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2003 J. Phys.: Condens. Matter 15 5511

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# Bose–Einstein condensation in confined geometry: thermodynamic mapping study

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Received 11 March 2003

Published 1 August 2003

Online at [stacks.iop.org/JPhysCM/15/5511](http://stacks.iop.org/JPhysCM/15/5511)

## Abstract

Quantum confinement shifts quantum phase transitions like the  $\lambda$ -point of liquid helium. This effect is calculated here for ideal Bose–Einstein condensates (BECs) using thermodynamic mapping (TM). TM is a procedure to obtain low temperature behaviour from high temperature information via elementary transformations. We report here a series of TM relations for thermodynamic quantities and the resulting transition properties for ideal BECs.

## 1. Introduction

Two of the most exciting lines of current research are studies of Bose–Einstein condensation (BEC) of dilute atomic gases confined in magnetic traps [1–3] and studies of nanostructures with quantum states controlled by confinement to wells small enough to determine and even tune allowed energies. Here we study the related problem of an ideal BEC in confined geometry and develop a technique for attacking a particular subset of the above problems.

While liquid  $^4\text{He}$  is not a non-interacting Bose gas, experiments in which  $^4\text{He}$  is confined in tiny pores, as in porous glasses, e.g. Vycor, have shown interesting changes in the  $\lambda$  transition due to quantum confinement [4]. For example, the  $\lambda$ -point is shifted to higher temperatures, and the transition temperature,  $T_c$ , is independent of the particle density, unlike bulk  $^4\text{He}$ . This work has stimulated the present study of a confined, non-interacting Bose gas [5].

The properties of a confined, ideal Bose gas are calculated by a new method in our work. We use a thermodynamic mapping (TM) theorem [6] to relate low temperature properties to high temperature properties.

## 2. Confinement effects

In the approximation that normal  $^4\text{He}$  can be described as an ideal Bose gas, the energy of a particle can be estimated from the Heisenberg uncertainty principle as follows:

$$\varepsilon = \frac{\overline{(\Delta p)^2}}{2m} \sim \frac{h^2}{2m} \frac{1}{(\Delta x)^2} = \frac{h^2}{2m} \left(\frac{N}{V}\right)^{2/3} \sim k_B T_c. \quad (1)$$

According to this estimate, it is clear that  $T_c$  is related to the particle density  $\bar{n} = N/V$ .

Confined  $^4\text{He}$  has very different properties from the bulk. Two striking effects are that  $T_c$  is independent of  $\bar{n}$  and that  $T_c$  increases as confinement size decreases. These differences are thought to be due to quantization effects, and that is consistent with the results reported in this paper. The interval of energy levels,  $\Delta\varepsilon$ , of an ideal system can be estimated as

$$\Delta\varepsilon \sim \frac{h^2}{2m} \frac{1}{a^2}, \quad (2)$$

where  $a$  is the cavity dimension. For  $a \sim 5$  nm, and  $m$  the mass of a helium atom,  $\Delta\varepsilon \sim 0.1$  K, easily observable relative to the critical temperature,  $T_c \sim 2$  K. So the size of the cavity makes quantum effects important and brings about significant changes in the system properties.

## 3. Thermodynamic mapping

It is an interesting dream to have TM to map the information at high temperature into that at low temperature. However, we know this is extremely difficult, and in general cases there is no unified method. But we can start from model studies and partly realize the TM. We think BEC in confined geometry is a perfect model for realizing the TM dream, because it is nontrivial and has a quantum phase transition at low temperature. So we start from the perfect gases in confined geometry first to realize the TM dream in a theoretical problem with some physical background and in a hot field.

TM is a method that maps low temperature properties from high temperature properties by elementary transformations. This is done by a finite procedure in contrast to infinite procedures like analytic continuation and the path from the zero-temperature Green function to the finite-temperature Green function, for which accumulation of error can be very serious.

The following classes of problems can be considered as some examples of our defined TM procedures.

- (1) In classical statistical physics, if the interaction potential is a  $p$ th-order homogeneous function of the differences of particle coordinates, then the configuration integrals satisfy the following general relation:

$$\left(\frac{1}{T_1}\right)^{3N/p} \int_{-\infty}^{\infty} e^{-U/k_B T_1} dq = \left(\frac{1}{T_2}\right)^{3N/p} \int_{-\infty}^{\infty} e^{-U/k_B T_2} dq. \quad (3)$$

- (2) For the Ising model, Kramers and Wannier [7] proved a dual transformation relating low and high temperature expansions. Three years later, Onsager [8] obtained the exact solution for the 2D Ising model. He also proved such a dual transformation. Similar dual transformations have only been found for finite level systems, i.e. spin systems.

