The finite-temperature thermodynamics of a trapped unitary Fermi gas within fractional exclusion statistics

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Abstract

We utilize the fractional exclusion statistics of the Haldane and Wu hypothesis to study the thermodynamics of a unitary Fermi gas trapped in a harmonic oscillator potential at ultra-low finite temperature. The entropy per particle as a function of the energy per particle and energy per particle versus rescaled temperature are numerically compared with the experimental data. The study shows that, except the chemical potential behaviour, there exists a reasonable consistency between the experimental measurement and theoretical attempt for the entropy and energy per particle. In the fractional exclusion statistics formalism, the behaviour of the isochore heat capacity for a trapped unitary Fermi gas is also analysed.

1. Introduction

The thermodynamics of a strongly interacting fermion system has attracted much attention, either experimentally or theoretically, in the many-body community in recent years [1]. For the dilute contact interacting atomic system, the scattering length $a$ describes the mutual interaction strength between two fermions. With the Feshbach resonance technology, it is possible to tune the $s$-wave scattering length $a$ by changing the external magnetic field. The scattering length $a$ can be changed from a negative value to the other side of the resonance where $a$ becomes positive. In the weak attraction Bardeen–Cooper–Schrieffer (BCS) regime with $k_F|a| \ll 1$ (with the Fermi wave vector $k_F$), the mean-field theory can give a reasonable description. With the increase of the interaction strength, the composite bosons can be formed in the fermion system, where the Bose–Einstein condensation (BEC) can occur [1, 2].

In the regime from negative scattering length to positive value, the two-body interaction strength can be singular with the existence of a zero-energy bound state. The limit $k_F|a| \to \infty$ is called the BCS–BEC crossover, which is also called the unitary regime [1]. The corresponding gas in this limit is called the unitary Fermi gas [2]. At unitarity, the gas has some properties of fermions and some of bosons, that is to say, the behaviour of this gas is between that of fermions and bosons. The fermion system will show a universal thermodynamic behaviour near the resonance point where the scattering length $a$ diverges [1, 2].

Initially, physicists concentrated on the energy density per particle of the unitary Fermi gas at zero temperature theoretically. For a homogeneous gas, the ground-state energy per particle is given by $E/N = \frac{2}{\xi} E_F$ with the ideal Fermi energy $E_F$ and the universal coefficient $\xi$ [2]. It is $E/N = \frac{1}{2} \sqrt{\xi} E_F$ for a trapped unitary gas, where $E_F$ is the Fermi energy of the trapped non-interacting Fermi gas [3]. Determining the dimensionless constant $\xi$ has been an important physical subject in the past few years.

Furthermore, exploring the thermodynamics of a unitary Fermi gas at finite temperature in theory to explain the experimental results is a more challenging task. A diagrammatic determinant Monte Carlo method for the negative-$U$ Hubbard model was used to calculate the finite-temperature thermodynamics of a homogeneous unitary gas [4]. Through the quantum Monte Carlo simulation, the finite-temperature thermodynamics of a homogeneous unitary gas can be given by [5, 6]. A self-consistent theory based on the combined Luttinger–Ward–De Dominicis–Martin variational formalism was also used to calculate it for a homogeneous unitary gas [7].

For the finite-temperature thermodynamics of a trapped unitary Fermi gas, the entropy and energy of the trapped unitary Fermi system have been experimentally measured...
in [8–10]. The quantum Monte Carlo simulation can also be used to calculate the finite-temperature thermodynamics of a trapped unitary gas [11]. Various theoretical attempts have been established to give the calculations for a trapped unitary Fermi gas. The pseudogap theory is one of them [12, 13]. A mean-field method by solving the Bogoliubov–de Gennes equations with an efficient and accurate method was used in [14]. A T-matrix calculation with a modified Nozières and Schmitt-Rink approximation was adopted to explore it [15]. The combined Luttinger–Ward–De Dominicis–Martin variational formalism was also proved to be a valuable approach [16]. We note that there are still differences among these attempts on the finite-temperature thermodynamic properties of a unitary Fermi gas.

Due to the scale invariance at unitarity, the thermodynamic properties of the universal strongly interacting unitary fermions are related to those of the non-interacting ideal fermions. This means that the dynamical details will not appear in the final thermodynamic analytical expressions. From the microscopic point of view, the unitary fermion system is in between the fermionic and composite bosonic phases. To characterize this crossover or intermediate unitary fermionic thermodynamics, Haldane–Wu fractional exclusion statistics was used to discuss the finite-temperature unitary Fermi gas thermodynamics [17, 18]. In physics, the thermodynamic behaviour of the fractional exclusion statistics is between those of Bose–Einstein and Fermi–Dirac statistics [19, 20], which is quite similar to the thermodynamics of real fermions at unitarity. As a hypothesis, the strongly interacting unitary gas is modelled by the non-interacting anyons. The priority is that the finite-temperature thermodynamic properties can be investigated analytically [21]. The quintessence hidden in this attempt is that the anyonic statistical parameter \( g \) characterizes the strongly interacting universal properties.

