Density of states of particles in a generic power-law potential in any dimensional space

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An ideal gas trapped in a generic power-law potential in any dimensional space is studied. The density of states of this system is derived. Both Fermi and Bose gases are discussed, and their properties are derived straightforwardly from the density of states. [S1050-2947(99)02204-0]

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Since the observations of Bose-Einstein condensation (BEC) in ultracold trapped atomic gases in 1995 [1–3], there have been studies analyzing the effects of external potential [4], interaction between particles [4], space dimensionality [5], and finite particle number [6] on a Bose system. However, the density of states of this system has rarely been studied. In most textbooks of statistical mechanics, the density of states is formulated for free noninteracting systems in three-dimensional space. The density of states takes an important role in statistical physics, so we think it deserves further investigation.

Although interactions are extremely important in a real system, the problems are made tractable and the essential physics is retained by assuming an ideal system of noninteracting particles. Furthermore, experiment [7] shows that the influence of the interaction between particles on the BEC transition temperature is about several percent, so that such a system is taken approximately as an ideal system. Besides, theoretical studies have revealed that space dimensionality has a significant effect on the properties of the system [5,8]. Although the harmonic potential is a good approximation in the cases of recent experiments, for the sake of universality, here we shall derive an expression for the density of states of particles in a generic power-law potential in any dimensional space.

Let us consider an ideal gas in a generic power-law potential in n-dimensional space with a single-particle Hamiltonian

$$H=\varepsilon_0\left(\frac{p}{p_0}\right)^s+\sum_{i=1}^{n} U_i\left|\frac{r_i}{L_i}\right|^{t_i}, \tag{1}$$

where ϵ_0, p_0, s, U_i, L_i, and t_i are all positive constants and p and r_i are the momentum and coordinate of particles, respectively. When the particle number of the system is large and the energy level spacing of the trapping potential is much smaller than $kT=\beta^{-1}$ (this condition is often satisfied), the Thomas-Fermi semiclassical approximation is valid [9]. Thus sums over quantum states may be replaced by integrals over phase space. The total number of quantum states may then be expressed as

$$\Sigma(\varepsilon)=\frac{g}{h^n}\int_{(H\leqslant\varepsilon)}\prod_{i=1}^{n}(dr_i dp_i), \tag{2}$$

where h is the Planck constant and g is the spin degenerate factor. The volume of an n-dimensional sphere $V_n=C_nR^n=[\pi^{n/2}/\Gamma(n/2+1)]R^n$ implies that

$$d^nR=S_n(R)dR=nC_nR^{n-1}dR, \tag{3}$$

where $S_n(R)$ is the surface of the n-dimensional sphere. By using Eq. (3) and the beta function $B(x,y)=\int_0^1\theta^{x-1}(1-\theta)^{y-1}d\theta=\Gamma(x)\Gamma(y)/\Gamma(x+y)$, the total number of quantum states Eq. (2) may be expressed as

$$\Sigma(\varepsilon)=F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\varepsilon^{\lambda}, \tag{4}$$

where

$$\lambda=\frac{n}{s}+\sum_{i=1}^{n}\frac{1}{t_i}, \tag{5}$$

$$F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)=\frac{g2^nC_n}{h^n}\frac{p_0^n}{\varepsilon_0^{n/s}}\frac{\Gamma(n/s+1)}{\Gamma(\lambda+1)}\prod_{i=1}^{n}\frac{L_i\Gamma(1/t_i+1)}{U_i^{1/t_i}}, \tag{6}$$

and $\Gamma(l)=\int_0^\infty\theta^{l-1}e^{-\theta}d\theta$ is the gamma function. Equation (4) gives the density of states as

$$D(\varepsilon)=\frac{\partial\Sigma(\varepsilon)}{\partial\varepsilon}=\lambda F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\varepsilon^{\lambda-1}. \tag{7}$$

For the case of an isotropic power-law potential, i.e., a system with a single-particle Hamiltonian $H=\varepsilon_0(p/p_0)^s+U_0(r/L_0)^t$, along similar lines, the total number of quantum states may be written as

$$\Sigma(\varepsilon)=F_0(n,\varepsilon_0,p_0,s,U_0,L_0,t)\varepsilon^{\lambda_0}, \tag{8}$$

where

$$\lambda_0=n/s+n/t, \tag{9}$$

$$F_0(n,\varepsilon_0,p_0,s,U_0,L_0,t)=\frac{gC_n^2}{h^n}\frac{p_0^n}{\varepsilon_0^{n/s}}\frac{L_0^n}{U_0^{n/t}}\frac{\Gamma(n/s+1)\Gamma(n/t+1)}{\Gamma(n/s+n/t+1)}. \tag{10}$$

Consequently, we have the density of states as

$$D(\varepsilon)=\lambda_0 F_0(n,\varepsilon_0,p_0,s,U_0,L_0,t)\varepsilon^{\lambda_0-1}. \qquad (11)$$

This is not trivial; Eq. (7) may be reduced to Eq. (11) only if $n=1$ or $t_i=2$ or $t_i\to\infty$.

