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**FERMI-DIRAC GAS OF ATOMS IN A BOX
WITH LOW ADIABATIC INVARIANT**

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Abstract

Quantum degenerate Fermi-Dirac gas of atoms, confined in a cubic box, shows an energy spectrum, which is discrete and strongly dependent on the atomic mass number, A_{at} , box geometry and temperature, for low product of A_{at} and the adiabatic invariant, $TV^{1/3}$, i.e. on $\gamma = A_{at}TV^{1/3}$. The present study compares the total number of particles and the total energy obtained by summing up the contributions of a finite number of states, defined by the values of γ , to the widespread approximations of the corresponding integrals. The sums show simple calculation algorithms and more precise results for a large interval of values of γ . A new accurate analytic formula for the chemical potential of the Fermi-Dirac quantum gas is also given.

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1. Introduction

The quantum atom gases are described usually by continuous thermodynamic functions, which are dependent on kinetic energy, temperature and chemical potential, but are independent on the container size and shape (considering the quantum gas with a very large number of identical particles, which is stored in a large container) [1-5].

In recent experiments, the quantum atom gases are confined in a trap using an external potential. This physical system may be reasonably replaced by an ideal quantum gas, which is placed inside of a virtual three-dimensional box. The effects of the container size on the atom gas thermodynamics are relatively small, but they increase when the box size decreases. More recently, a number of papers calculated the effect of trap dimension and size on quantum atom gases [6-19] taking account of the system discreteness in this phenomenon.

In this paper, we show that the number of particles and total energy of the discrete (finite) Fermi-Dirac systems with low adiabatic invariant can be calculated in a simple and precise way by summing up the contributions of a finite number of states, defined by the values of γ . The usual approximations of the corresponding integrals are restricted by conditions, which make them difficult to be used in the present experiments with ultra-cold Fermi-Dirac gases. A new accurate analytic formula for the chemical potential of the Fermi-Dirac quantum gas is also given.

When working with systems of identical particles, one can use the grand canonical ensemble in order to dispense of the particle number conservation. The grand canonical ensemble allows the number of particles and the energy in the system to fluctuate, but keeps the chemical potential fixed. For an ideal gas of identical particles, each of mass m , the grand partition function can be written in the form [see for example, 9]:

$$Z(T, V, \mu) = \text{Tr}[\exp(-(\mathbf{H} - \mu\mathbf{N})/k_B T)], \quad (1)$$

where \mathbf{H} and \mathbf{N} are the kinetic energy and total particle number operators, T is the absolute temperature of the quantum gas, V is the container volume, μ is the chemical potential, and k_B is the Boltzmann constant.

Assuming that the ideal quantum gas is confined in a cubic box, with size L and with periodic boundary conditions, the momentum operator for a particle has the following eigenvalues:

$$\mathbf{p}_q = \hbar\mathbf{k} = (h/L)(\mathbf{1}_x q_1 + \mathbf{1}_y q_2 + \mathbf{1}_z q_3), \quad (2)$$

where \mathbf{k} is the wave-vector of the particle and q_i are integer numbers or zero (each triplet defining a system state).

The kinetic energy operator for a single particle is $\mathbf{p}^2/2m$ and has eigenvalues:

$$\varepsilon_q = \frac{p_q^2}{2m} = \varepsilon_0 \cdot q; \quad \varepsilon_0 = \frac{h^2}{2m} \frac{1}{L^2}, \quad (3)$$

where q is an integer state (level) number and ε_0 – the inter-level energy. The energy levels, ε_q , of the particle in a box, can be obtained resorting to Brillouin's model of

momentum quantisation and to the assumption of the same energy-momentum relationship as in the classical mechanics [2]. This procedure allows the exchange of energy and particles between the box and the thermostat and accordingly, makes the use of quantum statistics possible via the grand ensemble partition.

