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A new approach to treat the problems of trapped ideal gases

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Abstract

By comparing the thermodynamic properties of ideal atomic gases in a powerlaw potential and in a rigid box, it is found that the power-law potential is equivalent to the rigid box as far as the macroscopic behaviors of the system are concerned. The dimensionality and volume of the equivalent box are dependent on the parameters charactering the power-law potential. This equivalent relation enables us to treat a trapped ideal gas as a free one, and consequently, several useful conclusions of the trapped-gas system can be easily derived from the corresponding results of the free-gas system.

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1. Introduction

The thermodynamic properties of an ideal atomic gas confined to a rigid box have been extensively studied in the textbooks [1, 2]. In most cases, however, the atoms are trapped in a spatially varying external potential. The constrained role of the external potential may significantly change the performance of atomic gases, and therefore the properties of the gases trapped in external potentials are also well investigated [3–7].

Of a variety of external potentials, a typical one is the power-law potential whose generic form is given by

$$U(x_1, x_2, \dots, x_D) = \sum_{i=1}^{D} U_i \left| \frac{x_i}{L_i} \right|^{t_i},$$
(1)

where *D* is the dimensionality of space, x_i (i = 1, 2, ..., D) is the *i*th component of coordinate of a particle, and L_i , U_i and t_i are all positive constants marking the characteristics of the potential. The power-law potential is of prominent importance both in theoretical and experimental research. One of the reasons is that the strength and shape of the potential

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can be continuously changed by varying the parameters L_i , U_i and t_i . This is important for controlling the behavior of atomic gases and quantitatively investigating their performance.

It is evident that the power-law potential and rigid box are different traps to restrict the atoms. However, it will be found that, as far as the macroscopic behaviors of the trapped atomic gases are concerned, the power-law potential can be equivalently replaced with a rigid box whose dimensionality and volume are dependent on the dimensionality D and parameters t_i , U_i and L_i of the power-law potential. This enables us to treat a trapped ideal gas as a free one, so that the problems about the trapped gases may be solved in an easy way.

2. Equivalence of the power-law potential and the rigid box

We consider a nonrelativistic ideal atomic gas trapped in a *D*-dimensional power-law potential with the energy spectrum

$$\varepsilon(p, x_1, x_2, \dots, x_D) = \frac{p^2}{2m} + \sum_{i=1}^D U_i \left| \frac{x_i}{L_i} \right|^{t_i},$$
(2)

where *p* and *m* are, respectively, the momentum and mass of a particle.

The generic form of the grand partition function Ξ of an ideal atomic system can be expressed as

$$\ln \Xi = \frac{1}{\delta} \sum_{k} \ln[1 + \delta z \exp(-\beta \varepsilon_k)], \qquad (3)$$

where $\beta = 1/k_BT$, k_B is the Boltzmann constant, T is the temperature, $z = \exp(\beta\mu)$ is the fugacity, μ is the chemical potential, ε_k is the energy of the kth single-particle state, and δ is equal to -1, 1 and 0 for Bose, Fermi and classical gases, respectively. Under the thermodynamic limit, it can be derived that

$$\ln \Xi = \ln \Xi_0 + \frac{1}{h^D \delta} \int \ln \left\{ 1 + \delta z \exp \left[-\beta \left(\frac{p^2}{2m} + \sum_{i=1}^D U_i \left| \frac{x_i}{L_i} \right|^{t_i} \right) \right] \right\} \prod_{i=1}^D \mathrm{d} p_i \, \mathrm{d} x_i$$
$$= \ln \Xi_0 + \frac{1}{\lambda^{D+2\eta}} \left(\frac{h^2}{2\pi m} \right)^\eta \left[\prod_{i=1}^D \frac{(2L_i)\Gamma(1/t_i+1)}{U_i^{1/t_i}} \right] h_{D/2+\eta+1}(z), \tag{4}$$

where *h* is the Planck constant, $\lambda = h/\sqrt{2\pi m k_B T}$ is the thermal wavelength, $\ln \Xi_0 = (1/\delta) \ln(1 + \delta z)$ is the contribution of the ground state to $\ln \Xi$, $\Gamma(x) = \int_0^\infty \exp(-t)t^{x-1} dt$ is the gamma function,

$$h_{l}(z) = \frac{1}{\Gamma(l)} \int_{0}^{\infty} \frac{x^{l-1} dx}{z^{-1} \exp(x) + \delta},$$
(5)

which is equal to the Bose integral, Fermi integral and z for the Bose, Fermi and classical systems [1], respectively, $\eta \equiv \sum_{i=1}^{D} 1/t_i$, and, for simplicity, the internal degeneracy is assumed to be unit.

