# DERIVATION OF THERMODYNAMIC QUANTITIES OF IDEAL FERMI GAS IN HARMONIC TRAP

**Ho Hoang Huy[1], Tran Duong Anh Tai[1], Tomotake Yamakoshi[2], Pham Nguyen Thanh Vinh[1]***

[1] Department of Physics, Ho Chi Minh University of Pedagogy,
280 An Duong Vuong St., District 5, Ho Chi Minh City

[2] Institute for Laser Science, University of Electro-Communications,
1-5-1 Chofugaoka, Chofu-shi, Tokyo 182-8585, Japan

**Abstract:** In this paper, we provide a comprehensive study of the thermodynamic quantities of the ideal Fermi gas confined in a three-dimensional harmonic trap by using the properties of the Fermi-Dirac integral function both analytically and numerically. The analytical formulae describing the dependences of the chemical potential, total energy and heat capacity on the temperature are obtained via the appropriate approximations. Afterwards, the results are compared with the well-converged numerical calculations in order to evaluate the applicability of these formulae.

**Keywords:** thermodynamic, harmonic trap, ideal Fermi gas

## 1    Introduction

In 1924–1925, Bose and Einstein theoretically predicted that non-interacting particles should experience a phase transition in a low-temperature regime. Only particles with an integer spin called bosons undergo this phase transition due to the fact that the same states can be occupied by many bosons. On the contrary, fermions following the Fermi-Dirac statistics with a half-integer spin obey the Pauli exclusion principle such that two or more identical fermions are not able to be in the same energy state. Thus, they are forbidden from condensing into Bose-Einstein condensate (BEC), and they can form a "Fermi sea", instead. This statistical effect plays a key role in the studies of solid-state physics, neutral stars and so forth, thus a lot of theoretical and experimental studies have been carried out. At the beginning of the new millennium, many articles regarding the observation of the quantum degenerate atomic Fermi gas have been published and attracted much attention because of their great promise for numerous applications. In 1999, DeMarco and Jin successfully trapped $7 \times 10^5$ of $^{40}K$ to $0.5\,T_F$ which was the onset of observing Fermi degeneracy [4] (here, $T_F$ is the Fermi temperature). Three years later, the observation of strongly-interacting fermionic $^6Li$ [9] was made. In this decade, the thermodynamic properties of such interacting Fermionic gases were still a hot topic [6, 8, 10].

In statistical physics, thermodynamic properties of the ideal Fermi gas in a free external potential are well-known and considered as textbook problems. However, those properties of

the ideal Fermi gas settled in a three-dimensional harmonic trap are vague. Here, the equation calculating the total number of particles $N = \int_0^{+\infty} f(\varepsilon,\mu,T) g(\varepsilon) d\varepsilon$ plays a significant role, in which $f(\varepsilon,\mu,T)$ and $g(\varepsilon)$ are the distribution function and the density of states, respectively. To deal with this integral, the mathematical properties of the Fermi function are used, then many thermodynamic quantities are able to be obtained such as chemical potential, total energy, heat capacity, entropy, and so forth. In the field of ultracold atomic systems, generally, the gases are captured by an optical parabolic trap which is called a far-off-resonant optical trap, thus the thermodynamics of such systems is important basic issues. In 1997, Butts and Rokhsar published their work [2] on the properties of the spin-polarized Fermi gas in a harmonic trap. They provided the formulae calculating the chemical potential without mentioning their accuracy. They also included the formulae of heat capacity at low temperatures and classical limits. One year later, Mingzhe Li and colleagues generally calculated these thermodynamic variables in an external potential with $U = br^t$ [7]. However, there were no rigorous evaluation of the errors and discussion about the applicability of the formulae. Therefore, a comprehensive study of important thermodynamic quantities of the ideal Fermi gas is deserved. In this work, we provide not only an analytical derivation on these formulae associating with each thermodynamic quantity for two regimes of low and high temperatures but also their precise calculation in order to classify and estimate the applicability of those analytical formulae within each temperature regime.

