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2002 J. Phys. A: Math. Gen. 35 9601

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Exact particle and energy densities for a noninteracting Fermi gas in a harmonic trap

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Received 26 June 2002, in final form 19 September 2002

Published 29 October 2002

Online at stacks.iop.org/JPhysA/35/9601

Abstract

The exact particle and energy densities for a noninteracting Fermi gas at any temperature in a d -dimensional harmonic trap are obtained, and they are expressed by the gamma function and the Laguerre polynomials. The obtained analytical expressions are rapidly converging series and may be conveniently used for the numerical calculations. These expressions can be used for the comparison with the experimental results and for the test of the local density approximation.

PACS numbers: 05.30.Fk, 03.75.Fi

1. Introduction

The ideal Fermi gas is an old and well-understood problem. There exist many physical systems for which the noninteracting Fermi gas is a good zeroth-order approximation. Historically, the noninteracting Fermi gas was applied to discuss the equilibrium states of white dwarf stars by Fowler (1926), to explain the paramagnetism of the alkali metals by Pauli (1927), to explain the properties of metals by Sommerfeld (1927), and to obtain rough estimates for electron distributions and the binding energies of heavy atoms by Thomas (1927) and Fermi (1928), respectively [1]. In these systems, the quantum degenerate effects dominate over the interaction.

The realization of Bose–Einstein condensation in the experiments on dilute vapours of alkali-metal elements [2, 3] has stimulated many further experimental and theoretical studies [4–7]. Recently, the evaporative cooling of dilute Fermi gases has been achieved using magnetic confinement techniques [8]. In these experiments, the interactions between atoms are weak. For dilute spin-polarized Fermi gases in the same hyperfine state, the Pauli exclusion principle forbids two-body s -wave scattering. The only remaining interaction is the dipole–dipole interaction between atoms, which is usually negligible. Therefore, a noninteracting Fermi gas is a very good approximation to an ultracold spin-polarized Fermi gas. This contrasts

strongly with the dilute ultracold Bose gas, where the weak interactions between atoms have pronounced effects.

Since the noninteracting Fermi gas can be used for comparison with the experimental results, there exist enormous investigations on the thermodynamic properties using the Thomas–Fermi approximation [9], the path-integration approach [10] and numerical calculations [11]. Recently, the ground state particle and kinetic energy densities for noninteracting Fermi gases in d -dimensional harmonic traps have been obtained using an inverse Laplace transform [12]. Very recently, the exact particle and energy densities for the trapped noninteracting Bose gas and for the trapped noninteracting Fermi gas with chemical potential less than the ground state energy have been obtained [13]. In this paper, we apply the Laplace transform method to the finite temperature noninteracting Fermi gas in a harmonic trap.

2. Formulation of the problem

The single-particle Schrödinger equation reads

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 \right] \psi_i(\vec{r}) = E_i \psi_i(\vec{r}) \quad (1)$$

with

$$E_i = \hbar\omega(l_1 + \cdots + l_d + d/2) \quad l_1, \dots, l_d = 0, 1, 2, \dots \quad (2)$$

and

$$\psi_i(\vec{r}) = \phi(l_1, \omega, x_1) \cdots \phi(l_d, \omega, x_d) \quad (3)$$

where d is the spatial dimension, $\phi(l, \omega, x)$ are the wavefunctions of one-dimensional harmonic oscillator,

$$\phi(l, \omega, x) = \left[\frac{m\omega}{\pi\hbar(2^l l!)} \right]^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_l\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \quad (4)$$

and

$$H_l(z) = (-1)^l e^{z^2} \frac{d^l}{dz^l} e^{-z^2}. \quad (5)$$

The single-particle density matrix is [14, 15]

$$\begin{aligned} C(d; \vec{r}, \vec{r}'; \beta) &= \sum_i \psi_i^*(\vec{r}') \psi_i(\vec{r}) e^{-\beta E_i} = \left[\frac{m\omega}{2\pi\hbar \sinh(\beta\hbar\omega)} \right]^{d/2} \\ &\times \exp\left\{ -\frac{m\omega}{4\hbar} [(\vec{r} + \vec{r}')^2 \tanh(\beta\hbar\omega/2) + (\vec{r} - \vec{r}')^2 \coth(\beta\hbar\omega/2)] \right\} \end{aligned} \quad (6)$$

where $\beta = 1/k_B T$.