According to equation (4), all the thermodynamic quantities of the system can be derived straightforwardly. For example, one can obtain the total number of particles and internal energy as

$$N = z \left(\frac{\partial \ln \Xi}{\partial z}\right)_{\beta} = N_0 + \frac{1}{\lambda^{D+2\eta}} \left(\frac{h^2}{2\pi m}\right)^{\eta} \left[\prod_{i=1}^{D} \frac{(2L_i)\Gamma(1/t_i+1)}{U_i^{1/t_i}}\right] h_{D/2+\eta}(z)$$
(6)

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and

$$E = -\left(\frac{\partial \ln \Xi}{\partial \beta}\right)_{z} = \left(\frac{D}{2} + \eta\right) \frac{k_{B}T}{\lambda^{D+2\eta}} \left(\frac{h^{2}}{2\pi m}\right)^{\eta} \left[\prod_{i=1}^{D} \frac{(2L_{i})\Gamma(1/t_{i}+1)}{U_{i}^{1/t_{i}}}\right] h_{D/2+\eta+1}(z), \quad (7)$$

respectively, where $N_0 = z/(1 + \delta z)$ is the number of particles in the ground state, which is negligible for Fermi and classical systems but significant for the Bose system below the critical temperature of Bose–Einstein condensation (BEC).

By introducing the following parameters,

$$D' = D + 2\eta \tag{8}$$

and

$$V'_{D'} = \left(\frac{h^2}{2\pi m}\right)^{\eta} \prod_{i=1}^{D} \frac{(2L_i)\Gamma(1/t_i+1)}{U_i^{1/t_i}},\tag{9}$$

equations (4), (6) and (7) can be, respectively, expressed as

$$\ln \Xi = \ln \Xi_0 + \frac{V'_{D'}}{\lambda^{D'}} h_{D'/2+1}(z), \tag{10}$$

$$N = N_0 + \frac{V'_{D'}}{\lambda^{D'}} h_{D'/2}(z), \tag{11}$$

and

$$E = \frac{D'}{2} \frac{V'_{D'} k_B T}{\lambda^{D'}} h_{D'/2+1}(z), \tag{12}$$

which are just the expressions of the grand partition function, total number of particles and internal energy of an ideal atomic gas confined in a rigid box with dimensionality D' and volume $V'_{D'}$. This implies the fact that, as far as the thermodynamic properties of the trapped atomic gas are concerned, the power-law potential can be equivalently replaced with a rigid box. The two parameters, D' and $V'_{D'}$, defined in equations (8) and (9) can be, respectively, taken as the reduced dimensionality and equivalent volume of the power-law potential.

It is known from equations (8) and (9) that the reduced dimensionality is dependent on the dimensionality D and the parameter $\eta = \sum_{i=1}^{D} 1/t_i$ of the power-law potential, while the equivalent volume $V'_{D'}$ is dependent on D, t_i , U_i and L_i of the power-law potential and the mass m of a particle of the trapped gas.

In the special case of $L_1 = L_2 = \cdots = L_D \equiv L$, $U_1 = U_2 = \cdots = U_D \equiv U$ and $t_1 = t_2 = \cdots = t_D \equiv t$, equation (9) can be simplified as

$$\frac{L'}{L} = \left[\frac{\Gamma(1/t+1)}{(U/\varepsilon_0)^{1/t}}\right]^{1/(1+2/t)},\tag{13}$$

