Chemical potential and internal energy of the noninteracting Fermi gas in fractional-dimensional space

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Abstract. Chemical potential and internal energy of a noninteracting Fermi gas at low temperature are evaluated using the Sommerfeld method in the fractional-dimensional space. When temperature increases, the chemical potential decreases below the Fermi energy for any dimension equal to 2 and above due to the small entropy, while it increases above the Fermi energy for dimensions below 2 as a result of high entropy. The ranges of validity of the truncated series expansions of these quantities are extended from low to intermediate temperature regime as well as from high to relatively low density regime by using the Padé approximant technique.

Keywords. Chemical potential; internal energy; Fermi gas; fractional-dimensional space; Padé approximation.

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1. Introduction

The chemical potential is a fundamental quantity in statistical mechanics which characterizes the many-particle systems in thermal equilibrium [1]. In the second law of thermodynamics, the change in total energy $(\mathrm{d}U)$ of the system exchanging the number of particles $(\mathrm{d}N)$ with the reservoir at a temperature (T) and under pressure (p) is given by $\mathrm{d}U = T\,\mathrm{d}S - p\,\mathrm{d}V + \mu\,\mathrm{d}N$, where $\mathrm{d}S$ is the change in entropy by T, $\mathrm{d}V$ is the change in volume by p and μ is the chemical potential. When S and V of the system are fixed, μ is defined as

$$\mu = \frac{\mathrm{d}U}{\mathrm{d}N}\bigg|_{S,V}. \tag{1}$$

In the ground state, S vanishes and μ is obtained under the condition that the number of particles in volume V does not depend on temperature [2]. The chemical potential is the energy necessary to add one particle to the system without changing both the entropy and volume. The quantum theory in solids and low-dimensional systems is essentially the physics deduced from the ideal Fermi gas model where the physical properties at a finite temperature are expressed in terms of the Fermi–Dirac distribution function characterized by μ.

Various techniques are described in the literature for evaluating μ of the non-interacting Fermi gas at low-temperature limit. In 1928, Sommerfeld [3] obtained μ as a low-temperature expansion in the three-dimensional systems. This method is not correct for an arbitrary value of $\mu/k_\mathrm{B}T$ (k_B is the Boltzmann constant) [2] because this method omits the term $\exp(-\mu/k_\mathrm{B}T)$ in the calculation. However, this method is accurate in the low-temperature limit as $\exp(-\mu/k_\mathrm{B}T)$ vanishes in this limit. Furthermore, the Sommerfeld method can be easily extended to calculate several ground state properties of the free fermion gas using the thermodynamic relations [2]. Both μ and U in 3D were calculated up to order T^6 by Kiess [4] and up to order T^8 by Aguilera-Navarro *et al* [5]. The only limitation of the Sommerfeld method is that it cannot be used for two-dimensional (2D) systems. However, the evaluation of μ and U in the 2D system is analytic and the expressions for these quantities are obtained in closed forms [6]. The other two procedures are the Cauchy's integral method [7] and polylogarithm method [8]. The results obtained in these methods are identical to those obtained in the Sommerfeld method.

The standard Padé approximant technique is well known for reproducing the correct behaviour of a function for which only a few terms are available [9]. In this technique, the truncated series is expressed as a ratio of the two polynomials of finite sizes so that the ratio is convergent. Using this method, the truncated series of μ and U valid in the low-temperature and high-density regimes are extended to intermediate-temperature and low-density regimes [5].

The multidimensional space method serves as a model for studying the dimensional dependence of the physical properties. For example, the properties of polaron are obtained as a function of n, an integer specifying the dimension [10]. The evaluation of μ and U in this space has been attempted by Cetina *et al* [6] using the series expansion method. It is more elegantly evaluated using the Cauchy's contour integration method [11] and the polylogarithm method [8]. All these methods are found to give identical results. In addition to these, the polylogarithm method in this space was employed to calculate μ in the one-dimensional (1D) [12] and zero-dimensional (0D) [13] systems.

The quantum well and quantum wire fabricated using the semiconductor hetero-junctions are 3D systems with embedded 2D and 1D structures, respectively. In 1986, Ishida [14] theoretically noticed the dimensional cross-over of the plasmon from 2D to 3D when the well width of the quantum well is increased. A narrow quantum well has only one level occupied by the electron so that the system manifests 2D behaviour. However, the level separation decreases with the increase of the well width so that higher and higher levels are occupied by electrons. When the well width is very large, the system shows 3D behaviour. Consequently, the system shows fractional-dimensional (FD) behaviour with the dimension varying between 2 and 3 when the well width is finite. Similarly, the quantum wire with

finite internal area shows FD behaviour with its dimensionality varying between 1 and 3.