The energies of the box states, $\varepsilon(q)$, are distributed in a discrete spectrum defined by the spatial quantisation rule for the momentum (wave-vectors):

$$q = q_1^2 + q_2^2 + q_3^2; \quad q_j = 0, \pm 1, \pm 2, \pm 3, \dots \quad (j = 1, 2, 3). \quad (4)$$

The number of degenerate states in the box is strongly and randomly fluctuating. The degeneracy occurs due to the discrete spatial orientations of the state wave-vectors with the same quantum number (q). The weight (degeneracy) of state with a quantum number q can be found, for large level numbers (asymptotic case), as [16-18]:

$$g_{asy} = 2\pi\sqrt{q}. \quad (5)$$

The average of the distribution $g(q)$ follows the asymptotic trend from Eq.(5).

For particle confinement in relatively small volumes and at relatively small temperatures (we shall define later what "relatively small" means), we have to account for the random distribution of the degeneracy. One can expect a discrete and irregular kinetic energy spectrum. We can define *the quantum degeneracy factor*:

$$\zeta(q) = \frac{g(q)}{g_{asy}(q)} = \frac{g(q)}{2\pi\sqrt{q}}, \quad (6)$$

which includes the spatial quantization effects. We have checked that *the factor $\zeta(q)$ is randomly fluctuating around the value 1* by the calculation of the average number of states on *constant frequency intervals*. The result is that the average number of states tends to the asymptotic value very rapidly, even in the case when the degeneracy fluctuations are large in a box with a small number of states. For a number of states larger than ≈ 100 , the classical equation (5) can be safely used.

The total degeneracy in an atomic gas, g_T , is the product of the state degeneracy, $g_q = g(q)$ and the intrinsic spin degeneracy of the atoms, $g_S = 2S+1$ (where S is the total spin of the atoms): $g_T = g_q \cdot g_S$.

Let us denote by n_q the number of particles with momentum \mathbf{p}_q . Then, the particle number operator can be written as $\mathbf{N} = \sum_q \mathbf{n}_q$ and the kinetic energy operator is $\mathbf{H} = \sum_q \mathbf{n}_q \varepsilon_q$. For fermions, the grand partition function becomes

$$Z(T, V, \mu) = \prod_q Z_q = \prod_q [1 + \exp(-(\varepsilon_q - \mu)/k_B T)]^{-g_T}. \quad (7)$$

Accordingly, the particle number in the fermion gas is:

$$N = k_B T \frac{\partial}{\partial \mu} \ln Z = \sum_q g_T [\exp((\varepsilon_q - \mu)/k_B T) + 1]^{-1} \quad (8)$$

and the total energy can be calculated as:

$$E = k_B T \left(T \frac{\partial \ln Z}{\partial T} + \mu \frac{\partial \ln Z}{\partial \mu} \right) = \sum_q g_T \varepsilon_q [\exp((\varepsilon_q - \mu)/k_B T) + 1]^{-1}. \quad (9)$$

We can also write:

$$\frac{\delta E}{\delta \varepsilon} = \frac{g_T \cdot q}{\exp[(\varepsilon - \mu)/k_B T] + 1} = \frac{g_T \cdot q}{\exp[-\mu/k_B T] \cdot \exp[\varepsilon/k_B T] + 1} = \frac{g_T \cdot q}{A^{-1} \exp(\alpha q / \gamma) + 1} \quad (10)$$

where $A = \exp(\mu/k_B T)$ is the fugacity, $\alpha = h^2/2m_{0p}k_B = 9.506 \cdot 10^{-14} [cm^2 K]$, $m = A_{at} m_{0p}$ is the particle mass, A_{at} is the atomic mass number and $\gamma = A_{at} L^2 T$ - the product of the atomic mass number, A_{at} and the adiabatic invariant, $TV^{2/3}$. Using the quantum degeneracy factor defined in (6), the fermion spectrum (10) can be put in the form:

$$u(q, A, \gamma) = \frac{\delta E}{\delta \varepsilon} = \frac{2\pi g_s \cdot q^{3/2}}{A^{-1} \exp(\alpha q / \gamma) + 1} \cdot \zeta(q). \quad (11)$$