This article is organized as follows: in section 2, we introduce a thorough procedure to obtain the approximated formulae to calculate the chemical potential, total energy and heat capacity of the Fermi gas in a harmonic trap, sequentially. The numerical results are provided and discussed; these results also give the evaluation of the accuracy as well as show the applicability of the formulae, then. Section 3 concludes the topic.

## 2    Thermodynamic functions

### 2.1    Chemical potential

We proceed to derive the most important thermodynamic quantities of the ideal Fermi gas confined in a three-dimensional harmonic trap. The chemical potential is the change in the internal energy when adding one extra particle to a system while keeping the volume and entropy unchanged [3]. The execution of the chemical potential as a function of temperature, to some extent, is helpful when calculating other thermodynamic quantities. The chemical potential is acquired by solving equation

$$N = \int_0^{+\infty} f(\varepsilon,\mu,T) g(\varepsilon) d\varepsilon \,, \qquad\qquad (1)$$

where $f(\varepsilon,\mu,T) = \dfrac{1}{\exp[\beta(\varepsilon-\mu)+1]}$ and $g(\varepsilon) = \dfrac{\varepsilon^2}{2(\hbar\omega)^3}$ are the Fermi-Dirac distribution and the density of the state functions, respectively, with $k_B$, $T$, $\varepsilon$ and $\mu$ being the Boltzmann constant, absolute temperature, energy and chemical potential, respectively, and $\beta = 1/(k_B T)$. We note that the rigorous derivation of the density of the state function $g(\varepsilon)$ for a harmonic oscillator is deferred to the appendix.

At the absolute temperature, all the available single-particle states below Fermi energy $\epsilon_F = \mu(T=0)$ are occupied, while above this critical energy they are unoccupied. Taking into account that the Fermi-Dirac distribution is a step function whose value is equal to unity for energy below $\epsilon_F$ and is zero elsewhere, the Fermi energy can be deduced from equation (1) as

$$\varepsilon_F = \hbar\omega\sqrt[3]{6N} \ . \tag{2}$$

At low temperatures ($T \ll T_F$), due to the fact that the fugacity $z = \exp(\beta\mu)$ is extremely large, the chemical potential of the nearly degenerated Fermi gas can only be obtained using the Sommerfeld expansion

$$\int\limits_{0}^{+\infty} g(\varepsilon)f(\varepsilon,\mu,T)d\epsilon \approx \int\limits_{0}^{\epsilon_F} g(\varepsilon)d\varepsilon + (\mu-\varepsilon_F)g(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2\, g'(\varepsilon)\big|_{\varepsilon=\varepsilon_F} + O[(k_B T)^4]. \tag{3}$$

Taking into account that the density of state $g(\varepsilon)$ is a quadratic function, the terms higher than the second one can be eliminated. The formula describing the chemical potential as a function of reduced temperature $\tau = T/T_F$ at low-temperature approximation (LTA) is obtained in terms of Fermi energy $k_B T_F$ can be straightforwardly deduced

$$\frac{\mu}{k_B T_F} = 1 - \frac{\pi^2}{3}\tau^2 \ . \tag{4}$$

We proceed to derive the chemical potential for high-temperature approximation (HTA) where $z = exp(\beta\mu)$ is sufficiently small so that a power series [1] can be introduced to the Fermi-Dirac integral in equation (1) as

$$f_\nu[z] = \frac{1}{\Gamma[\nu]}\int\limits_{0}^{\infty} \frac{\varepsilon^{\nu-1}}{z^{-1}e^\varepsilon + 1}dx = -\sum_{k=1}^{\infty}\frac{(-z)^k}{k^\nu}, \tag{5}$$

where $\Gamma[\nu]$ is the Gamma function. Substituting equation (5) into equation (1) with $\nu=3$ one obtains

$$\frac{1}{3}\tau^{-3} = f_3[z]\Gamma[3] \ . \tag{6}$$

Due to the complexity of solving the cubic or high-order equation, the Fermi-Dirac integral function $f_3[z]$ is expanded up to the second order then substituted to equation (6) to obtain

$$\frac{1}{6}\tau^{-3} \approx z - \frac{z^2}{8} + O(z^3).$$

(7)