The FD space is termed as dynamic space which differs from the geometric space in that its dimensionality is determined by physical interactions as seen from the viewpoint of the excitation dynamics. The formalism for calculating the physical properties in the FD space was introduced by He [15]. The anisotropic low-dimensional space in 3D structures becomes isotropic in the FD space and the dimension provides a measure for the degree of anisotropy in the actual physical system. The dimension is determined from the extension of radius of bosons such as exciton [16], polaron [17], exciton–polaron [18] and plasmon [19] with respect to the well width in quantum well and the square root of the internal area in quantum wire [20]. The quasi-2D layered structures of high-temperature superconducting thin films are actually not 2D objects, but fractals with Hausdorff dimensionalities between 2D and 3D in the real laboratory situation [21,22]. The formalism of He [15] has been used to describe the superconductivity [23] and the transport properties in fractals [24]. An accurate evaluation of μ is necessary to find the temperature dependence of the excitation spectra in these systems.

In the present work, we have used the Sommerfeld method to find μ and U in FD space at low-temperature and high-density limits. Finally, the results are fitted to Padé approximant forms to extend their validity to intermediate-temperature and low-density limits.

2. Method of calculation

Recently, we have derived an interpolating formula for μ of the noninteracting Fermi gas in the FD space valid in the high-temperature limit at an arbitrary density of particles [19]. In the present work, we will present the derivation of μ valid for low-temperature and high-density limits only. The number of particles is defined as

$$N = 2 \sum_{\mathbf{k}} \frac{1}{\exp((\epsilon_k - \mu)/k_{\mathrm{B}}T) + 1}, \tag{2}$$

where $\epsilon_k = \hbar^2 k^2/2m^*$ is the energy variable with m^* being the effective mass of the particle and the factor 2 accounts for the spin degeneracy.

The internal energy is defined as

$$U = 2 \sum_{\mathbf{k}} \frac{\epsilon_k}{\exp((\epsilon_k - \mu)/k_{\mathrm{B}}T) + 1}. \tag{3}$$

In the FD space, $\mathbf{k}$ is not a vector space and the coordinates in this space are termed as pseudocoordinates [25]. The vector operations are not allowed in this space. Since the FD space is taken as isotropic in the method of calculation [25], the sum over $\mathbf{k}$ can be transformed into integral over positive k as

$$\sum_{\mathbf{k}} \cdots = \frac{V}{(2\pi)^\alpha} \frac{2\pi^{(\alpha-1)/2}}{\Gamma((\alpha-1)/2)} \int k^{\alpha-1}\mathrm{d}k \int_0^\pi \mathrm{d}\theta \sin^{\alpha-2}\theta \cdots, \tag{4}$$

where V is the volume in FD space and $\Gamma(x)$ is the Euler's gamma function. This transformation is also the same as in the multidimensional space where α is replaced by n. This transformation is not valid for the 1D system since $\Gamma(0) = \infty$. However, such a transformation can be used when $\alpha \to 1$. This formalism can be applied to quantum dots [13] since $\Gamma[(\alpha - 1)/2] = -2\sqrt{\pi}$ when $\alpha = 0$.

At $T = 0$, using eq. (4) in eq. (2) and carrying out the integration over θ, we find

$$\rho = 2\rho_0 \int_0^{E_F} \epsilon_k^{(\alpha-2)/2} \, d\epsilon_k, \tag{5}$$

where the density of particles $\rho = N/V$ and $\rho_0 = (m^*/2\pi\hbar^2)^{\alpha/2}/\Gamma(\alpha/2)$. Here $\Gamma[(\alpha-1)/2]$ in eq. (5) gets cancelled after θ integration except when $\alpha = 1$. Therefore, this method raises the validity of the previous work on the applicability of the multidimensional space method to 1D system [12]. Carrying out the trivial integration in eq. (5), we find the expression for E_F as

$$E_F = \left(\frac{\alpha\rho}{4\rho_0}\right)^{2/\alpha} = \frac{\hbar^2}{2m^*} \left(\frac{(4\pi)^{\alpha/2}\Gamma(1+\frac{\alpha}{2})\rho}{2}\right)^{2/\alpha}. \tag{6}$$