The Fermi-Dirac energy spectrum (FDES), from Eq.(11), is discrete for a small number of states in the cubic box. One observes that the quantum effects may occur in cubic cavities with micrometer sizes, at temperatures around μK , which are presently reached by evaporation and laser cooling [6]. These spectra show that, the higher the adiabatic invariant, $L^2 T$, the higher the number of levels, for specified particles (atoms) in the cavity. At a certain resolution limit, the spectrum is obtained by averaging the energy lines ($\zeta \rightarrow 1$) and the continuous FDES is reached.

We can introduce a reasonable superior limit of the number of states in the box, q_T , which bring a significant contribution to the FDES. At high energies, the exponential term dominates and $\zeta(q) \rightarrow 1$, so that Eq.(11) can be approximated by:

$$u(x) \approx Bx^{3/2} \exp(-x), \text{ with } x = \alpha q / \gamma.$$

Considering $A < 1$ and neglecting the levels which bring a contribution of less than 10^{-3} , one can parametrically truncate the Fermi-Dirac distribution at *the highest significant level number (HSL)* in the box:

$$q_T \approx 15\gamma / \alpha. \quad (12)$$

One can observe that, for any of its values, Eq.(12) ensures an over-evaluated value for q_T . For example, $A_{at} = 40$ (Potassium), $L = 10^{-4}$ cm and $T = 10^{-6}$ K, Eq.(12) leads to: $q_T \approx 64$. For Li⁶, one can find in the same box: $q_T \approx 10$.

2. The average number of fermions in a gas confined in a cubic box with low adiabatic invariant

With the above notations, the average fermion number in the gas from Eq.(8) can be written in the form:

$$N = g_s \sum_{q=0}^{\infty} \frac{g_q}{A^{-1} \exp[\alpha q / \gamma] + 1} \approx 2\pi g_s \sum_{q=0}^{q_T} \frac{q^{1/2}}{A^{-1} \exp[\alpha q / \gamma] + 1}, \quad (13)$$

by summing up the contributions of the quantum states up to the highest significant one (given by (12)) and by leaving apart the factor $\zeta(q)$ of state degeneracy (which

have a negligible effect in the sums, as we previously demonstrated [16-18]). For finite FD systems, which are characterized by low adiabatic invariant (in quantum regime), one can take $A > 1$.

The total number of particles and the total energy of the ideal Fermi-Dirac gas are described in many textbooks passing rapidly from sums to integrals [see for example, 1, 2]:

$$N = \frac{g_s L^3 m^{3/2}}{\sqrt{2\pi^2 \hbar^3}} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{\exp[(\varepsilon - \mu)/k_B T] + 1}; \quad (14)$$

Introducing the new dimensionless variable $z = \varepsilon/k_B T$, one can write Eqs. (14) in the form:

$$N = 2\pi g_s \left(\frac{\gamma}{\alpha}\right)^{3/2} \int_0^\infty \frac{z^{1/2}}{A^{-1}e^z + 1} dz = 2\pi g_s \left(\frac{\gamma}{\alpha}\right)^{3/2} \cdot f_1(A), \quad (15)$$

where $f_1(A)$ is the integral.

In the quantum regime, it is usually to approximate the integral from Eq. (15) using a power series expansion leading to [2-5]:

$$f_1(A) \cong \frac{2}{3} (\ln A)^{3/2} \left[1 + \frac{\pi^2}{8} (\ln A)^{-2} + \frac{7\pi^4}{640} (\ln A)^{-4} + \frac{31\pi^6}{3072} (\ln A)^{-6} + \dots \right], \quad (16)$$

where $\ln A = \frac{\mu}{k_B T} \approx \frac{E_F}{k_B T} = \frac{T_F}{T}$ and T_F is Fermi temperature ($T_p = \varepsilon_F / k_B$). This

approximation provides reasonable precision for $\mu/k_B T \geq 5$ only, which could be hardly met in the present experimental conditions. Moreover, for $\mu/k_B T > 1$, the series expansion from (16) does not converge. Certainly, with mathematical efforts (e.g., using Pade-type approximations), one can improve the classical approximations of the type (16) [19].