For most practical systems the number of single-particle energy levels is infinite. We have found an exact TM relation for confined systems. We first discuss the thin film case.

Consider free electrons in a thin film of thickness  $t$ , with large lateral dimensions, so  $t \ll L_1 = L_2 \equiv L$ . The energy levels are

$$\varepsilon_i = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n_1^2 + n_2^2}{L^2} + \frac{n_3^2}{t^2} \right). \quad (4)$$

Motions in the plane of the film are quasi-classical. Quantum effects may be important in the direction normal to the film, due to the smallness of  $t$ .

For Boltzmann statistics, the free energy is

$$F = -k_B T \ln \left[ \frac{1}{N!} \left( L^2 \frac{mk_B T}{2\pi\hbar^2} \sum_i e^{-\varepsilon_i/k_B T} \right)^N \right]. \quad (5)$$

With  $\varepsilon_i$  as given in equation (4), the remaining summation in equation (5) is of the form

$$w(\alpha) \equiv \sum_{n=0}^{\infty} e^{-\alpha n^2}. \quad (6)$$

For convenience, rewrite this sum over both positive and negative integers, so

$$Z(\alpha) \equiv \sum_{-\infty}^{\infty} e^{-\alpha n^2} = 2w(\alpha) - 1. \quad (7)$$

The sum in equation (6) appears in both classical and quantum partition functions and thermodynamic potentials, at least for non-interacting systems. So the TM relation we prove below,

$$Z(\alpha) = \sqrt{\frac{\pi}{\alpha}} Z\left(\frac{\pi^2}{\alpha}\right), \quad (8)$$

is applicable more generally than just to the thin film problem. In the remainder of this paper we apply equation (8) to the problem of BEC in confined geometries. The TM relation could also be used for a suitable nonideal system for which one can transform the sums over states into the form of equation (6).

### 3.1. Proof of the TM relation equation (8)

We first prove

$$w\left(\frac{\pi^2}{\alpha}\right) = \sqrt{\frac{\alpha}{\pi}} \left[ w(\alpha) - \frac{1}{2} \right] + \frac{1}{2}. \quad (9)$$

For real  $\gamma$  and  $\beta$  with  $\beta > 0$ ,

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}\beta\xi^2} \cos(\gamma\xi) d\xi = \sqrt{\frac{2\pi}{\beta}} e^{-\gamma^2/2\beta} \quad (\beta > 0). \quad (10)$$

Letting  $\gamma = nx$  ( $n = 0, \pm 1, \pm 2, \dots$ ) and  $\beta = 2$  and summing both sides of equation (10), we have

$$\sqrt{\pi} \sum_{n=0}^{\infty} e^{-(x/2)^2 n^2} = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} e^{-\xi^2} \cos(nx\xi) d\xi. \quad (11)$$

The left-hand side of equation (11) is just  $\sqrt{\pi} w(x^2/4)$  (see equation (6)). Now we use the identity [9]

$$\sum_{n=1}^{\infty} \cos(nx) = -\frac{1}{2} + \pi \sum_{n=-\infty}^{\infty} \delta(x - 2\pi n), \quad (12)$$

to obtain for the right-hand side of equation (11)

$$\int_{-\infty}^{\infty} \left[ \frac{1}{2} + \pi \sum_{n=-\infty}^{\infty} \delta(x\xi - 2\pi n) \right] e^{-\xi^2} d\xi = \frac{\sqrt{\pi}}{2} - \frac{\pi}{|x|} + \frac{2\pi}{|x|} w \left[ \left( \frac{2\pi^2}{x} \right) \right], \quad (13)$$

proving equation (9) and the following two equivalent relations:

$$w(\alpha) = \sqrt{\frac{\pi}{\alpha}} \left[ w \left( \frac{\pi^2}{\alpha} \right) - \frac{1}{2} \right] + \frac{1}{2}, \quad (14)$$

$$Z(\alpha) = \sqrt{\frac{\pi}{\alpha}} Z \left( \frac{\pi^2}{\alpha} \right). \quad (15)$$

Since  $\alpha \sim 1/T$  in statistical physics, the above equations realize a mapping relation between the high temperature region and the low temperature region, divided at  $\alpha = \pi$ . For numerical calculations we can select either temperature region for the simplest calculation and map the opposite region.