It is clear that $k_F = ((4\pi)^{\alpha/2}\Gamma(1+\alpha/2)\rho/2)^{1/\alpha}$. For $T \neq 0$, ρ is obtained as

$$\rho = 2\rho_0 \int_0^{\infty} \frac{\epsilon_k^{(\alpha-2)/2}}{\exp((\epsilon_k - \mu)/k_B T) + 1} d\epsilon_k. \tag{7}$$

For $\alpha = 2$, the integration in eq. (7) is carried out exactly to obtain,

$$\rho = 2\rho_0 \left[\mu + k_B T \log\left\{1 + \exp\left(\frac{\mu}{k_B T}\right)\right\}\right]. \tag{8}$$

The Fermi energy is calculated as

$$E_F = \mu + k_B T \log\left[1 + \exp\left(\frac{\mu}{k_B T}\right)\right]. \tag{9}$$

It is easy to invert eq. (9) to find μ as [6]

$$\frac{\mu}{E_F} = 1 + \frac{k_B T}{E_F} \log\left[1 - \exp\left(-\frac{E_F}{k_B T}\right)\right]. \tag{10}$$

At $T = 0$, $\mu = E_F$.

2.1 *Sommerfeld method*

For $\alpha \neq 2$, ρ can be obtained by using the method of Cetina *et al* [6]. Taking the low-temperature expansion in powers of $k_B T$, ρ is obtained as [1,6]

$$\rho = \frac{4\rho_0}{\alpha} \left[\mu^{\alpha/2} + \sum_{l=1}^{\infty} (k_{\mathrm{B}}T)^{2l} \zeta(2l) \frac{4^l - 2}{4^l} \frac{\mathrm{d}^{2l-1} \mu^{\frac{\alpha}{2}-1}}{\mathrm{d}\mu^{2l-1}} \right], \tag{11}$$

where $\zeta(x)$ is the Riemann zeta function. This is the Sommerfeld expansion for density. The Fermi energy is calculated as

$$E_{\mathrm{F}} = \mu \left[1 + \frac{\alpha - 2}{12} \left(\frac{\pi k_{\mathrm{B}}T}{\mu} \right)^2 + \frac{(\alpha - 2)(\alpha^2 - 25\alpha + 74)}{1440} \left(\frac{\pi k_{\mathrm{B}}T}{\mu} \right)^4 \right.$$

$$+ \frac{(\alpha - 2)(4\alpha^4 - 259\alpha^3 + 4419\alpha^2 - 23996\alpha + 41252)}{362880} \left(\frac{\pi k_{\mathrm{B}}T}{\mu} \right)^6$$

$$+ \frac{\left\{ \begin{array}{c} (\alpha - 2)(18\alpha^6 - 2167\alpha^5 + 81924\alpha^4 - 1303409\alpha^3 \\ + 9638270\alpha^2 - 33428844\alpha + 44072968) \end{array} \right\}}{87091200}$$

$$\left. \times \left(\frac{\pi k_{\mathrm{B}}T}{\mu} \right)^8 + \cdots \right]. \tag{12}$$

For finding μ when $\alpha \neq 2$, the inversion of eq. (12) is carried out using the isotherm approach. In this approach the number of particles does not depend upon temperature at a given volume. Therefore, E_{F} is independent of temperature,

$$\left(\frac{\partial E_{\mathrm{F}}}{\partial T} \right)_V = 0. \tag{13}$$

A series expansion of μ/E_{F} in terms of $k_{\mathrm{B}}T/E_{\mathrm{F}}$ is taken as

$$\frac{\mu}{E_{\mathrm{F}}} = 1 + a_2 \left(\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}} \right)^2 + a_4 \left(\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}} \right)^4 + a_6 \left(\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}} \right)^6 + a_8 \left(\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}} \right)^8 + \cdots, \tag{14}$$

where a_2, a_4, etc. are the coefficients of expansion. The coefficients of odd powers of T vanish since E_{F} contains only even powers of T. These coefficients are easily obtained as

$$a_2 = -\frac{(\alpha - 2)\pi^2}{12},$$

$$a_4 = -\frac{(\alpha - 2)(\alpha - 6)(\alpha - 9)\pi^4}{1440},$$

$$a_6 = -\frac{(\alpha - 2)(\alpha - 4.2231)(\alpha - 8.6476)(\alpha - 10)(\alpha - 20.8794)\pi^6}{90720},$$

$$a_8 = -\frac{\left\{ \begin{array}{c} (\alpha - 2)(\alpha - 4.0247)(\alpha - 6.3142)(\alpha - 9.5286) \\ \times (\alpha - 14)(\alpha - 14.8860)(\alpha - 37.9687)\pi^8 \end{array} \right\}}{4838400}. \tag{15}$$