However, the direct summation (with finite number of terms) implies simple algorithms and gives more precise results than the summation in the approximate series for the classical integral (15). In Fig.1, we have shown the average number of fermions in a cubic box with low adiabatic invariant calculated by direct summation with Eq. (13) and by approximate summation (16) (with the first three terms of the power series, at very low temperatures), i.e:

$$N \approx \frac{4\pi g_s}{3} \left(\frac{\gamma}{\alpha}\right)^{3/2} \cdot (\ln A)^{3/2} \left[1 + \frac{\pi^2}{8} (\ln A)^{-2} + \frac{7\pi^4}{640} (\ln A)^{-4} \right]. \quad (17)$$

The theoretical procedure of building the grand canonical ensemble is compatible to the present experimental cooling procedure based on evaporation, which eliminates progressively the particles with the highest kinetic energy and implies a variable particle number in the system. In this case, the Fermi-Dirac gas finds a straightforward description in the direct summations (Eq.(13)), for given fugacity and adiabatic invariant.

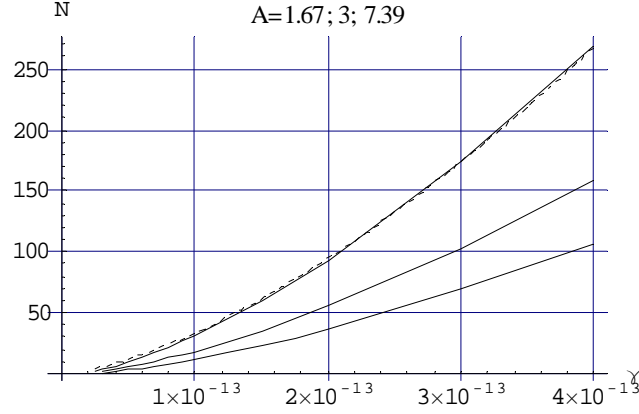


Fig.1. The plot of the number of particles in Fermi-Dirac gas, N , versus the adiabatic invariant multiplied by the atomic mass number, $\gamma = A_{at} L^2 T$ [$\text{cm}^2 \cdot \text{K}$], at fixed fugacity, A , using direct summation (continuous lines, from bottom to top: $A = 1.67, 3$ and 7.39) and the integral approximation from Eq.(17) (for $A = 7.39$, dashed line). The value $A = 1.67$ is close to the onset of quantum regime, while $A = 7.389$ is close to the lowest experimental limits.

Often, the function $f_1(A)$ is inverted in order to obtain the fugacity. In the Appendix, we give an analytical procedure for the accurate calculation of the chemical potential.

3. The total energy of discrete Fermi-Dirac system in the cubic box

In the cubic box, the total energy, from Eq.(9), should be written by summing the state energies up to the highest significant one (characterized by q_T):

$$\frac{E}{k_B T} = g_s \left(\frac{\alpha}{\gamma} \right) \sum_{q=1}^{\infty} \frac{2\pi q^{3/2} A}{\exp[\alpha q / \gamma] + A} \approx 2\pi g_s \left(\frac{\alpha}{\gamma} \right) \sum_{q=1}^{q_T} \frac{q^{3/2} A}{\exp[\alpha q / \gamma] + A}. \quad (18)$$