In the study of confined BEC, derivatives of  $Z(\alpha)$  will be needed. Here are TM relations for first, second and third derivatives.

(1) *First derivative:*

$$Z'(\alpha) = - \sum_{n=-\infty}^{\infty} n^2 e^{-\alpha n^2}; \quad (16)$$

$$Z'(\alpha) = - \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}} Z \left( \frac{\pi^2}{\alpha} \right) - \left( \frac{\pi}{\alpha} \right)^{5/2} Z' \left( \frac{\pi^2}{\alpha} \right). \quad (17)$$

(2) *Second derivative:*

$$Z''(\alpha) = \sum_{n=-\infty}^{\infty} n^4 e^{-\alpha n^2}; \quad (18)$$

$$Z''(\alpha) = \frac{3\sqrt{\pi}}{4} \alpha^{-5/2} Z \left( \frac{\pi^2}{\alpha} \right) + \frac{3\pi^{5/2}}{\alpha^{7/2}} Z' \left( \frac{\pi^2}{\alpha} \right) + \left( \frac{\pi}{\alpha} \right)^{9/2} Z'' \left( \frac{\pi^2}{\alpha} \right). \quad (19)$$

(3) *Third derivative:*

$$Z'''(\alpha) = - \sum_{n=-\infty}^{\infty} n^6 e^{-\alpha n^2}; \quad (20)$$

$$\begin{aligned} Z'''(\alpha) = & - \frac{15\sqrt{\pi}}{8\alpha^{7/2}} Z \left( \frac{\pi^2}{\alpha} \right) - \frac{45\pi^{5/2}}{4\alpha^{9/2}} Z' \left( \frac{\pi^2}{\alpha} \right) \\ & - \frac{15\pi^{9/2}}{2\alpha^{11/2}} Z'' \left( \frac{\pi^2}{\alpha} \right) - \left( \frac{\pi}{\alpha} \right)^{13/2} Z''' \left( \frac{\pi^2}{\alpha} \right). \end{aligned} \quad (21)$$

#### 4. Mapping relation for confined BEC

Noticing that the interaction in liquid  $^4\text{He}$  is a strong one and many theories studying even weak interaction and homogeneous models are in not consistence, in order to emphasize the effect of geometric confinement, we consider an ideal Bose gas, neglecting interactions. Just as one of the referees said, 'it is often useful to consider the interaction-free limit'.

We consider rectangular cavities of size  $L_1 \times L_2 \times L_3$ . For numerical calculations we use parameters suitable for a hypothetical non-interacting gas of  $^4\text{He}$ . In order to show the effect of confinement on quantum states of the gas, we consider two common boundary conditions:

(1) periodic boundary conditions, giving the wavefunctions and energies

$$\psi_{\vec{p}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{p}\cdot\vec{r}/\hbar}, \quad p_i = \frac{\hbar n_i}{L_i} \quad (i = 1, 2, 3), \quad (22)$$

$$\varepsilon(\vec{n}) = \frac{\hbar^2}{2m} \sum_{i=1}^3 \left( \frac{n_i}{L_i} \right)^2 \quad (n_i = 0, \pm 1, \pm 2, \dots), \quad (23)$$

(2) rigid boundary conditions, with wavefunctions and energies

$$\psi_n(\vec{r}) = \prod_{i=1}^3 \sqrt{\frac{2}{L_i}} \sin\left(\frac{n_i \pi}{L_i} x_i\right) \quad (n_i = 1, 2, \dots), \quad (24)$$

$$\varepsilon(\vec{n}) = \frac{\hbar^2}{2m} \sum_{i=1}^3 \left( \frac{n_i}{L_i} \right)^2 \quad (n_i = 1, 2, 3, \dots). \quad (25)$$

Both boundary conditions can be applied to this problem. There are some differences: rigid boundary conditions have no state with zero energy and the quantum numbers  $\{n_i\}$  are positive integers. These differences give slight differences in the results, but the analysis is identical, and physical conclusions are the same.