For quantum wire, it has been derived earlier [26] that $\mu/E_{\mathrm{F}} = 1 + (\pi^2/12)(k_{\mathrm{B}}T/E_{\mathrm{F}})^2$. Our derivation reproduces this, however, at $\alpha \to 1$. For $\alpha > 2$,

we find that μ/E_F decreases with T. On the other hand, for $\alpha < 2$, μ/E_F increases with T which is unphysical as $\mu/E_F \to \infty$ when $T \to \infty$. Grether *et al* [27] have shown that μ/E_F increases in the low-temperature limit and then becomes negative at $T \to \infty$ with a hump in the intermediate temperature limit.

The internal energy U can be calculated using the general thermodynamic relationship [4]

$$(\alpha + 2)U - 2T\left(\frac{\partial U}{\partial T}\right)_{V,N} - \alpha N\mu + \alpha NT\left(\frac{\partial \mu}{\partial T}\right)_{V,N} = 0. \tag{16}$$

A series expansion of U in terms of even powers of $k_B T/E_F$ is taken as

$$U = U_0\left[1 + A_2\left(\frac{k_B T}{E_F}\right)^2 + A_4\left(\frac{k_B T}{E_F}\right)^4 \right.$$
$$\left. + A_6\left(\frac{k_B T}{E_F}\right)^6 + A_8\left(\frac{k_B T}{E_F}\right)^8 + \cdots\right], \tag{17}$$

where U_0 is the internal energy at $T = 0$ and A_2, A_4 etc. are the coefficients to be determined. These coefficients are obtained by substituting eqs (17) and (14) in eq. (16),

$$U_0 = \alpha N E_F/(\alpha + 2),$$
$$A_2 = \frac{(\alpha + 2)\pi^2}{12},$$
$$A_4 = \frac{(\alpha + 2)(\alpha - 2)(\alpha - 9)\pi^4}{480},$$
$$A_6 = \frac{(\alpha + 2)(\alpha - 2)(\alpha - 4.2231)(\alpha - 8.6476)(\alpha - 20.8794)\pi^6}{18144},$$
$$A_8 = \frac{\left\{\begin{array}{c} 7(\alpha + 2)(\alpha - 2)(\alpha - 4.0247)(\alpha - 6.3142) \\ \times(\alpha - 9.5286)(\alpha - 14.8860)(\alpha - 37.9687)\pi^8 \end{array}\right\}}{691200}. \tag{18}$$

Substituting $E_F = (\alpha N/4n_0 V)^{2/\alpha}$ in eq. (17) and using eq. (1), we can obtain eq. (14). The internal energy increases for all α.

2.2 *Padé approximant method*

We find that the truncated series for μ and U correctly finds the low-temperature limit of the numerical method. We need to express the series as a ratio of two finite-sized polynomials in the Padé approximant technique for extending their validity to intermediate temperature and relatively low-density regimes. This method has been described by Baker [9]. As pointed out earlier, this method has been applied to truncated series of μ/E_F and U/U_0 in 3D containing terms up to the 8th power of T [5], where different Padé approximant forms have been fitted to the series expansions. Among three different forms, [0/3], [2/1] and [1/2], [0/3] form has

been found to be the best. In order to include a_8 term in the fitting, the entire series in the present work is expressed in terms of [0/4], [1/3], [2/2] and [3/1] forms and it is found that [1/3] is the best among them. Using this form, μ/E_F is expressed as

$$\frac{\mu}{E_F} = \frac{1 + p_2(k_B T/E_F)^2}{1 + q_2(k_B T/E_F)^2 + q_4(k_B T/E_F)^4 + q_6(k_B T/E_F)^6},\qquad(19)$$

where the coefficients are obtained using the Mathematica package [28] as $p_2 = (a_2^4 - 3a_2^2 a_4 + a_4^2 + 2a_2 a_6 - a_8)/A$, $q_2 = (a_2^4 - a_2^2 a_4 + a_2 a_6 - a_8)/A$, $q_4 = (a_2^4 - a_2^2 a_4 + a_2 a_6 - a_8)/A$ and $q_6 = (-a_3^4 + 2a_2 a_4 a_6 - a_6^2 - a_2^2 a_8 + a_4 a_8)/A$, where $A = a_2^3 - 2a_2 a_4 + a_6$. These coefficients are evaluated using eq. (15).