The total energy integral, which characterizes large particle ensembles in classical conditions, is:

$$E = \frac{g_s L^3 m^{3/2}}{\sqrt{2\pi^2 \hbar^3}} \int_0^{\infty} \frac{\varepsilon^{3/2} d\varepsilon}{\exp[(\varepsilon - \mu) / k_B T] + 1}; \quad \varepsilon = \varepsilon_0 \cdot q; \quad \varepsilon_0 = \frac{\alpha}{\gamma} k_B T, \quad (19)$$

Considering the quantum regime and temperatures much lower than the Fermi one ($T < 0.2 T_F$), (19) is written as:

$$\begin{aligned} \frac{E}{k_B T} &= 2\pi g_s \left(\frac{\gamma}{\alpha} \right)^{3/2} \int_0^{\infty} \frac{A z^{3/2}}{e^z + A} dz = 2\pi g_s \left(\frac{\gamma}{\alpha} \right)^{3/2} \cdot f_2(A) \\ f_2(A) &\cong \frac{2}{5} (\ln A)^{5/2} \left[1 + \frac{5\pi^2}{8} (\ln A)^{-2} - \frac{7\pi^4}{384} (\ln A)^{-4} - \frac{155\pi^6}{21504} (\ln A)^{-6} - \dots \right] \end{aligned} \quad (20)$$

Again, the direct summation (with finite number of terms) implies simple algorithms and gives more precise results than the summation in the approximate

series for the classical integral. We can calculate the ratio of total energies of the fermion gas in the box and in a classical (large) container with Eqs. (13) and (18), in the universal form:

$$F = \frac{E}{(3/2)g_S N k_B T} = \frac{2\pi}{(3/2)N} \left(\frac{\alpha}{\gamma} \right) \sum_{q=1}^{\infty} \frac{q^{3/2}}{A^{-1} e^{\alpha q/\gamma} + 1} \approx \frac{4\pi}{3N} \left(\frac{\alpha}{\gamma} \right)^{g_T(\gamma)} \sum_{q=1}^{\infty} \frac{q^{3/2}}{A^{-1} \cdot e^{\alpha q/\gamma} + 1} \geq 1. \quad (21)$$

The corrective factor, F , depends on the parameter α/γ (i.e. on the adiabatic invariant multiplied by the atomic mass number of the fermions).

In the first order of approximation, F can be obtained by replacing both the total energy and the number of fermions by (20) and (17):

$$\begin{aligned} F &\approx \frac{2}{5} (\ln A) \frac{1 + (5\pi^2/8)(\ln A)^{-2} - (7\pi^4/384)(\ln A)^{-4}}{1 + (1/8)\pi^2 (\ln A)^{-2} + (7\pi^4/640)(\ln A)^{-4}} \\ &\approx \frac{2}{5} \left(\frac{T}{T_F} \right)^{-1} \frac{1 + (5\pi^2/8)(T/T_F)^2 - (7\pi^4/384)(T/T_F)^4}{1 + (\pi^2/8)(T/T_F)^2 + (7\pi^4/640)(T/T_F)^4}, \end{aligned} \quad (22)$$

which shows its dependence on the ratio of the absolute and Fermi temperatures, which is related, at very low temperatures, to the number of fermions and adiabatic invariant, as: $T/T_F \approx (8\pi/3)^{2/3} (\gamma/\alpha) \cdot N^{-2/3} [S + (1/2)]^{2/3}$.

Thus, with specified atoms and box size, *the total energy in the box with low adiabatic invariant has a strong dependence on temperature* (Fig.2).

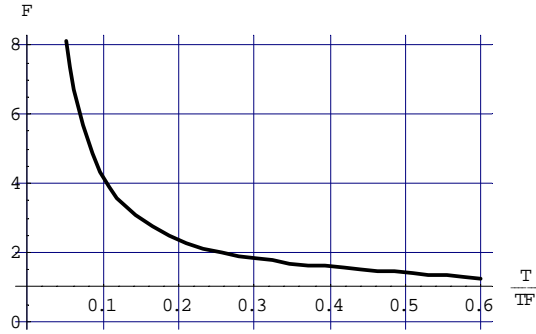


Fig.2. The ratio between the total energy of fermions in the quantum box and in the classical (large) container, F , in function of the ratio of fermion and Fermi temperatures (when $T/T_F \ll 1$).