where $L' = (V'_{D'})^{1/D'}/2$ is the semi-side-length of the equivalent box, and $\varepsilon_0 \equiv h^2/(8\pi mL^2)$. Figure 1 shows the curves of $L'/L \sim U/\varepsilon_0$ for the different values of the parameter t. It is found that L'/L decreases with U/ε_0 for a given parameter t. The decreasing rate will increase as the parameter t is decreased. For the special case of $t \to \infty$, L'/L = 1 is independent of U/ε_0 . The physical meaning of the result is evident, because in the case of $t \to \infty$, the power-law potential becomes

$$U(x_1, x_2, \dots, x_D) = \begin{cases} 0 & |x_i| \le L \\ \infty & |x_i| > L, \end{cases}$$
(14)

which corresponds to a D-dimensional rigid box with the semi-side-length L.



Figure 1. Scaled semi-side-length L'/L of an equivalent box varying with the parameter U/ε_0 of a power-law potential for a different parameter *t*.

It should be noted that the power-law potential with $L_1 = L_2 = \cdots = L_D$, $U_1 = U_2 = \cdots = U_D$ and $t_1 = t_2 = \cdots = t_D$ is, in general, different from the spherical symmetric power-law potential with the form of

$$U(r) = U_0 \left(\frac{r}{r_0}\right)^r,\tag{15}$$

where t, U_0 and r_0 are positive constants, and $r = (\sum_{i=1}^{D} x_i^2)^{1/2}$. In the case of spherical symmetry, the grand partition function of the ideal atomic gas can be derived as

$$\ln \Xi = \ln \Xi_0 + \frac{1}{h^D \delta} \int \ln \left(1 + \delta z \exp \left\{ -\beta \left[\frac{p^2}{2m} + U_0 \left(\frac{r}{r_0} \right)^t \right] \right\} \right) \prod_{i=1}^D \mathrm{d} p_i \, \mathrm{d} x_i$$
$$= \ln \Xi_0 + \frac{1}{\lambda^{D+2D/t}} \left(\pi r_0^2 \right)^{D/2} \left(\frac{h^2}{2\pi m U_0} \right)^{D/t} \frac{\Gamma(D/t+1)}{\Gamma(D/2+1)} h_{D/2+D/t+1}(z)$$
(16)

and the reduced dimensionality and equivalent volume are given by

$$D' = D + 2D/t \tag{17}$$

and

$$V'_{D'} = \left(\pi r_0^2\right)^{D/2} \left(\frac{h^2}{2\pi m U_0}\right)^{D/t} \frac{\Gamma(D/t+1)}{\Gamma(D/2+1)},\tag{18}$$

respectively.

Another special power-law potential is the harmonic potential, which corresponds to the parameters $t_i = 2$ and $U_i/L_i^{t_i} = m\omega_i^2/2$ (i = 1, 2, ..., D), where ω_i is the frequency of the harmonic potential along the *i*th direction. It is found from equations (8) and (9) that, for the harmonic potential, D' = 2D and $V'_{D'} = \prod_{i=1}^{D} (h/m\omega_i)$. If L'_j (j = 1, 2, ..., D') denotes the *j*th semi-side-length of the equivalent box, i.e., $V'_{D'} = \prod_{j=1}^{D'} (2L'_j)$, we have $L'_j = (h/m\omega_j)^{1/2}/2 = (\pi/2)^{1/2}a_{hj}$, where $\omega_j = \omega_{j-D}$ for j > D, $a_{hj} = (h/m\omega_j)^{1/2}$ is the *j*th characteristic length of the harmonic potential with the frequency ω_j along the *j*th direction,

and $\hbar = h/2\pi$. The above analysis shows that the ideal atomic gas trapped in a *D*-dimensional harmonic potential can be treated as the same gas confined to a 2*D*-dimensional rigid box with the semi-side-length proportional to the characteristic length of the harmonic potential.

3. Some useful inferences

According to the equivalent relation of a power-law potential and a rigid box discussed above, some important results concerning the atomic gases trapped in a power-law potential can be easily derived from the familiar results for the free-gas system. Some typical examples are given below.