Then, HTA of the chemical potential of the ideal Fermi gas in terms of Fermi energy $k_B T_F$ is obviously derived

$$\frac{\mu}{k_B T_F} = \tau \ln\left(\frac{\tau^{-3}}{6} + \frac{\tau^{-6}}{288}\right).$$

(8)

Besides, we also provide the precise data by numerically solving equation (1) with the frequency of the trap ($\omega = 200\pi$ $rad/s$) and the total number of particles ($N = 10^5$), then compare the results with those obtained using the analytical formulae in order to estimate the applicability of the approximately analytical work. For the sake of intuitive evaluation, the matching between the numerical and analytical results was performed. Throughout this paper, we present the relative error as

$$\sigma = \left|\frac{a_{num} - a_{approx}}{a_{num}}\right|,$$

(9)

where $a_{num}$, $a_{approx}$ are the well-converged numerical and approximated analytical values, respectively. We note that the accuracy of the numerical solution is not verified below 0.02T$_F$ due to the computational limitation, thus causing the divergence of the relative errors.
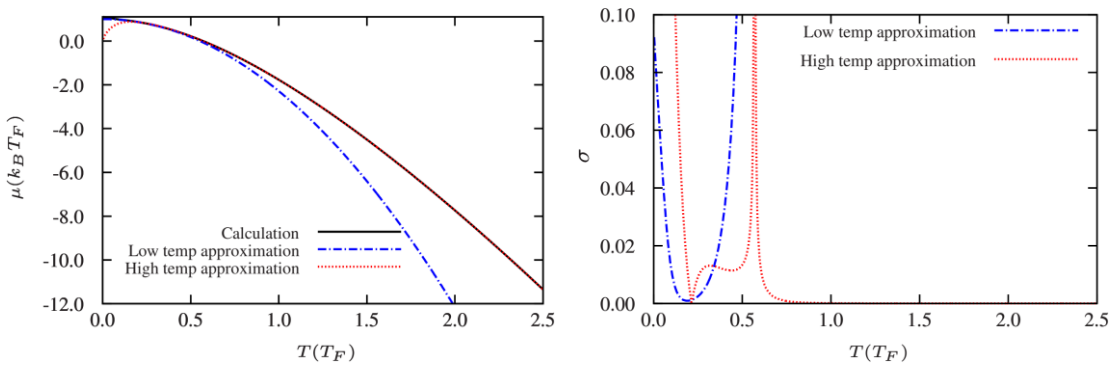


**Fig. 1.** Chemical potential of the Fermi gas in the harmonic trap as a function of reduced temperature $\tau$ (left panel) and the relative error between results obtained from precise and approximation approaches (right panel). The solid black, dashed red and dotted blue curves represent results received from the numerical calculation, LTA (equation 4), and HTA (equation 8), respectively.

We now present the chemical potential of the Fermi gas in the harmonic trap obtained by numerical calculation (solid black curve), LTA (dashed red curve), and HTA (dotted blue curve) in the left panel of Figure 1 for a wide range of temperatures to estimate the applicability of each approximation limit. The relative error between numerical and analytical results are also shown in the right panel of Figure 1 to intuitively classify the applicable range of each approximation limit. The results indicate that below $T \approx 0.4T_F$, the LTA is well consistent with

the numerical calculation with the relative error of less than 0.06. For the wide range of temperature from 0.4 to $2.5\,T_F$, the HTA is identical to the numerical result with the relative error being always of less than 0.06 and even approximately equal to 0 for $\tau > 0.8$. There is also an overlap between two approximation formulae in $0.2 < \tau < 0.3$ which implies the boundary between nearly degenerated and normal regions. We note that the shape of the curve corresponding to the numerical calculation (solid red) is universal regardless of the total number of particles used in our numerical calculations since the considered chemical potential is dimensionless and independent of the total number of particles of the system.