For given atoms, the box size and the temperature are reciprocal parameters in the box, i.e. the same effects (in the thermodynamics of the fermion gas) can be obtained either by varying $L^2 = V^{2/3}$ or by varying T , if their product remains constant.

4. Accurate formula for chemical potential of the Fermi-Dirac quantum gas

The chemical potential can be calculated, in a large domain around T_F , by using a derivative method combined with the saddle-point method for inverting the integral from Eq.(15)[19]:

$$\frac{\mu(T, N)}{k_B T} = -\ln[1 - f_3(w) - f_4(w)], \quad (23)$$

$$\text{where } w = 1.8654019 f_1(A) - 1.2649177. \quad (24)$$

$f_1(A)$ is the integral from (15):

$$f_1(A) = \frac{1}{2\pi g_s} N \left(\frac{\alpha}{\gamma} \right)^{3/2} \approx \frac{4}{3g_s} \left(\frac{E_F}{k_B T} \right)^{3/2} = \frac{4}{3g_s} \left(\frac{T_F}{T} \right)^{3/2}, \quad (25)$$

$$f_3(w) = \frac{w + 9.687028 \cdot 10^{-2} w^2 + 3.536258 \cdot 10^{-3} w^3}{1 + 0.91105858w + 9.9727494 \cdot 10^{-2} w^2 + 3.5307381 \cdot 10^{-3} w^3} \quad (26)$$

$$\text{and } f_4(w) = \frac{10^{-6} w^4}{7.5961894 - 0.7579328w + 0.1731814w^2}. \quad (27)$$

One can observe that (23) is a universal representation of the chemical potential for Fermi-Dirac quantum gas (containing any number of particles) (Fig. 3).

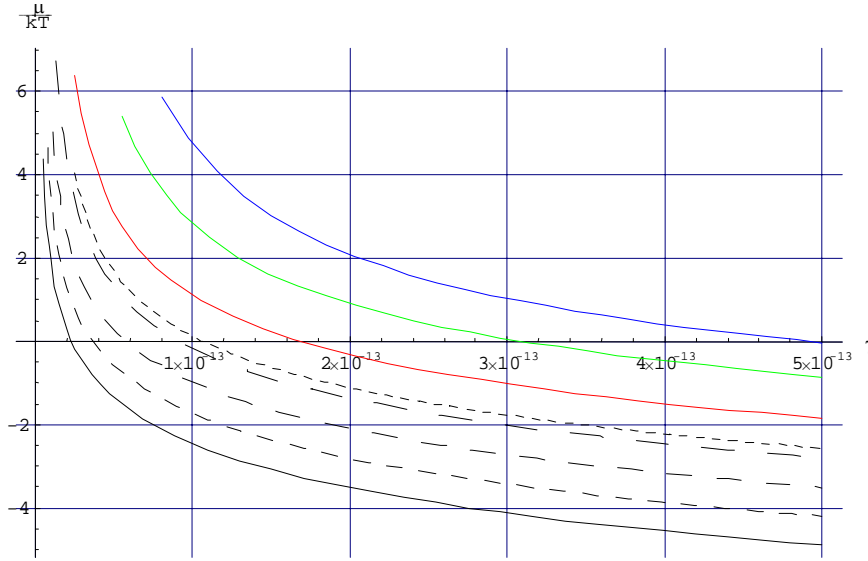


Fig.3. The chemical potential of Fermi-Dirac quantum gas in function of the adiabatic invariant, γ and for increasing number of fermions, $N = 1, 2, 4, 8, 10, 20, 50, 100$, bottom to top, calculated with our Eq. (23). One can remark that for a constant chemical potential, the number of particles grows with the adiabatic invariant, as expected from Eq. (15).