3.1. The condition of the occurrence of BEC and the critical temperature

It is well known that BEC can occur for an ideal Bose gas in a *D*-dimensional free space with D > 2 (the particles discussed in this paper are all assumed to be nonrelativistic). Thus, one can deduce that the condition of the occurrence of BEC in a *D*-dimensional power-law potential is

$$D' = D + 2\sum_{i=1}^{D} \frac{1}{t_i} > 2.$$
(19)

The result is in accordance with that obtained in [4]. In the special case of harmonic potential, the above condition is reduced to D > 1.

Similarly, according to the expression of the critical temperature for an ideal Bose gas in a D-dimensional free space [8], we can get the critical temperature for the corresponding system trapped in a D-dimensional power-law trap to be

$$T_{C} = \frac{h^{2}}{2\pi m k_{B}} \left[\frac{N}{V'_{D} \zeta(D'/2)} \right]^{2/D'}$$
$$= \frac{1}{k_{B}} \left[\frac{N h^{D}}{\zeta(\eta + D/2)(2\pi m)^{D/2}} \prod_{i=1}^{D} \frac{U_{i}^{1/t_{i}}}{(2L_{i})\Gamma(1/t_{i}+1)} \right]^{1/(D/2+\eta)}, \quad (20)$$

where $\zeta(x) = \sum_{l=1}^{\infty} 1/l^x$ is the Riemann zeta function. Equation (20) is in agreement with the result obtained in [4].

3.2. Discontinuity of the heat capacity at the critical temperature

According to the fact that, for an ideal Bose gas in a *D*-dimensional free space, the heat capacity at the critical temperature of BEC is discontinuous when D > 4 [8], we can get the condition of discontinuity of the heat capacity at the critical temperature for the system of ideal bosons trapped in a *D*-dimensional power-law potential as

$$D' = D + 2\sum_{i=1}^{D} \frac{1}{t_i} > 4,$$
(21)

which is reduced to D > 2 in the special case of the harmonic potential. It is the same as that obtained in [4].

3.3. Equivalence of the heat capacity between Bose and Fermi gases

It has been found that in a two-dimensional space the heat capacity at a constant volume for an ideal Bose gas is identical with that for an ideal Fermi gas [9, 10]. The equivalent relation between the power-law potential and the rigid box implies that the equality of the heat capacity is also valid for the ideal Bose and Fermi gases trapped in a power-law potential with

$$D' = D + 2\sum_{i=1}^{D} \frac{1}{t_i} = 2.$$
(22)

According to equation (22), one can deduce that the heat capacity for an ideal Bose gas trapped in a one-dimensional harmonic potential is identical with that for the corresponding Fermi gas trapped in the same potential.

3.4. Equation for a reversible adiabatic process

For ideal atomic gases (including Bose, Fermi and classical gases) in a *D*-dimensional free space, it is familiar that in a reversible adiabatic process, the relation between the temperature and the volume of the system is determined by $TV_D^{2/D} = \text{const.}$ Thus, we can infer that there will be the following relationship for an ideal atomic gas trapped in a *D*-dimensional power-law potential when the system undergoes a reversible adiabatic process:

$$TV_{D'}^{2/D'} = T\left[\left(\frac{h^2}{2\pi m}\right)^{\eta} \prod_{i=1}^{D} \frac{(2L_i)\Gamma(1/t_i+1)}{U_i^{1/t_i}}\right]^{1/(D/2+\eta)} = \text{const.}$$
(23)

It is seen from equation (23) that the temperature of the system in an adiabatic process will reduce if the equivalent value, $V_{D'}^{2/D'}$, is increased through the control of the parameters t_i , U_i and L_i of the power-law potential. This technique has successfully been employed in the experiment of BEC carried out at MIT [11].

4. Conclusions

In summary, we come to a conclusion that a power-law potential is equivalent to a rigid box, and the reduced dimensionality and equivalent volume are dependent on the parameters related to the power-law potential and the mass of gas particles. The equivalent relation enables us to treat a trapped atomic gas as a free one, so that the problems of trapped atomic gases may be solved more easily and some new characteristics of trapped atomic gases may be conveniently revealed. Finally, it is worthwhile to point out that the method mentioned above is of general significance and is also suitable for the ideal gas systems trapped in other external potentials such as the cylindrical power-law potential given in [12] and so on.

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