Thermodynamics of Generalized Fermi Systems in a Harmonic Trap

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Abstract. Thermodynamics of the generalized ideal Fermi systems in the two- and three-dimensional harmonic traps are respectively calculated by the Tsallis entropy in this paper. The influences of the trap and q-number on the thermodynamic parameters (epically the heat capacity) are analysed in detail. The results yield a well agreement with the classical cases.

1. Introduction
There are two subsystems named fermions and bosons in the nature. Fermions obey Fermi-Dirac distribution. Bosons obey Bose-Einstein distribution. This results that they appear completely different physical properties, especially at the region of low temperature. Under the region of low temperature, Bose system in a harmonic trap shows the unique Bose-Einstein condensation (BEC) phenomenon. Fermi system also can produce the similar BCS (Bardeen, Cooper and Schrieffer)-BEC crossover in certain special cases due to their mutual attraction of the nearest particles. Therefore, by studying the characteristics of Fermi system in an external potential, the researchers can better understand the BEC phenomenon.

Recently, many researchers develop and improve q-generalized entropy theory proposed by Tsallis through introducing the atomic interactions. The new q-generalized entropy theory yields a better case with the actual system. It is necessary to study the thermodynamic properties of Fermi system by using the extensive statistical theory [1-8]. In this paper, we firstly discuss the thermodynamic properties of the generalized ideal Fermi system in the free space based on the Fermi-Dirac distribution function in section 2. Furtherly, we obtain the corresponding cases of the generalized ideal Fermi system in the two-(2D) and three-dimensional (3D) harmonic traps in section 3 and section 4, respectively. Lastly, we calculate the related particle number, internal energy and heat capacity and discuss the influence of changing q-number.

2. Theory and Method
According to the non-generalized statistical theory, Tsallis entropy is expressed by

$$S_q = \left( \ln_q \left( \frac{1}{p_i} \right) \right) = \sum_{i=1}^{w} p_i \ln_q \frac{1}{p_i} = 1 - \sum_{i=1}^{w} p_i^q \frac{1}{q-1}.$$  (1)

After approximate factorization Eq. (1), one can obtain the following generalized Fermi-Dirac distribution function
\[ n_q = \frac{1}{\left[1 + (q-1)\beta(\epsilon - \mu)\right]^{1/(q-1)} + 1}. \]  

In Eq. (2), \( n_q \) is the average particle number of the micro states with energy \( \epsilon \). \( \mu \) is the chemical potential. \( q \) is the extensive parameter. When \( q \) is fixed to 1, Eq. (2) is transitioned into the classical Fermi Dirac distribution, which yields to

\[ a_i = \frac{\omega_i}{e^{\beta \epsilon_i} + 1}. \]  

Because of the limitation of Pauli exclusion principle, the Fermi system should have the limitation \( 0 \leq n_q \leq 1 \). Therefore, according to Eq. (2), one can obtain

\[ 1 + (q - 1)\beta(\epsilon - \mu) \geq 0. \]  

Eq. (4) is rewritten as the following expression for arbitrary \( q \)

\[ \begin{align*}
\epsilon &\leq \mu + \frac{1}{(1-q)\beta} \quad (q \leq \cdot) \\
\epsilon &\geq \mu - \frac{1}{(q-1)\beta} \quad (q \geq \cdot).
\end{align*} \]  

When it satisfies the condition \( \mu - \epsilon > 0 \), the equation will become \( [1 + (q-1)\beta(\epsilon - \mu)]^{1/(q-1)} > 1 \). When it satisfies the condition \( \epsilon - \mu < 0 \), the equation becomes \( [1 + (q-1)\beta(\epsilon - \mu)]^{1/(q-1)} < 1 \). One can introduce a generalized fugacity \( z_q \), which is denoted by

\[ z_q = [1 + (1-q)\beta\mu]^{1/q}. \]  

Thus, we obtain

\[ [1 + (1-q)\beta(\epsilon - \mu)]^{1/(q-1)} = z_q^{-1} [1 + (q-1)\beta z_q^{q-1}\epsilon]^{1/(q-1)}. \]  

By Eq. (2), Eq. (4) and the Taylor series \( \frac{1}{1+z} = \sum_{i=0}^{\infty} (-1)^iz^i \), which reads

\[ n_q = \begin{cases} 
\sum_{i=0}^{\infty} \frac{(-1)^i}{i+1} z_q^i [1 + (q-1)\beta z_q^{q-1}\epsilon]^{i/q-1} & (\epsilon > \mu) \\
\sum_{i=0}^{\infty} \frac{(-1)^i}{i+2} z_q^i [1 + (q-1)\beta z_q^{q-1}\epsilon]^{i/q-1} & (\epsilon = \mu) \\
\sum_{i=0}^{\infty} \frac{(-1)^i}{i+1} z_q^i [1 + (q-1)\beta z_q^{q-1}\epsilon]^{i/q-1} & (\epsilon < \mu)
\end{cases}. \]  