As an example, to check (23), one can take: $f_1(A) = 1$. This value successively leads to: $w = 0.6004842$; $f_3(w) = 0.401679$; $f_4(w) = 1.804938 \cdot 10^{-8}$. From (23), we get the chemical potential: $\mu(T) = 0.5136279 \cdot k_B T$ and the fugacity: $A = \exp(\mu/k_B T) = 1.6713436$ (which is a bit higher than the onset of the quantum regime, at $\mu = 0$, $A = 1$). Then, using the approximations of the integral $f_1(A)$, from (16) (or more precise, from [18]), we can arrive to: $f_1(A) = 0.9999574$, which compares very favorably with the starting value, we have considered for this test.

Our formula (23) has the form:

$$\frac{\mu}{k_B T} = -\log \left[f_5 \left(\frac{T}{T_F} \right) \right], \quad f_5 \equiv (1 - f_3 - f_4), \quad (23a)$$

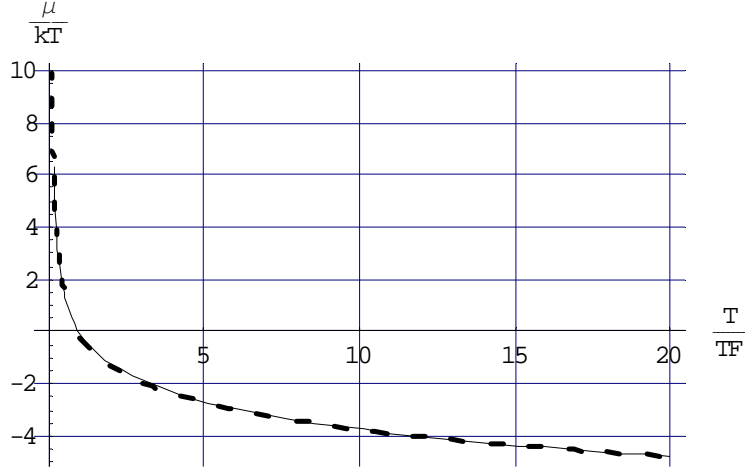


Fig. 4. The chemical potential of Fermi-Dirac quantum gas in function of the ratio between the absolute temperature and Fermi temperature calculated with: (a) accurate analytic formula (26) (continuous line); (b) Sommerfeld approximation at low temperature (28) (small dashed line); approximate (semi-classical) formula for high temperature (large dashed line).

and is very useful to complete the Sommerfeld formula (valid at very low temperatures [2-5]):

$$\frac{\mu}{k_B T} = \left(\frac{T}{T_F}\right)^{-1} \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_F}\right)^2 \right] \quad (28)$$

and the semi-classical one, at high temperatures [2-5] (Fig.4).

4. Conclusions

The energy spectrum of a Fermi-Dirac system, which is confined in a rigid cubic box with low adiabatic invariant, is discrete and depends strongly on the box size and temperature. We have introduced a reasonable superior limit of the number of states in the box, which brings a significant contribution to this discrete spectrum and which is to be considered in the calculations of the particle number and of the total energy by summing up the quantum level contributions.

We have shown that the number of particles and total energy of the discrete (finite) Fermi-Dirac systems with low adiabatic invariant can be calculated in a simple and precise way by summing up the contributions of a finite number of states, defined by the values of γ . These procedures complete successfully the usual approximations of the corresponding integrals, which are restricted by conditions difficult to be met in the present experiments with ultra-cold Fermi-Dirac gases.

In Fermi-Dirac systems with low adiabatic invariant, the box size and the temperature are reciprocal parameters in the sense that the same effects can be obtained either by varying L or by varying T , if their product remains constant.

A new accurate formula for chemical potential of the Fermi-Dirac quantum gas is given, which completes well the previously used approximations.

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