## 2.2    Total energy

In this subsection, a pair of formulae is provided to demonstrate the total energy of the system for both LTA and HTA by using the same treatment as in subsection 2.1. The average energy of a single particle is defined as

$$\bar{\varepsilon} = \frac{\displaystyle\int_0^{+\infty} \epsilon g(\epsilon) f(\epsilon, \mu, T)}{\displaystyle\int_0^{+\infty} g(\epsilon) f(\epsilon, \mu, T)} = \frac{\displaystyle\int_0^{+\infty} \epsilon g(\epsilon) f(\epsilon, \mu, T)}{N} \; . \tag{10}$$

Then the total energy of this system can be sought as

$$E = N\bar{\varepsilon} = \frac{1}{2(\hbar\omega)^3} \int_0^{+\infty} \frac{\varepsilon^3}{\exp[\beta(\varepsilon - \mu)] + 1} d\epsilon \; . \tag{11}$$

Again at low temperatures ($T \ll T_F$), due to the extremely large fugacity $z = \exp(\beta\mu)$, the total energy in terms of $Nk_BT_F$ can be derived using the Sommerfeld expansion and has the form of the quadratic polynomial

$$\frac{E}{Nk_BT_F} = \frac{3}{4} + \frac{\pi^2}{2}\tau^2 \; . \tag{12}$$

Then for the high-temperature limit, the Fermi-Dirac integral function and power series are still the key tools to derive the formula. Equation (10) can be rewritten in the form

$$\frac{E}{Nk_BT_F} = 3\tau^4\Gamma[4]f_4[z] \; . \tag{13}$$

By substituting the definition of $f_4[z]$ given by equation (4) into equation (13), the approximated total energy for HTA is then derived

$$\frac{E}{Nk_BT_F} = 3\tau + \frac{\tau^{-2}}{32} \; . \tag{14}$$

Note that in equation (14), the first term is identical to the classical limit derived in [8]. The second term in our treatment is the quantum correction for the total energy of the Fermi gas. For sufficiently high temperatures, our treatment and classical limit merge.

The precise result is also sought by directly solving equation (11) numerically using the chemical potential obtained in the previous step as shown in subsection 2.1 and is shown in Figure 2 together with those analytically obtained from LTA (equation 12) and HTA (equation 14). For $\tau < 0.4$, the LTA formula has the relative error of less than 0.08 with respect to the numerical result. While for $\tau \sim 0.4$, the HTA result has the relative error of less than 0.08, which decreases continuously as the temperature increases. At the absolute zero temperature, the total energy of the completely degenerating system is non-zero ($0.75\,Nk_BT_F$) due to the well-known Pauli exclusive principle, i.e., two fermions are not able to occupy an identical state. There is also a divergence as seen in Figure 1 for $0.2 < \tau < 0.3$, which supports the idea that this region is the boundary between nearly degenerate and ordinary states. As the temperature rises, the non-degenerating Fermi gas approaches the classical limit and behaves like the classical gas as expected.
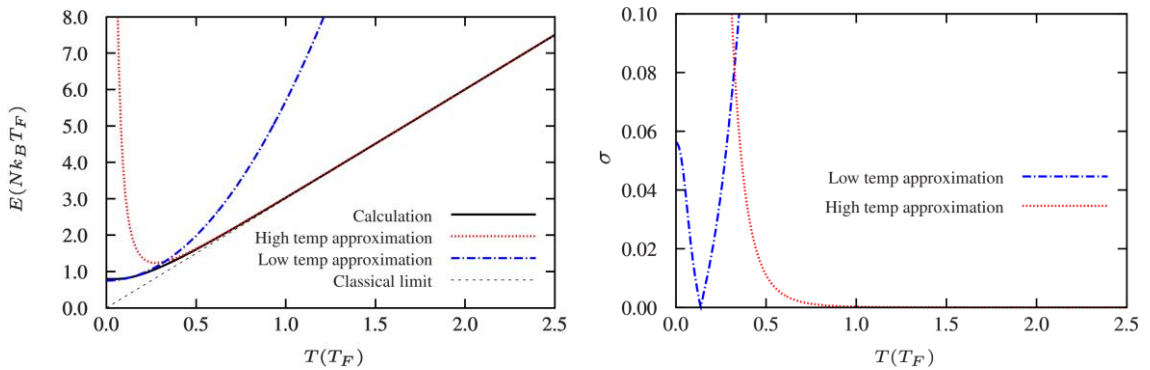


**Fig. 2.** Total energy of Fermi gas in the harmonic trap as a function of temperature T(T$_F$) (left panel) and the relative error between results obtained from precise and approximation approaches (right panel). Here the classical limit (dotted black curve) is also presented in the left panel.