Following the fractional exclusion statistics formalism, the aim of this work is to give a detailed discussion on the thermodynamic behaviour of the fractional exclusion statistics was used to discuss the finite-temperature unitary Fermi gas thermodynamics [17, 18]. In physics, the thermodynamic behaviour of the fractional exclusion statistics is between those of Bose–Einstein and Fermi–Dirac statistics [19, 20], which is quite similar to the thermodynamics of real fermions at unitarity. As a hypothesis, the strongly interacting unitary gas is modelled by the non-interacting anyons. The priority is that the finite-temperature thermodynamic properties can be investigated analytically [21]. The quintessence hidden in this attempt is that the anyonic statistical parameter \( g \) characterizes the strongly interacting universal properties.

Following the fractional exclusion statistics formalism, the aim of this work is to give a detailed discussion on the trapped gas thermodynamics. By generalizing the discussion for the homogeneous unitary system [22], we want to give the expressions and the corresponding numerical results of entropy, physical chemical potential and isochore heat capacity of a trapped unitary system. The concrete comparisons with experimental measurements are made.

The natural units \( k_B = \hbar = 1 \) are used throughout the paper.

2. Finite-temperature thermodynamics within fractional exclusion statistics

2.1. Framework of fractional exclusion statistics

In this subsection, we will briefly review the formalism of the fractional exclusion statistics. By generalizing the simple formula with the fractional exclusion statistics, one can get the microscopic quantum states \( W \) of \( N \) identical particles occupying a group of \( G \) states [20, 22]

\[
W = \prod_i \frac{[G_i + (N_i - 1)(1 - g)]!}{N_i![G_i - gN_i - (1 - g)]!},
\]

where \( g \) is a statistical parameter, which denotes the number of states that one particle can occupy. For bosons, \( g = 0 \) and \( g = 1 \) for fermions. If \( G_i \) and \( N_i \) are very large, one has the approximate expression of the logarithm of \( W \)

\[
\log W \approx \sum_i \left[ G_i + (1 - g)N_i \right] \log \left( G_i + (1 - g)N_i \right)
- \left( G_i - gN_i \right) \log \left( G_i - gN_i \right) - N_i \log N_i,
\]

through the Stirling formula \( \log N! = N(\log N - 1) \).

The variational formulation of \( \log W \) is

\[
\delta \log W = \sum_i \left[ (1 - g) \log (G_i + (1 - g)N_i)
+ g \log (G_i - gN_i) - \log N_i \right] \delta N_i.
\]

However, \( \delta N_i \) is not arbitrary, it must satisfy the conditions below:

\[
\delta N = \sum_i \delta N_i = 0,
\]

\[
\delta E = \sum_i \epsilon_i \delta N_i = 0.
\]

Setting the two Lagrange multipliers \( \alpha = -\mu / T \) and \( \beta = 1 / T \), one can have

\[
\delta \log W - \alpha \delta N - \beta \delta E
= \sum_i \left[ (1 - g) \log (G_i + (1 - g)N_i)
+ g \log (G_i - gN_i) - \log N_i + (\mu - \epsilon_i) / T \right] \delta N_i
= \sum_i \left[ (1 - g) \log \left( 1 + \frac{G_i}{N_i} - g \right)
+ g \log \left( \frac{G_i}{N_i} - g \right) + \left( \frac{\mu - \epsilon_i}{T} \right) \right] \delta N_i,
\]

where \( \mu \) is the chemical potential, \( T \) is the system temperature and \( \epsilon_i \) is the single-particle energy for the state of species \( i \).

Defining the average occupation number \( \bar{N}_i \equiv N_i / G_i \), through the Lagrange multiplier method \( \delta \log W - \alpha \delta N - \beta \delta E = 0 \), the most probable distribution of \( \bar{N}_i \) can be derived from equation (5)

\[
\bar{N}_i = \frac{1}{\omega_i + g},
\]

where \( \omega_i \) obeys the relation

\[
\mu - \epsilon_i = -T \left[ (1 - g) \log (1 + \omega_i) + g \log \omega_i \right].
\]

In equation (7), we define \( \omega_0 \) as the value of \( \omega_i \) at \( \epsilon_i = 0 \). Consequently, one has

\[
\mu = -T \left[ (1 - g) \log (1 + \omega_0) + g \log \omega_0 \right].
\]