The grand thermodynamic potential for an ideal Bose gas is

$$\Omega = k_B T g \sum_{\vec{n}} \ln[1 - e^{\frac{\mu - \varepsilon(\vec{n})}{k_B T}}], \quad (26)$$

where  $k_B$  is the Boltzmann constant,  $g$  is the spin degeneracy,  $T$  is the temperature and  $\mu$  is the chemical potential. Expanding the logarithm,  $\ln(1 - x) = -\sum x^l/l$ , ( $|x| < 1$ ), the thermodynamic potential can be expressed as

$$\begin{aligned} \Omega &= -k_B T g \sum_{\vec{n}} \sum_l \frac{1}{l} e^{l \frac{\mu - \varepsilon(\vec{n})}{k_B T}} \\ &= -k_B T g \sum_l \frac{1}{l} e^{l\mu/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right). \end{aligned} \quad (27)$$

In the usual approach, the above sum would be transformed to an integral in the thermodynamic limit ( $N \rightarrow \infty$ ,  $V \rightarrow \infty$ ,  $N/V \rightarrow \text{constant}$ ). But in a confined system we cannot take the thermodynamic limit, which takes the energy intervals to zero and makes the integral a good approximation for the sum. In fact, in a confined system the energy intervals are of appreciable size, so the sums must be calculated as sums. This makes the problem more difficult but also gives the new results seen in the experiments with confined  $^4\text{He}$ .

In order to calculate the sums we make use of the TM relation for  $Z(\alpha)$ , equation (15), and the derivative relations, equations (16)–(21). Hence we write the relevant thermodynamic relations in terms of the function  $Z$ . The pressure is

$$p = -\Omega/V = \frac{k_B T g}{V} \sum_l \frac{1}{l} e^{l\mu/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right). \quad (28)$$

The total particle number and particle density of the system are

$$N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = g \sum_l e^{l\mu/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right); \quad (29)$$

$$\bar{n} = \frac{N}{V} = \frac{N}{\prod_{i=1}^3 L_i}. \quad (30)$$

Equation (29) can be used to determine the chemical potential  $\mu$  as a function of  $T$  and  $\bar{n}$ , expressed by  $\mu(T, \bar{n})$ , or abbreviated as  $\mu(T)$ , one of the basic relations in our analysis.

To obtain the heat capacity of this system, we need the internal energy,  $\bar{E}$ .

$$\begin{aligned}\bar{E} &= g \sum_{\bar{n}} \frac{\varepsilon(\bar{n})}{e^{(\varepsilon(\bar{n})-\mu(T))/k_B T} - 1} \\ &= k_B T^2 g \sum_{l=1}^{\infty} \frac{1}{l} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right].\end{aligned}\quad (31)$$

So the heat capacity is

$$\begin{aligned}c_V = \left( \frac{\partial \bar{E}}{\partial T} \right)_V &= 2 \frac{\bar{E}}{T} + k_B T^2 g \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + k_B T^2 g \sum_{l=1}^{\infty} \frac{1}{l} e^{l\mu(T)/k_B T} \frac{\partial^2}{\partial T^2} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right].\end{aligned}\quad (32)$$

The derivative of the heat capacity is needed to precisely define the  $\lambda$  transition. It is

$$\begin{aligned}c'_V = \left( \frac{\partial c_V}{\partial T} \right)_V &= -2 \frac{\bar{E}}{T^2} + 2 \frac{c_V}{T} \\ &\quad + 2k_B T g \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + k_B T^2 g \frac{\partial}{\partial T} \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + k_B T^2 g \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right]^2 \sum_{l=1}^{\infty} l e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + 2k_B T^2 g \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial^2}{\partial T^2} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + 2k_B T g \sum_{l=1}^{\infty} \frac{1}{l} e^{l\mu(T)/k_B T} \frac{\partial^2}{\partial T^2} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right] \\ &\quad + k_B T^2 g \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial^3}{\partial T^3} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right].\end{aligned}\quad (33)$$

In order to calculate the quantities

$$\frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \quad \text{and} \quad \frac{\partial}{\partial T} \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right]\quad (34)$$

needed for equations (32) and (33), while avoiding the numerical calculation of derivatives, we use the invariance of the system particle density:

$$\frac{d\bar{n}}{dT} = 0.\quad (35)$$

Then

$$\begin{aligned}\frac{V}{g} \frac{d\bar{n}}{dT} &= \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} l e^{l\mu(T)/k_B T} \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \\ &\quad + \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z \left( \frac{lh^2}{2mk_B T L_i^2} \right) \right],\end{aligned}\quad (36)$$