### 2.3    Heat capacity

One more important thermodynamic quantity is the heat capacity defined as the sufficient energy required to increase the temperature of a system by one degree and is directly related to the total energy as

$$C = \frac{\partial E}{\partial T}. \tag{15}$$

For LTA, the heat capacity can be derived by directly taking differential of the total energy in equation (12) and takes the form

$$\frac{C}{Nk_B} = \pi^2 \tau \tag{16}$$

In case of HTA, since the power series has to be truncated in acquiring the total energy, the inaccuracy uncontrollably grows on the occasion that the total energy in equation (14) is directly differentiated. Thus, we have to consider the comprehensive form of total energy before treating to obtain the heat capacity. By combining equations (6) and (13), we have the total energy $E$ defined in equation (11) in the form

$$E = Nk_BT_F\, 3\tau\, \frac{f_4[z]}{f_3[z]}\,, \tag{17}$$

Substituting equation (17) into equation (15) and taking into account the recursion relation $\frac{\partial f_\nu[z]}{\partial z} = \frac{1}{z} f_{\nu-1}[z]$, we acquire the relationship between heat capacity and Fermi-Dirac integral function

$$\frac{C}{Nk_B} = 3\left[\frac{f_4[z]}{f_3[z]} - 3\left(\frac{f_3[z]}{f_2[z]} - \frac{f_4[z]}{f_3[z]}\right)\right]. \tag{18}$$

Again, the power series equation (5) is used and truncated at the second order to derive the formula describing the heat capacity for HTA

$$\frac{C}{Nk_B} = 12 + \frac{\tau^{-3}}{8} - \frac{3}{\dfrac{1}{3} - \dfrac{\tau^{-3}}{144}}. \tag{19}$$

Formula (19) is well consistent with the classical limit for the first term [8], and the last two terms are the correction which widens the applicable region of HTA in our work. The results obtained from LTA and HTA are compared with those from the numerical calculation of equation (15) using the numerical total energy from the previous step as discussed in subsection 2.2. The comparison is shown in Figure 3. Overall, the heat capacity of the Fermi gas in the harmonic trap is a linear function of reduced temperature in the nearly degenerate region, then it exponentially grows and approaches the classical limit [8] as the temperature increases. Obviously, in case of heat capacity, the relative error between the approximation and numerical calculation is well noticeable. LTA (equation 16) can be applied only for a narrow region of $0.1 < \tau < 0.3$ with the error value of around 0.2. However, as the temperature approaches zero, LTA totally diverges from the numerical calculation. While for sufficiently high temperatures, HTA can be applied for $\tau > 0.5$ with the relative error of less than 0.2. The interesting feature observed from Figure 3 is that the heat capacity obtained from both LTA and HTA in the region $0.3 < \tau < 0.5$ is completely departed from that of the numerical calculation. There are two possible reasons for such divergence. The first one is the accumulation of inaccuracy while deriving heat capacity approximately. The second reason is due to the truncation up to second order of the power series in equation (5) throughout our treatment. However, the expansion to a higher order for the extension, the applicability of HTA is so tedious and deferred to our next project.
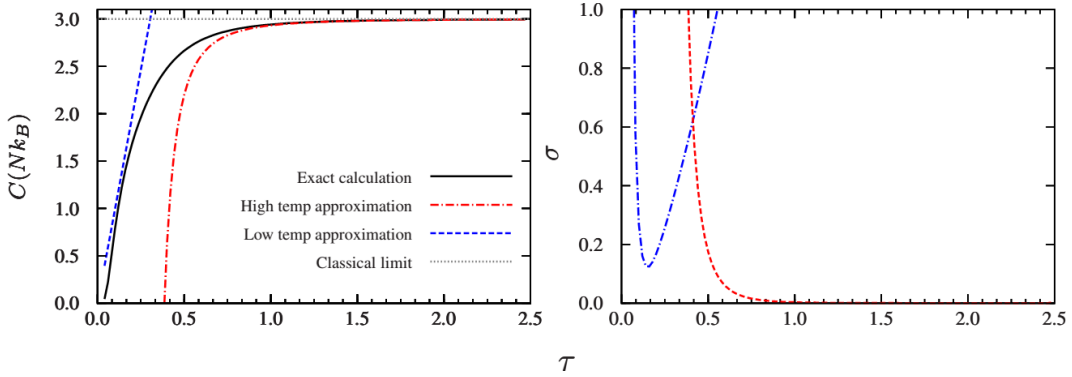
**Fig. 3.** Heat capacity of Fermi gas in the harmonic trap as a function of temperature *T(Tꜰ)* (left panel) and the relative error between results obtained from well-converged and approximation approaches (right panel). Here the classical limit (dotted black curve) is also presented in the left panel.

