansatz solution is obtained for the case of bounded states (i.e., $\text{Im} k_j = 0$), so the range of the integration is $[-V_0, V_0]$. In terms of the distribution function of roots, we can write out the energy per particle

$$E/N = D^{-1} \int \rho(k) k^2 dk, \quad (6)$$

where

$$D = N/L = \int \rho(k) dk. \quad (7)$$

On the basis of the strategy of Ref. 18, the total entropy of the system is obtained

$$S/N = D^{-1} \int [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h] dk, \quad (8)$$

where the Boltzmann constant is set to unit.

In the thermal equilibrium, the free energy $\Omega = (E - TS - \mu N)$ should be in minimum. Writing

$$\frac{\rho_h(k)}{\rho(k)} = \exp[\epsilon(k)/T], \tag{9}$$

we obtain from the minimizing requirements, $\delta\Omega = 0$, the following equations:

$$\epsilon(k) = -\mu + k^2 - \frac{T}{2\pi} \int \left[\frac{c}{c^2 + (k-k')^2} + \frac{c}{c^2 + (k+k')^2} \right] \ln(1 + e^{-\epsilon(k')/T}) dk'. \tag{10}$$

Equation (5) is readily written as

$$2\pi(1 + e^{\epsilon/T})\rho(k) = 1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + \int dk' \rho(k') \left[\frac{c}{c^2 + (k-k')^2} + \frac{c}{c^2 + (k+k')^2} \right]. \tag{11}$$

Principally, Eq. (10) can be solved by iteration and then Eq. (5) can be a Fredholm-type equation for $\rho(k)$.

We would like to mention some points about the parameter μ . If minimizing the Helmholtz free energy $F = E - TS$ under the condition that the concentration D in (7) is a constant, one will have a Lagrangian multiplier. The multiplier function is just the same as the chemical potential μ when considering a grand assemble. So both procedures are equivalent.

Multiplying Eq. (10) with ρD^{-1} and integrating over k , we obtain

$$\mu = D^{-1} \int (k^2 - \epsilon)\rho dk - \frac{T}{2\pi D} \int \left[2\pi(\rho + \rho_h) - 1 - \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \ln(1 + e^{-\epsilon/T}) dk. \tag{12}$$

The argument k of ρ and ϵ are always omitted in our notions as long as it does not bring about confusion. With the help of Eq. (9), the entropy (8) is rewritten as

$$\frac{S}{N} = D^{-1} \int [(\rho + \rho_h)\ln(1 + e^{-\epsilon/T}) + \rho\epsilon/T] dk. \tag{13}$$

The Helmholtz free energy per particle is

$$\frac{F}{N} = \frac{1}{D} \int (k^2 - \epsilon)\rho dk - \frac{T}{D} \int [(\rho + \rho_h)\ln(1 + e^{-\epsilon/T})] dk. \tag{14}$$

Comparison of Eq. (12) and Eq. (14) gives rise to

$$F = \mu N - \frac{TL}{2\pi} \int \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \ln(1 + e^{-\epsilon/T}) dk. \tag{15}$$

Thus the free energy will be obtained once the $\epsilon(k)$ is solved from Eq. (10). As in thermodynamics $F = -PL + \mu N$, the pressure is $P = -(\partial F / \partial L)_T$. It was shown²² that if ϵ, μ are implicit functions of some thermodynamic quantities x (such as T, L), the derivative of Eq. (15) with respect to x is the same as the partial derivative of Eq. (15) with respect to the explicit variable x . Then it is easy to calculate the pressure in terms of the ϵ , namely,

$$P = \frac{T}{2\pi} \int \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \ln(1 + e^{-\epsilon/T}) dk. \tag{16}$$

It is formally similar to the results of Ref. 18 except that one more term arising from the boundary condition is involved. Likewise, the entropy is

$$S = \frac{L}{2\pi} \int \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \left[\ln(1 + e^{-\epsilon/T}) + \frac{\epsilon/T}{1 + e^{\epsilon/T}} \right] dk. \quad (17)$$

The other thermal quantities such as specific heat, etc., are also obtainable if one is able to solve $\epsilon(k)$ from Eq. (10). We will calculate them in some special cases in the following sections.