and repeating this procedure,

$$\frac{d^2\bar{n}}{dT^2} = 0, \quad (37)$$

gives

$$\begin{aligned} \frac{V}{g} \frac{d^2\bar{n}}{dT^2} &= \frac{\partial}{\partial T} \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} l e^{l\mu(T)/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \\ &+ \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right]^2 \sum_{l=1}^{\infty} l^2 e^{l\mu(T)/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \\ &+ 2 \left[ \frac{\mu'(T)}{k_B T} - \frac{\mu(T)}{k_B T^2} \right] \sum_{l=1}^{\infty} l e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \right] \\ &+ \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \frac{\partial^2}{\partial T^2} \left[ \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \right]. \end{aligned} \quad (38)$$

Finally, the entropy of the system can be expressed as

$$\begin{aligned} S &= - \left( \frac{\partial \Omega}{\partial T} \right)_{V, \mu} = - \frac{\Omega}{T} - g \frac{\mu(T)}{T} \sum_{l=1}^{\infty} e^{l\mu(T)/k_B T} \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \\ &+ k_B T g \sum_{l=1}^{\infty} \frac{1}{l} e^{l\mu(T)/k_B T} \frac{\partial}{\partial T} \left[ \prod_{i=1}^3 Z\left(\frac{lh^2}{2mk_B T L_i^2}\right) \right]. \end{aligned} \quad (39)$$

With the aid of equations (15), (17), (19) and (21), all the mapping relations for the fundamental thermodynamic functions are now available.

In order to guarantee the accuracies of the series calculation to be better than a fixed level, e.g.  $10^{-10}$ , the numbers of terms are controlled automatically. For example,  $\alpha = 10^{-4}$ , in order to have accuracy  $10^{-10}$ , in the direct calculation, the function  $Z(\alpha)$  needs more than 320 terms. In our computer program, the calculation will be switched to the TM relation; it only needs two terms to guarantee the same accuracy,  $10^{-10}$ .

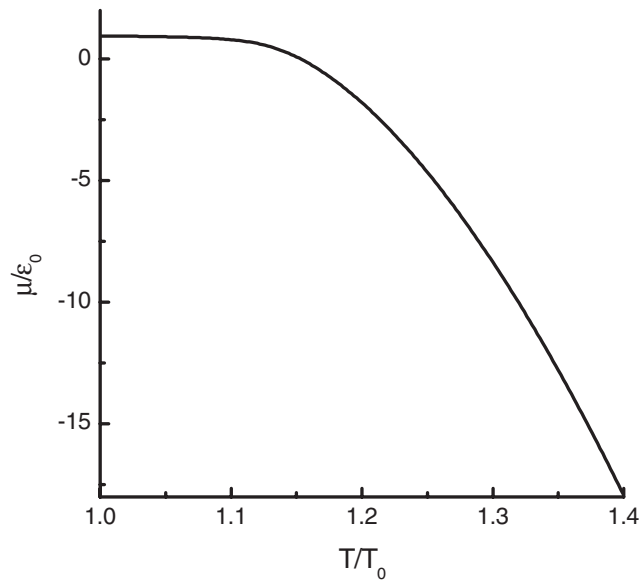
## 5. Determination of the critical temperature

It is important to note that the range of the chemical potential is different for the two boundary conditions:  $\mu \leq 0$  for periodic boundary conditions, while  $\mu \leq \varepsilon_0$  for rigid boundary conditions.

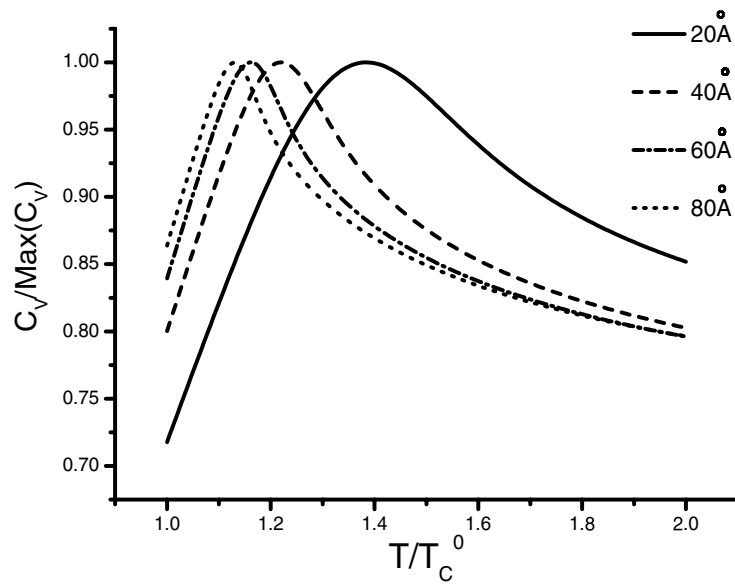
To obtain the chemical potential,  $\mu(T)$ , it is necessary to evaluate and invert equation (29). The results of this calculation are shown in figure 1, where it can be seen that the chemical potential changes significantly in one temperature range, perhaps indicating a phase transition. However, because this is a rather smooth function, a transition temperature cannot be obtained from this numerical result.