## 3    Conclusion

In this work, we successfully derived the formulae describing chemical potential and total energy of ideal Fermi gas trapped inside the three-dimensional harmonic trap for whole temperatures by using the Sommerfeld expansion and Fermi – Dirac integral function. In the low temperature and classical regime, these formulae completely agree with those proposed in [2]. Nevertheless, the applicability of these thermodynamic functions for each corresponding region is verified by comparing with the numerical results provided by rigorous and precise method. However, for heat capacity, there is still a wide temperature range that cannot be described either LTA or HTA. Thus, the expansion of the applicability of the approximation approach for heat capacity has to be included in our next work.

**Appendix: Calculating the density of state function of harmonic oscillator**

In the classical limit, the energy of a fermion in a three-dimensional harmonic trap is given as [5]

$$\varepsilon = \hbar\omega(n_x + n_y + n_z),\tag{A1}$$

where $n_x, n_y, n_z > 0$ are the quantum numbers corresponding to three dimensions *x*, *y*, and *z*, respectively, and the zero-point energy has been neglected. Equation (A1) is also the equation of a surface of a specific energy in a three-dimensional space consisting of three mutually orthogonal coordinates $n_x, n_y, n_z$ as shown in Figure 4.
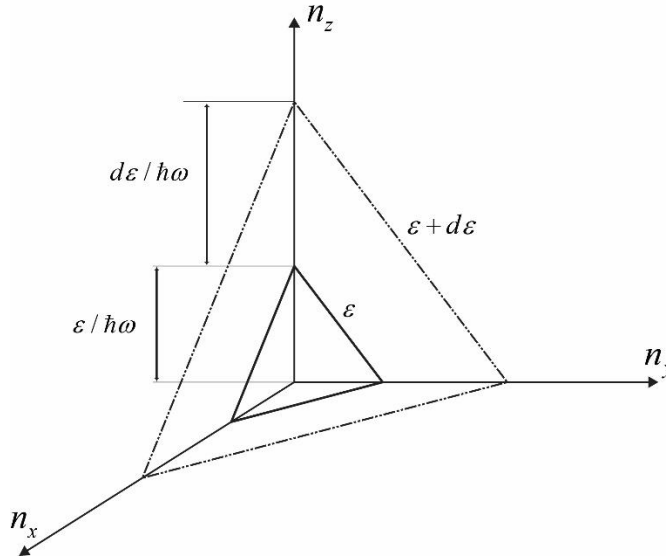
**Fig. 4.** Surface presentation of the energy of a three-dimensional harmonic oscillator

When the total number of states is sufficiently large, the total number of states corresponds to the volume of the tetrahedron is

$$N = \frac{n^3}{6} , \tag{A2}$$

in which $n = \frac{\varepsilon}{\hbar\omega}$ . Thus, it leads to

$$dN = \frac{n^2}{2} dn = \frac{\varepsilon^2}{2(\hbar\omega)^3} d\varepsilon . \tag{A3}$$

The density of states describing the total number of quantum states within an interval of energy is now straightforwardly derived

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{\varepsilon^2}{2(\hbar\omega)^3} . \tag{A4}$$

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