3. Generalized Fermi Systems in a 2D Harmonic Trap

For the generalized ideal Fermi system in the 2D isotropic harmonic trap, the single particle Hamiltonian is written as

\[ H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m \omega^2 \left( x^2 + y^2 \right). \]
For the case of $q \leq 1$ and $\mu < 0$, one can obtain the analytical expressions of particle number, internal energy and heat capacity as follows

$$N = \frac{4 g \pi^2 (k_B T)^2}{(\hbar \omega)^2} f_{q,2}(z_q),$$

$$E = 4 k_B T N \frac{f_{q,3}(z_q)}{f_{q,2}(z_q)},$$

$$C_{V,q} = 4 k_B N \left[ 3 \frac{f_{q,3}(z_q)}{f_{q,2}(z_q)} - 2 \frac{f_{q,2}(z_q)}{f_{q,1}(z_q)} \right].$$

The above-mentioned generalized Fermi integral $f_{q,D}(z_q)$ satisfies

$$f_{q,D}(z_q) = \sum_{i=0}^{\infty} \frac{(-1)^i z_q^{i+\alpha} q \Gamma(i)}{(1-q)^i \Gamma(i+D)}.$$

For the case of $\mu \geq 0$, one can obtain the analytical expressions of particle number, internal energy and heat capacity as follows

$$N = \frac{4 g \pi^2 (k_B T)^2}{(\hbar \omega)^2} f_{q,2}(z_q),$$

$$E = 2 k_B T N \frac{f_{q,3}(z_q)}{f_{q,2}(z_q)},$$

$$C_{V,q} = k_B N \left[ 3 \frac{f_{q,3}(z_q)}{f_{q,2}(z_q)} - 2 \frac{\partial f_{q,2}(z_q)}{\partial z_q} \right].$$

Generalized Fermi integral $f_{q,D}(z_q)$ satisfies

$$f_{q,D}(z_q) = \sum_{i=0}^{\infty} \frac{(-1)^i z_q^{i+\alpha} D}{(1-q)^D \Gamma(i+D)} H \left[ \frac{i}{1-q}, D+1, 1-z_q^{i+1} \right].$$

$$+ \sum_{i=1}^{\infty} \frac{(-1)^i z_q^{i+\alpha}(D+1)}{1-q^{i+1}} H \left[ 1-D, i, i+2, z_q^{i+1} \right].$$

Here, $H[a,b,b+1,C] = b \int_0^1 (1-Ct)^{-a} t^{b-1} dt$ is the hypergeometric function. The parameters $a, b, C$ are all independent on $t$. 

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4. Generalized Fermi Systems in a 3D Harmonic Trap

For the generalized ideal Fermi system in the 3D isotropic harmonic trap, the single particle Hamiltonian is written as

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2).$$ (18)

For the case of $q \leq 1$ and $\mu < 0$, one can obtain the analytical expressions of particle number, internal energy and heat capacity as follows

$$N = \frac{8g\pi^3 (k_B T)^3}{(\hbar \omega)^3} f_{q,3}(z_q),$$ (19)

$$E = 9Nk_BT \frac{f_{q,4}(z_q)}{f_{q,3}(z_q)},$$ (20)

$$C_{V,q} = 9Nk_B \left[ 4 \frac{f_{q,4}(z_q)}{f_{q,3}(z_q)} - 3 \frac{f_{q,3}(z_q)}{f_{q,2}(z_q)} \right].$$ (21)

Generalized Fermi integral $f_{q,D}(z_q)$ satisfies Eq. (13).

For the case of $\mu \geq 0$, one can obtain the analytical expressions of particle number, internal energy and heat capacity as follows

$$N = \frac{4g\pi^3 (k_B T)^3}{(\hbar \omega)^3} f_{q,3}(z_q),$$ (22)

$$E = 3Nk_BT \frac{f_{q,4}(z_q)}{f_{q,3}(z_q)},$$ (23)

$$C_{V,q} = Nk_B \left[ 4 \frac{f_{q,4}(z_q)}{f_{q,3}(z_q)} - 3 \frac{\partial f_{q,4}(z_q) / \partial z_q}{\partial f_{q,3}(z_q) / \partial z_q} \right].$$ (24)

Generalized Fermi integral $f_{q,D}(z_q)$ satisfies Eq. (17).

Absolutely, thermodynamics of generalized ideal Fermi system in harmonic trap are related to the generalized parameter $q$. Although they have the similar expression form, the generalized Fermi integrals are completely different, which lead to the major differences. The numerical results of heat capacity versus temperature are shown in figure 1 by setting particle number as a fixed parameter. Fig. 1(a), (b) and (c) depict the cases of free space, 2D and 3D harmonic traps, respectively. It can be seen that heat capacity is the approximate monotone increasing function of temperature, which increases with the rising of temperature. When the generalized parameter tends to one, that is $q \rightarrow 1$, the system is transitioned to the classical Fermi-Dirac distribution. The results calculated by generalized Tsallis statistics are consistent with the classical equipartition theorem [9-11]. Due to the limitation of Pauli principle, the value of the heat capacity converges to zero near the absolute temperature. The numerical difference of heat capacity becomes bigger as the temperature increases, which needs more energy to stimulate the same number of particles.
Figure 1. Heat capacity of generalized Fermi system versus temperature in (a) free space, (b) 2D and (c) 3D traps, respectively.
5. Conclusions
Starting from the generalized Fermi-Dirac distribution function, the thermodynamic properties of generalized ideal Fermi system in free space, 2D and 3D harmonic traps are discussed based on the non-extensive Tsallis theory. Through the analytical and numerical results of heat capacity, the relevant characteristics of the system are reported in detail.

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