Similarly, U is expressed in the [1/3] Padé approximant form as

$$\frac{U}{U_0} = \frac{1 + P_2 \left(k_B T/E_F\right)^2}{1 + Q_2 \left(k_B T/E_F\right)^4 + Q_4 \left(k_B T/E_F\right)^6 + Q_6 \left(k_B T/E_F\right)^8},\qquad(20)$$

where P_2, Q_2, Q_4 and Q_6 are related to A_2, A_4, A_6 and A_8 as in $\mu/k_B T$.

3. Results and discussions

We have calculated μ/E_F as a function of $k_B T/E_F$ numerically at a constant density for $\alpha = 1.01$, 1.5, 2.5 and 3 and compared them with those obtained in the Sommerfeld and Padé approximant methods in figure 1. The numerical results also show similar behaviour as in the other two methods at extremely low-temperature limit. For $\alpha \geq 2$, we find that μ/E_F decreases with T. On the other hand, for $\alpha < 2$, μ/E_F increases with T which is unphysical as $\mu/E_F \to \infty$ when $T \to \infty$. Grether *et al* [27], in the numerical method, have shown that μ/E_F increases in the low-temperature limit and then becomes negative at $T \to \infty$ with a hump in the intermediate temperature limit. The overall behaviour of the temperature dependence of μ in 3D has been described by Cook and Dickerson [29]. At zero temperature, the system is in the ground state with zero entropy. At a small T the sharpness of the edge of the Fermi surface is lost. In the Sommerfeld expansion method the entropy up to order T^3 in FD space is obtained as

$$\frac{S}{\alpha N k_B} = \frac{\pi^2}{6} \left(\frac{k_B T}{E_F}\right) \left[1 + \frac{(\alpha - 2)(\alpha - 9)\pi^2}{20} \left(\frac{k_B T}{E_F}\right)^2 + \cdots\right].\qquad(21)$$

It is clear that the second term is negative for $\alpha > 2$ and it is positive for $\alpha < 2$. As the temperature rises, the total internal energy of the system increases and some of the fermions begin to occupy excited states. In order to keep entropy as zero, the added fermions for $\alpha \geq 2$ must go into the low-lying vacant single-particle states little below E_F left open by the excited fermions. The number of available microstates must be minimized by cooling the gas. The change in internal energy of the Fermi gas must be positive, but a little below E_F. As the temperature increases, more of the low-lying states become vacant. To add a new particle
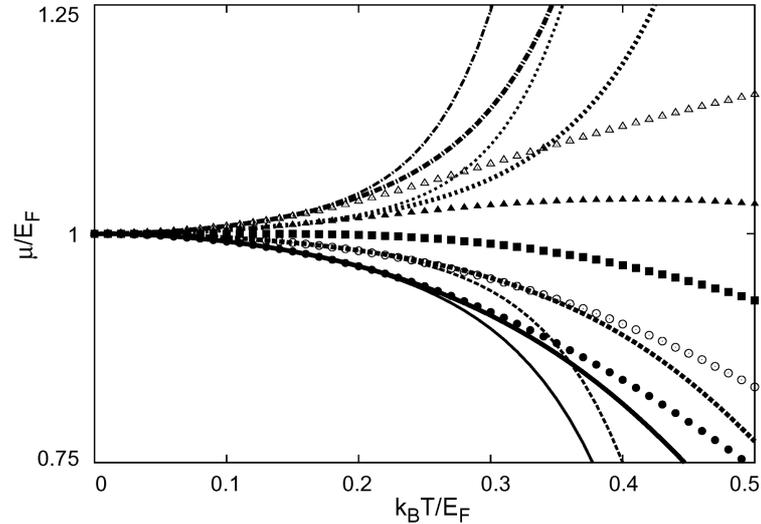
Figure 1. Chemical potentials scaled with respect to Fermi energy as a function of thermal energy scaled with the same Fermi energy for $\alpha = 1.01$, 1.5, 2, 2.5 and 3. The chemical potentials calculated in the numerical method are compared with those estimated in the series expansion method and Padé approximant methods. In the numerical method: closed circles ($\alpha = 3$), open circles ($\alpha = 2.5$), closed squares ($\alpha = 2$), closed triangles ($\alpha = 1.5$) and open triangles ($\alpha = 1.01$). In the series expansion and Padé approximant methods: solid line ($\alpha = 3$), dashed line ($\alpha = 2.5$), dotted line ($\alpha = 1.5$) and dot-dashed line ($\alpha = 1.01$). Here thick and thin lines correspond to Padé approximant and series expansion methods, respectively.