Although only particles in an external potential have been studied, the above results may be used to describe a free system. As long as the external potential in Eq. (1) is chosen, when $t\to\infty$, $U\to\infty$, and $U\to 0$ in the regions $r_i>L_i$ and $r_i<L_i$, respectively. This is just the condition of a free system confined in an n-dimensional container with a length $2L_i$ of each side. Applying this condition, Eq. (7) gives the form for a free system as

$$D(\varepsilon)=\left[\frac{g}{h^n}\frac{n}{s}C_n V_n \frac{p_0^n}{\varepsilon_0^{n/s}}\right]\varepsilon^{n/s-1}. \qquad (12)$$

If we further let $n=3$, $g=1$, $s=2$, and $\varepsilon_0=p_0^2/2m$, Eq. (12) may be reduced to

$$D(\varepsilon)=\frac{2\pi V_3}{h^3}(2m)^{3/2}\varepsilon^{1/2}. \qquad (13)$$

Equation (13) describes a nonrelativistic free ideal gas in three-dimensional space, and coincides with the result in current textbooks of statistical mechanics [10] as it should.

For the case of nonrelativistic spinless gas trapped in a generic power-law potential in three-dimensional space, $n=3$, $g=1$, and $\varepsilon_0=p_0^2/2m$, the density of states Eq. (7) then gives

$$D(\varepsilon)=\frac{V_3}{h^3}(2\pi m)^{3/2} \times\frac{\Gamma(1/t_1+1)\Gamma(1/t_2+1)\Gamma(1/t_3+1)}{U_1^{1/t_1}U_2^{1/t_2}U_3^{1/t_3}\Gamma(3/2+1/t_1+1/t_2+1/t_3)} \times\varepsilon^{1/2+1/t_1+1/t_2+1/t_3}. \qquad (14)$$

Reference [11] gives an expression of density of states, in fact, if we finish the integrations in it, we may obtain a result that coincides with this specific case.

With the density of states, one can obtain the thermodynamic quantities of systems straightforwardly. We shall show some examples.

From first principles of statistical mechanics, we have the distribution function

$$n_\varepsilon=\frac{1}{e^{(\varepsilon-\mu)/kT}+\delta}, \qquad (15)$$

where δ is -1, 1, and 0 for the case of the Bose, Fermi, and classical system, respectively. The total particle number N may be expressed as

$$N=\int_0^\infty D(\varepsilon)n_\varepsilon d\varepsilon =F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\Gamma(\lambda+1)I_\lambda(z)(kT)^\lambda, \qquad (16)$$

where $z=\exp(\mu/kT)$ is the fugacity; $I_\lambda(z)$ is equal to $g_\lambda(z)$, $f_\lambda(z)$, and z, respectively, for the Bose, Fermi, and classical systems; and $g_\lambda(z)=[1/\Gamma(\lambda)]\int_0^\infty[(\theta^{\lambda-1}d\theta)/(z^{-1}e^\theta-1)]$, $f_\lambda(z)=[1/\Gamma(\lambda)]\int_0^\infty[(\theta^{\lambda-1}d\theta)/(z^{-1}e^\theta+1)]$ are, respectively, the Bose and Fermi integrations. Similarly, the total energy E of the system may be written as

$$E=\int_0^\infty \varepsilon D(\varepsilon)n_\varepsilon d\varepsilon =\lambda F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\Gamma(\lambda+1)I_{\lambda+1}(z)(kT)^{\lambda+1} =NkT\lambda\frac{I_{\lambda+1}(z)}{I_\lambda(z)}. \qquad (17)$$