At zero temperature, there is

\[
\bar{N}_i = 0, \quad \text{for } \epsilon_i > \mu,
\]

\[
\bar{N}_i = \frac{1}{g}, \quad \text{for } \epsilon_i < \mu.
\]

Furthermore, by inserting equation (6) into equation (2), one obtains the expression for entropy as

\[
S = \log W = \sum_i \frac{G_i}{\omega_i + g} \left[ (\omega_i + 1) \log (\omega_i + 1) - \omega_i \log \omega_i \right].
\]
2.2. Thermodynamics of a trapped unitary Fermi gas

The finite-temperature thermodynamics can be derived for the unitary Fermi gas trapped in a harmonic oscillator $mσ^2r^2/2$, where the oscillator parameter $σ$ is defined as $σ = (ω_x, ω_y, ω_z)^{1/3}$ and $r$ denotes the position of particles. The corresponding density of states is $D(ϵ) = ω^2/σ^3$. At zero temperature, the particle number and system energy are

$$N = \frac{1}{g} \int_0^{E_F} E^{3/2} d(ϵ) = \frac{E_F^3}{3σ^3},$$

$$E = \frac{1}{g} \int_0^{E_F} ϵ D(ϵ) d(ϵ) = \frac{g^{1/3} E_F^4}{4σ^2},$$

where $E_F$ obeys the relation $E_F = g^{1/3} E_F$ with the ideal Fermi energy $E_F = (3N)^{1/3} σ$ in a harmonic oscillator.

Comparing equation (11) with equation (12) to eliminate $σ$, it is shown that

$$\frac{E}{N E_F} = \frac{3}{4} \frac{g^{1/3}}{σ}.$$  

(13)

If the statistical parameter $g$ in the fractional exclusion statistics is fixed through the zero-temperature ground-state energy, the finite-temperature thermodynamic quantities for a trapped unitary Fermi gas can be calculated. For the trapped system, the ground-state energy is related to the universal coefficient according to $E/(\frac{3}{4} N E_F) = \sqrt{g}$ [3]. From equation (13), it is found that $E/(\frac{3}{4} N E_F) = g^{1/3}$. So the statistical parameter could be calculated as $g = \xi^{3/2} = \frac{9}{27}$, with $ξ = \frac{9}{2}$ given by the developed quasi-linear approximation method [23–28].

For the finite-temperature trapped unitary Fermi system, the particle number and energy can be represented by turning the sum of quantum state into integral and changing the variable from $dϵ$ to $dω$

$$N = \sum_i G_i N_i = \int_0^{∞} \frac{D(ϵ) d(ϵ)}{ω + g} = \left( \frac{T}{\sigma} \right)^3 h_2(ω_0),$$

$$E = \sum_i G_i N_i ϵ_i = \int_0^{∞} \frac{ϵ D(ϵ) d(ϵ)}{ω + g} = \left( \frac{T}{\sigma} \right)^3 T h_3(ω_0),$$

(14)

(15)

where

$$h_2(ω_0) = \int_0^{∞} \frac{dω}{ω(1 + ω)} \left[ \ln \left( \frac{ω}{ω_0} \right)^{g} \left( \frac{1 + ω}{1 + ω_0} \right)^{1−g} \right]^n$$

may be referred to as the generalized Fermi integral function of the fractional exclusion statistics.

By replacing equation (11) into equations (14) and (15), one gets

$$3 \left( \frac{T}{T_F} \right)^3 h_2(ω_0) = 1,$$

$$E/N E_F = 3 \left( \frac{T}{T_F} \right)^4 h_3(ω_0),$$

(16)

(17)

with the Fermi characteristic temperature $T_F$.

One can turn the sum of equation (10) to an integral. With equation (16), one can get the explicit integral expression of entropy per particle

$$S/N = 3 \left( \frac{T}{T_F} \right)^3 \int_0^{∞} \left[ \ln \left( \frac{ω + 1}{ω} \right) - \ln \omega + 1 \right] \times \left( \ln \left( \frac{ω}{ω_0} \right)^{g} \left( \frac{1 + ω}{1 + ω_0} \right)^{1−g} \right)^2 d(ω).$$

(18)

In order to derive the expression of the isochore heat capacity, let us further discuss the particle number. From equation (14), the partial derivative of the particle number $N$ to temperature $T$ for fixed $N$ and $σ$ is given by

$$\left( \frac{∂N}{∂T} \right)_{N,σ} = \frac{3T^2}{σ^3} h_2(ω_0) + \left( \frac{T}{σ} \right)^3 \left[ \left( \frac{∂h_2}{∂T} \right)_μ \right]$$

$$+ \left( \frac{∂h_2}{∂μ} \right)_T \left( \frac{∂μ}{∂T} \right)_{N,σ}.$$  

(19)