III. STRONG COUPLING LIMIT

It is difficult to obtain an explicit expression of $\epsilon(k)$ from Eq. (10). However, in some special cases, we are able to obtain some plausible results. In the strong coupling limit $c \gg V_0$, Eq. (10) becomes

$$\epsilon(k) = -\mu + k^2 - \frac{T}{2\pi} \int \ln[1 + e^{(\mu - k'^2)/T}] \frac{d}{dk'} \left[\tan^{-1}\left(\frac{k' - k}{c}\right) + \tan^{-1}\left(\frac{k' + k}{c}\right) \right] dk'. \quad (18)$$

Integrating by part under the consideration of the approximation that $\tan^{-1}(k/c) \approx k/c$ for $c \gg V_0$, we have

$$\epsilon = -\mu' + k^2, \quad (19)$$

where

$$\mu' = \mu + \frac{2}{\pi c} \int \frac{k'^2}{1 + e^{(-\mu + k'^2)/T}} dk'. \quad (20)$$

Because of $(2/L)\sqrt{V_0^2 - k^2} \ll 1$ and $c \gg V_0$, we obtain up to the first order that

$$2\pi(\rho + \rho_h) = 1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + \frac{4V_0}{c}. \quad (21)$$

From Eqs. (9), (19), and (21), we obtain an analytic expression of $\rho(k)$:

$$2\pi\rho(k) = \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + \frac{4V_0}{c} \right] [1 + e^{(-\mu' + k^2)/T}]^{-1}. \quad (22)$$

Obviously, the $\rho(k)$ is a Fermi-type distribution. When $c, L \rightarrow \infty$,

$$2\pi\rho(k) = \frac{1}{1 + e^{(-\mu + k^2)/T}}, \quad (23)$$

which is just the distribution of free Fermi gas. The chemical potential μ should be positive-definite for the positive-definite density of roots.

As all particles are bounded in the potential well, i.e., $\text{Max}(k) \sim V_0$, $\rho(k)$ should vanish almost for $k > V_0^{1/2}$. This requirement together with Eq. (22) gives

$$(V_0^2 - \mu')/T \gg 1.$$

The system being thermal equilibrium exhibits a simple dependence on the large momentum cutoff $T_0(T_0 = V_0^2 - \mu')$, due to boundary effects. Therefore, the system can be in a state of

thermal equilibrium only when $T \ll T_0$. Otherwise some particles may overcome the potential energy at the boundary and escape out of the well. Substituting the obtained ϵ into Eq. (15), we obtain

$$F = \mu N - \frac{TL}{2\pi} \int \ln[1 + e^{(\mu' - k^2)/T}] \frac{d}{dk} \left[k + \frac{2}{L} \sin^{-1} \left(\frac{k}{V_0} \right) \right] dk. \tag{24}$$

As $k \ll V_0$, we can replace $\sin^{-1}(k/V_0)$ by k/V_0 , then

$$F = \mu N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \int_0^{V_0} \frac{k^2}{1 + e^{(-\mu' + k^2)/T}} dk. \tag{25}$$

In the low-temperature condition, the free energy becomes

$$F = \mu N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \left(\frac{1}{3} \mu'^{3/2} + \frac{T^2 \pi^2}{24 \mu'^{1/2}} \right), \tag{26}$$

where

$$\mu' = \mu + \frac{1}{c} \left(\frac{4}{3\pi} \mu^{3/2} + \frac{T^2 \pi}{6 \mu^{1/2}} \right). \tag{27}$$

The μ' is regarded as a mandation of chemical potential according to Eq. (22). However, we are not able to get an explicit result for the specific heat by partial derivative of Eq. (26), because the chemical potential μ might be temperature dependent. In order to observe some properties of specific heat at low temperature, we let $c \rightarrow \infty$ and let μ_0 denote chemical potential at zero temperature. The μ_0 is determined by

$$D = \frac{1}{2\pi} \int_{-\sqrt{\mu_0}}^{\sqrt{\mu_0}} \left(1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right) dk. \tag{28}$$

Considering $\lim_{T \rightarrow 0} \mu(T)/\mu_0 = 1$, we have

$$F = \mu_0 N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \left(\frac{1}{3} \mu_0^{3/2} + \frac{T^2 \pi^2}{24 \mu_0^{1/2}} \right). \tag{29}$$

We find that the specific heat at low temperature is Fermi-liquid-like,

$$C_V = \frac{\pi L}{6 \mu_0^{1/2}} \left(1 + \frac{2}{LV_0} \right) T. \tag{30}$$

Thus the interaction between the particles plays an important role to their statistical properties though the system we considered is a boson system. This is a model belonging to the class of Haldane's exclusion statistics.²³

IV. WEAK COUPLING LIMIT

Obviously, Eq. (10) can be written as

$$\epsilon = -\mu + k^2 - \frac{T}{2\pi} \int e^{-c|\omega|} e^{ik\omega} \cos(k'\omega) \ln(1 + e^{-\epsilon/T}) dk' d\omega. \tag{31}$$