In order to determine carefully the critical temperature of the system, we sought the maximum in the heat capacity, as occurs at the  $\lambda$  point in the thermodynamic limit. We thus identified  $T_c$  as the temperature where the derivative of the heat capacity goes to zero with  $c'_V(T_c^-) > 0$  and  $c'_V(T_c^+) < 0$ . The heat capacity is shown in figure 2, in which a  $\lambda$ -like transition is apparent. But there is no cusp, as occurs in the thermodynamic limit. In figures 2 and 3,  $T_c^0$  denotes the transition temperature in the thermodynamic limit.





**Figure 1.** Chemical potential versus temperature (typical for  $L$  a few nm in size). In this figure,  $L_1 = L_2 = L_3 = 10$  nm,  $\bar{n} = 20 \times 10^{23} \text{ m}^{-3}$ .



**Figure 2.** Heat capacity of an ideal Bose gas as a function of temperature for cavity sizes 2–8 nm.

$$T_c^0 = \frac{2\pi\hbar^2}{mk_B} \left[ \frac{\bar{n}}{\zeta(\frac{3}{2})} \right]^{2/3} \quad (40)$$

where  $m$  is the mass of the boson, and  $\zeta(x)$  is the Riemann zeta function.

Having determined  $T_c$  by the sign change of the derivative of the heat capacity, we calculated the relation between  $T_c$  and cavity size for cubic cavities of side  $L$  from 1 to 10 nm, as shown in figure 3.

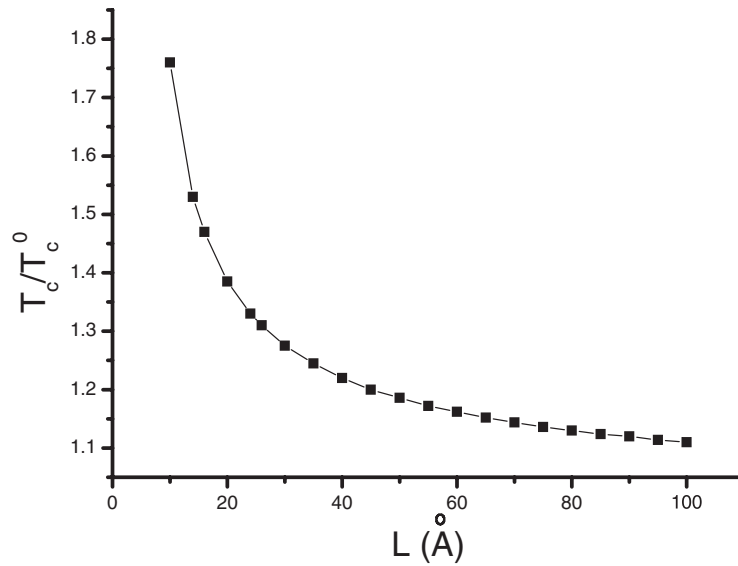


Figure 3.  $T_c$  versus cavity size.

It is worth mentioning that in a finite system the temperature of the maximum of the specific heat no longer coincides with other characteristic temperatures like the one for the onset of superfluidity, because in our recent work [10] there are at least five different definitions of the ‘transition’ temperatures for a finite system of dilute Bose gases. They are different, but will approach only one  $T_c$  as the systems approach the thermodynamic limit.

For studies we should be very careful, especially for confined geometry cases. We have not presented these here, but we may come back to this topic later.

Some interesting works have been done on the effects of finite size of dilute Bose gases in traps, e.g. [11–13]. For comparison, one should notice the following characters.

- (1) The  $T_c$  expansion is obtained under the condition  $\frac{\hbar\omega}{k_B T} \ll 1$ .
- (2) In harmonic traps, the dispersion relation (the energy-momentum relation) is linear, while in our case, it is quadratic.
- (3) The density is increasing with the total number of particles, but in our case, the density is fixed.