without increasing the entropy, it requires the new particle to go into a low-lying single-particle state, considerably well below E_F while once again cooling the gas slightly to avoid an increase in the number of microstates. However, a particle in the system with $\alpha < 2$ is prevented from going below E_F as its paths are blocked by other excited particles due to greater entropy than in $\alpha \geq 2$. This suggests that the particles which are taken out of the Fermi sea are more dispersed for $\alpha < 2$ resulting in greater entropy than in $\alpha \geq 2$.

For $\alpha < 2$, μ/E_F slowly rises with temperature compared to that in the Sommerfeld method. The comparison shows that the results in the Sommerfeld method fail to match with those obtained numerically beyond a certain temperature T_c and T_c decreases with decreasing α. The series expansion method is described reasonably well when $\alpha > 2$. Figure 1 also shows that at a fixed temperature μ is correctly calculated only when the density is high. For lower density there is no agreement between numerical and series expansion methods. As shown in figure 1, the chemical potentials in the Padé approximant method are extended to higher temperatures and lower density of particles for $\alpha > 2$. However, it does not give any substantial improvement for $\alpha < 2$.

The internal energies obtained in eq. (17) are compared with those obtained in the numerical method in figure 2. Unlike μ, U is found to increase for all α values.
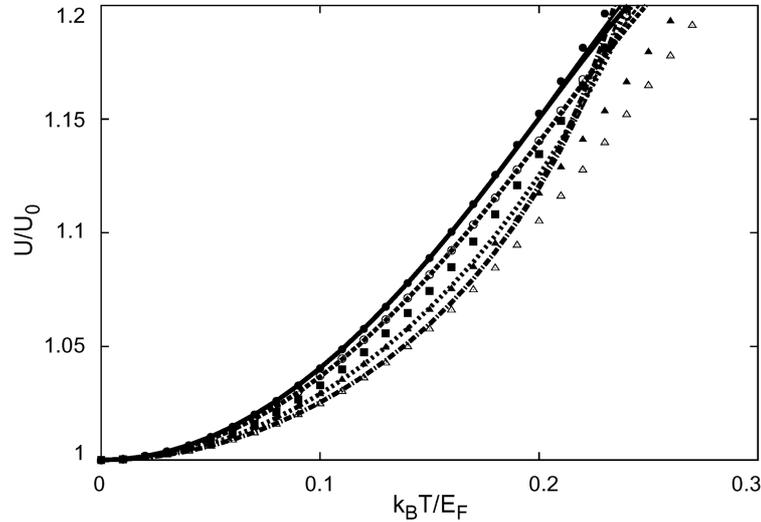
Figure 2. Internal energy of finite temperature scaled with respect to internal energy at zero temperature as a function of thermal energy scaled with Fermi energy for $\alpha = 1.01$, 1.5, 2, 2.5 and 3. The internal energies calculated in the numerical method are compared with those estimated in the series expansion and Padé approximant methods. The symbols carry the same meaning as in figure 1.

The agreement between the series expansion and numerical results is qualitatively the same as shown earlier for μ/E_F. The series expansion method is good for lower temperature and higher density of particles and it is better for $\alpha \geq 2$ than for $\alpha < 2$. The internal energies obtained in this method are compared with those obtained in the series expansion and numerical methods. While the Padé approximant method gives an improvement from low-temperature limit to intermediate-temperature limit and higher density of particles to lower density of particles when $\alpha > 2$, it is not so appreciable for dimensionalities below 2.

4. Summary

In summary, both μ and U of the noninteracting Fermi gas are calculated in the numerical and series expansion methods for α =1.01, 1.5, 2.5 and 3. Comparison of these quantities in the numerical and series expansion methods shows that the results obtained in the latter method are valid in the low-temperature and high-density regimes. These quantities in 2D are obtained in closed forms. In order to extend their validity to higher temperature and lower density, the results are expressed in the Padé approximant method. The [1/3] Padé approximant form is found to be the most suitable for the truncated series expansions of μ and U.

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