Because in the weak coupling limit $c \ll 1$, we have

$$\epsilon(k) = -\mu + k^2 - T \ln(1 + e^{-\epsilon/T}) - f(k, c), \tag{32}$$

where

$$f(k, c) = \frac{T}{2\pi} \sum_{n=1}^{\infty} \int \frac{(-1)^n c^n |\omega|^n}{n!} e^{ik\omega} \cos(k'\omega) \ln(1 + e^{(\mu - k^2)/T}) dk' d\omega.$$

This leads to

$$e^{-\epsilon/T} = [e^{(-\mu + k^2 - f(k, c))/T} - 1]^{-1}. \quad (33)$$

Likewise, Eq. (5) gives rise to

$$2\pi\rho_h(k) = 1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + g(k, c), \quad (34)$$

where

$$g(k, c) = \sum_{n=1}^{\infty} \int \frac{(-1)^n c^n |\omega|^n}{n!} e^{ik\omega} \cos(k'\omega) dk' d\omega.$$

With the help of (33), we obtain the distribution function of roots

$$2\pi\rho(k) = \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} + g(k, c) \right] \frac{1}{e^{[-\mu + k^2 - f(k, c)]/T} - 1}. \quad (35)$$

Physically, it represents the distribution of quasimomenta of the system as a collection. Because the density of root should be positive-definite, $\mu + f(k, c)$ must be always smaller than the corresponding k^2 , particularly, $\mu + f(0, c) \leq 0$. So Eq. (35) is a bosonlike distribution. If considering the boundary effects so that $\rho(V_0) \approx 0$ we have $V_0^2 - \mu - f(V_0, c) \gg T$. There is a large-momentum cutoff $T_0 = V_0^2 - f(V_0, c) - \mu$ such that the system can be in a thermal equilibrium only when $T \ll T_0$.

Now we consider the free energy, and only take account of the leading terms for $c \ll 1$,

$$2\pi\rho(k) = \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \frac{1}{e^{(k^2 - \mu)/T} - 1}. \quad (36)$$

The free energy (15) becomes

$$F = \mu N + T \frac{L}{2\pi} \int \left[1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right] \ln[1 - e^{(\mu - k^2)/T}] dk. \quad (37)$$

Since $k \ll V_0$, $\sin^{-1}(k/V_0) \approx k/V_0$, we have

$$F = \mu N - \frac{L}{\pi} \left(1 + \frac{2}{LV_0} \right) \int \frac{k^2}{e^{(k^2 - \mu)/T} - 1} dk. \quad (38)$$

As for free bosons (i.e., $c = 0$), the chemical potential should be nonpositive-definite and smaller than the energy of any particles. Moreover, for a fixed concentration ($D = N/L$), it is a function of temperature decreasing as the temperature increases according to Eq. (36). Hence when temperature goes to zero, the chemical potential will approach to zero from a negative value.

At low temperature, Eq. (38) becomes

$$F = \mu N - \frac{LT^{3/2}}{2\sqrt{\pi}} \left(1 + \frac{2}{LV_0} \right) Li_{3/2}(e^{\mu/T}), \quad (39)$$

where $Li_n(z)$ is polylogarithm function with $Li_{3/2}(1) = \zeta(3/2)$ and $\zeta(x)$ is Riemann's Zeta function. Since $Li_n(z)$ can be expanded into series of z and the chemical potential μ should be zero at zero temperature, we neglect the $Li_{3/2}(e^{\mu/T})$'s dependence on T . Then the entropy has the form

$$S = \frac{3LT^{1/2}}{4\sqrt{\pi}} \left(1 + \frac{2}{LV_0} \right) Li_{3/2}(e^{\mu/T}), \quad (40)$$

and the specific heat

$$C_V = \frac{3LT^{1/2}}{8\sqrt{\pi}} \left(1 + \frac{2}{LV_0} \right) Li_{3/2}(e^{\mu/T}), \quad (41)$$

which has boson-gas-like behaviors.

V. CONCLUSIONS AND REMARKS

In the above, we discussed the thermodynamics of bosons in a one-dimensional potential well on the basis of the exact solution of the model. Using the strategy of Yang and Yang,¹⁸ we studied the general thermodynamic properties of the system. We considered the problem in the strong coupling limit and found that the behavior of the system at low temperature is Fermi liquidlike even though it is a boson system. Therefore, the interaction plays an important role. Meanwhile we obtained the specific heat which is linearly dependent on the temperature T . For the weak coupling limit, we found that the system behaves like boson gas at low temperature.

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