So we can expect that the effects can be different.

The expressions and their mapping relations for the thermodynamic functions developed above have already been used to obtain the energy,  $\bar{E}$ , heat capacity,  $c_V$ , derivative of the heat capacity,  $c'_V$ , chemical potential,  $\mu(T)$ , and its derivatives,  $\mu'(T)$  and  $\mu''(T)$ , as well as other properties, such as the pressure,  $p$ , entropy,  $S$ , etc that could be developed using this approach.

The TM has also been applied to study the sharpness  $R$  for the specific heat peak. We set up the width of the peak  $T_d$  in advance for comparison, e.g.  $T_d = 5$  K, then  $R = \frac{c_V(T_c+T_d)+c_V(T_c-T_d)}{2T_d}$ . In figure 4, it is shown that the peak becomes sharper and sharper as the  $L$  increases. Thus just as one could expect, in the thermodynamic limit, the peak becomes a cusp.

TM is also useful in studies on pressure. As we noticed, equation (28) is only an average expression of pressure. It is very interesting that for anisotropic cases the pressure becomes a tensor. For example, its value in the principal axis  $x$  is  $p_x = -\frac{1}{L_y L_z} \frac{\partial \Omega}{\partial L_x}$ ; in these cases, the TM is still very useful.

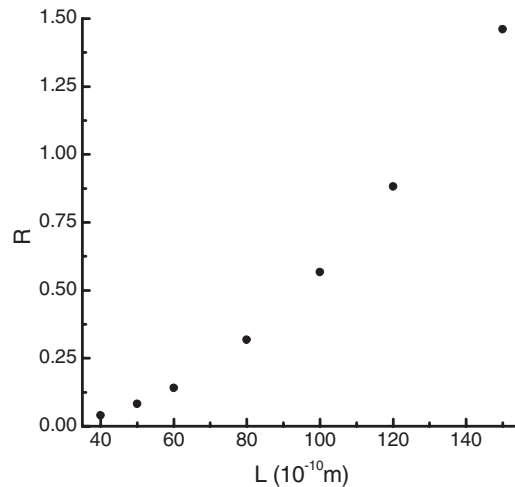


Figure 4.  $R$  versus cavity size.

## 6. Discussion

In this paper we have found and proven a TM relation that enables us to calculate the partition function and thermodynamic quantities for a confined system by carrying out the summations to high accuracy. Neither integral approximations to these sums nor approximate densities of states are necessary. These two points are significant, because in BEC the low-lying states are extremely important and the approximation of the density of states is very sensitive to the properties of the BEC, especially the ground state. The thermodynamic quantities of interest are all expressed in terms of  $Z(\alpha)$  and the derivatives,  $Z'(\alpha)$ ,  $Z''(\alpha)$ ,  $\mu'(T)$  and  $\mu''(T)$  with TM relations that are exact for this model, because on a computer the derivatives are difficult to obtain with high accuracy. Therefore, all these thermodynamic quantities can be calculated to high accuracy using the TM relations.

We emphasize that all the derivatives, including first and second derivatives of the chemical potential (notice that  $\mu(T)$  is obtained by solving a functional equation), are carried out by exact analytic operations to find equations that are evaluated by the TM process. So accuracy is maintained even for derivatives.

The singularity of the  $\lambda$ -transition disappeared, due to the finite size of the system. Nevertheless, the general characteristics of the transition in the bulk system remain. We find, as expected, that the sharpness of the transition increases as the size of the system increases.

The relation between  $T_c$  and cavity size ( $L$ ) shows that energy quantization in the confined geometry is the main reason for the shift of  $T_c$ .  $T_c$  increases as  $L$  gets smaller because the energy interval increases, requiring more thermal energy to create excitations from the ground state. This calculation is also consistent with experimental results in confined geometries.

In addition to allowing the calculation of the thermodynamic properties for confined BECs, the present work has illustrated the practical utility of TM, a general tool for statistical physics.

## Acknowledgments

This work was supported in part by the National Science Foundation of China, projects 19975009, 19834010 and 10174016. One of the authors (XXD) would like to thank the

Department of Physics and Astronomy at Brigham Young University for their hospitality, Professors C N Yang and Yu Lu and the Brigham Young University research group in theoretical physics for significant discussions.

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