From equation (19), one can get

$$\left( \frac{∂μ}{∂T} \right)_{N,σ} = \frac{μ}{T} \left[ \frac{3h_3(ω_0)}{2h_1(ω_0)} \right].$$

(20)

Furthermore, with equation (15) and the thermodynamic relation between the isochore heat capacity $C_V$ and internal energy $E$, one has

$$C_V = \left( \frac{∂E}{∂T} \right)_{N,σ}$$

$$= 4 \left( \frac{T}{σ} \right)^3 h_3(ω_0) + \left( \frac{T}{σ} \right)^3 \left[ \left( \frac{∂h_3}{∂T} \right)_μ \right]$$

$$+ \left( \frac{∂h_3}{∂μ} \right)_T \left( \frac{∂μ}{∂T} \right)_{N,σ}.$$  

(21)

Substituting equations (14) and (20) into equation (21), one obtains the isochore heat capacity per particle

$$\frac{C_V}{N} = \frac{4h_3(ω_0)}{h_2(ω_0)} - \frac{9h_2(ω_0)}{2h_1(ω_0)}.$$  

(22)

3. Discussions

Based on the above analytical expressions, we will give the numerical results.

The energy per particle versus the rescaled temperature can be calculated from equations (16) and (17). As indicated by figure 1, the energy for the trapped unitary Fermi gas with the statistical parameter $g = \frac{9}{27}$ versus the rescaled temperature is consistent with the experimental data [8]. Through equations (17) and (18), the relation between the entropy per particle and the energy per particle is given explicitly in figure 2. The entropy increases with increasing energy, and in the Boltzmann regime, the curve for a trapped unitary Fermi gas gets closer to and almost overlaps with that
Figure 1. The energy per particle versus the rescaled temperature. The solid curve denotes that for the trapped unitary Fermi gas, and the dashed one is that for the trapped ideal Fermi gas. The dots with error bars are the experimental data of [8].

Figure 2. The entropy per particle plotted as a function of the rescaled energy per particle. The line styles are similar to figure 1. The dots with error bars are the experimental data of [9, 10].

of the trapped ideal Fermi gas. It is found that the theoretical result is reasonably consistent with that of the experiment.

The agreements in figures 1 and 2 between the theoretical curves and the experimental data show that the statistical parameter $g$ can be capable of describing the strong interaction of unitary Fermi gas at extremely low temperature.

With equations (8), (16) and (17), we have also shown the plot of the chemical potential varying with the rescaled energy per particle in figure 3. It is a monotonically decreasing function of the energy per particle. In the Boltzmann regime, the curve for a trapped unitary Fermi gas gets closer to that of the trapped ideal one. In the extremely low-temperature regime ($E/(NE_F) < 1.2$), the departure between the theoretical result and the experimental data is not obvious. However, the chemical potential differs explicitly from the experimental result for $E/(NE_F) > 1.2$. As the temperature increases, the experimental data also diverge from the curve of the trapped ideal gas. We also plot the chemical potential versus the rescaled temperature in figure 4.

From equations (16) and (18), the entropy per particle as a function of the rescaled temperature is indicated in figure 5. In figure 6, the isochore heat capacity per particle related to the rescaled temperature is presented. The numerical results are obtained by solving the coupled equations (16) and (22).

Near the Boltzmann regime, the energy, chemical potential, entropy and isochore heat capacity of a trapped unitary Fermi gas get closer to and almost overlap with those of the trapped ideal Fermi gas. In the low-temperature strong degenerate regime, the thermodynamic quantities of the unitary gas are lower than those of the ideal gas at the same
The energy, chemical potential and entropy of a unitary gas are always lower than the ideal ones at the same temperature. However, as shown in figure 6, the isochore heat capacity per particle given by the fractional exclusion statistics is not a naive monotonously increasing function with the increase of the scaled temperature. This behaviour is different from that of the trapped ideal Fermi gas.

4. Conclusion

The finite-temperature thermodynamic quantities of a trapped unitary Fermi gas have been discussed in terms of the approved fractional exclusion statistics framework. The study shows that the thermodynamic quantities of a trapped unitary Fermi gas will overlap with those of the trapped ideal Fermi gas in the Boltzmann regime. The thermodynamic quantities given by this formalism are lower than the trapped ideal ones at the same temperature except for the isochore heat capacity. The energy and entropy per particle manifest the consistency with the low-temperature experimental measurement. However, the detailed numerical study of the chemical potential shows that there is an explicit difference between the result given in terms of fractional exclusion statistics and experimental data in the weakly degenerate regime. For the three-dimensional trapped unitary Fermi gas, the high-temperature weakly degenerate behaviour of chemical potential given by a simple fractional exclusion statistics hypothesis needs clarifying further.

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