For an ideal Bose gas, Eq. (16) illustrates the number of particles in the gaseous state. The zero momentum state can become macroscopically occupied, and the system then undergoes a phase transition — BEC at the critical temperature T_c. The chemical potential cannot be positive and is a monotonically decreasing function of temperature. When $T\to T_c,\mu\to 0$, the particle number of the ground state is still macroscopically negligible. Therefore, Eq. (16) gives

$$kT_c=\left(\frac{N}{F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\Gamma(\lambda+1)\zeta(\lambda)}\right)^{1/\lambda}, \qquad (18)$$

where $\zeta(\lambda)=g_\lambda(1)=\Sigma_{J=1}^\infty J^{-\lambda}(\lambda\geqslant 1)$ is the Riemann zeta function. At a temperature T below T_c, from Eq. (16) we can obtain the fraction of condensation

$$\frac{N_0}{N}=1-\frac{N_e}{N}=1-\left(\frac{T}{T_c}\right)^\lambda. \qquad (19)$$

The total energy (17) gives a jump of heat capacity at critical temperature as

$$\Delta C_{T=T_c}\equiv C_{T_c^-}-C_{T_c^+}=Nk\lambda^2\frac{g_\lambda(1)}{g_{\lambda-1}(1)}, \qquad (20)$$

where we have made use of

$$\frac{\partial g_{\lambda+1}(z)}{\partial(\ln z)}=g_\lambda(z), \qquad (21)$$

and

$$\frac{\partial N}{\partial T}=0, \qquad (22)$$

at a temperature T above T_c. We can obtain a general criterion for BEC occurrence from Eq. (18) to be

$$\lambda\equiv\frac{n}{s}+\sum_{i=1}^n\frac{1}{t_i}>1. \qquad (23)$$

That is, BEC may take place only when criterion (23) is satisfied. Criterion (23) mirrors the fact that it relates not only to the dimensionality of space and kinematic characteristics of particles, but also to the shape (not the strength) of the external potential. Similarly, Eq. (20) implies a criterion on the continuity of heat capacity at the critical temperature. If

$$\lambda \equiv \frac{n}{s} + \sum_{i=1}^{n} \frac{1}{t_i} > 2, \tag{24}$$

there is a jump of heat capacity at critical temperature, otherwise, there exists no jump if $1 < \lambda \leqslant 2$ or even no BEC if $\lambda \leqslant 1$.

At low temperatures, the Fermi integration may be written as a quickly convergent series by using the Sommerfeld lemma [10],

$$f_\lambda(z) = \frac{(\ln z)^\lambda}{\Gamma(\lambda+1)}\left[1 + \lambda(\lambda-1)\frac{\pi^2}{6}\frac{1}{(\ln z)^2} + \lambda(\lambda-1)(\lambda-2)(\lambda-3)\frac{7\pi^4}{360}\frac{1}{(\ln z)^4} + \cdots\right]. \tag{25}$$

For an ideal Fermi gas, when $T=0$ K, there is only the first term in Eq. (25). Substituting it into Eq. (16) gives

$$N = F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)E_F^\lambda. \tag{26}$$

Consequently, the Fermi energy may be expressed as

$$E_F = \left(\frac{N}{F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)}\right)^{1/\lambda}. \tag{27}$$

When $T>0$ K and, however, the temperature is very low, the chemical potential in the limit of low temperatures may be derived from Eq. (17) and Eq. (25) to be

$$\mu = E_F\left[1 - (\lambda-1)\frac{\pi^2}{6}\left(\frac{kT}{E_F}\right)^2\right]. \tag{28}$$

Integrations $g_\lambda(z)$ and $f_\lambda(z)$ may be expanded as series

$$g_\lambda(z) = \sum_{i=1}^{\infty} \frac{z^i}{i^\lambda}, \tag{29}$$

$$f_\lambda(z) = \sum_{i=1}^{\infty} (-1)^{i-1}\frac{z^i}{i^\lambda}. \tag{30}$$

At high temperatures, z is very small, and both of the above series are quickly convergent. Consequently, in the limit of high temperatures, $I_\lambda(z) \to z$, and both Eq. (16) and Eq. (17) unify at their respective classical limits

$$N = F(n,\varepsilon_0,p_0,s,U_i,L_i,t_i)\Gamma(\lambda+1)z(kT)^\lambda, \tag{31}$$

and

$$E = NkT\lambda z. \tag{32}$$

Letting $t \to \infty$, the above thermodynamic quantities may be used to describe a free system. Equations (7) and (11) are general, they favor discussing the effects of external potential, space dimensionality, and kinematic characteristics of particles.

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