The particle and energy densities are given by

$$\rho(\vec{r}) = g \sum_i |\psi_i(\vec{r})|^2 \frac{1}{e^{\beta(E_i - \mu)} + 1} \quad (7)$$

and

$$e(\vec{r}) = g \sum_i |\psi_i(\vec{r})|^2 E_i \frac{1}{e^{\beta(E_i - \mu)} + 1} \quad (8)$$

where the factor g accounts for spin. The chemical potential μ is determined by the total number of particles $N = g \sum_i 1/[e^{\beta(E_i - \mu)} + 1]$.

The kinetic energy density is given by

$$e_K(\vec{r}) = e(\vec{r}) - \frac{1}{2}m\omega^2 r^2 \rho(\vec{r}). \tag{9}$$

Substituting equations (3) and (4) into (7) gives

$$\begin{aligned} \rho(\vec{r}) = g \left[\frac{m\omega}{\pi\hbar} \right]^{d/2} \exp\left(-\frac{m\omega}{\hbar} r^2\right) \sum_{l_1, l_2, \dots, l_d=0}^{\infty} \frac{1}{2^{l_1+l_2+\dots+l_d} l_1! l_2! \dots l_d!} H_{l_1}^2\left(\sqrt{\frac{m\omega}{\hbar}} x_1\right) \\ \times H_{l_2}^2\left(\sqrt{\frac{m\omega}{\hbar}} x_2\right) \dots H_{l_d}^2\left(\sqrt{\frac{m\omega}{\hbar}} x_d\right) \frac{1}{e^{\beta[\hbar\omega(l_1+\dots+l_d+d/2)-\mu]} + 1}. \end{aligned} \tag{10}$$

From equation (5) we see that for l large enough, the explicit expressions of H_l are not available. Hence, the evaluation of equation (10) by summing over Hermite polynomials is not feasible. We must seek a method to evaluate equations (7) and (8).

The particle and energy densities are given by the following.

Theorem 1. For the weak degenerate case $\mu < E_0$, we have

$$\rho(\vec{r}) = g \sum_{n=1}^{\infty} (-1)^{n+1} e^{n\beta\mu} C(d; \vec{r}, \vec{r}; n\beta) \tag{11}$$

and

$$e(\vec{r}) = -g \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n} e^{n\beta\mu} \frac{\partial}{\partial\beta} C(d; \vec{r}, \vec{r}; n\beta). \tag{12}$$

This result is obtained in [13].

Proof. Since $E_i > \mu$, in equations (7) and (8) we may expand $1/[e^{\beta(E_i-\mu)} + 1]$ as a power series in $e^{-\beta(E_i-\mu)}$. Making use of equation (6), we obtain the desired results. \square

Theorem 2. For the strong degenerate case $\mu > E_0$, $\rho(\vec{r})$ is given by

$$\rho(\vec{r}) = g \sum_{n=0}^{\infty} (-1)^n \mathcal{L}_\mu^{-1} \left[\frac{C(d; \vec{r}, \vec{r}; \beta')}{\beta' + n\beta} \right] + g \sum_{n=1}^{\infty} (-1)^n \mathcal{L}_\mu^{-1} \left[\frac{C(d; \vec{r}, \vec{r}; \beta')}{\beta' - n\beta} \right] \Big|_{\text{Re}(\beta' - n\beta) < 0}. \tag{13}$$

Here the Laplace transform is defined as follows [16]. Let $f(x)$ be a real function defined in the interval $(0, \infty)$ such that $f(x)$ is piecewise continuous and $|f(x)| < M e^{c_1 x}$. Here $M > 0$ and $c_1 > 0$ are constants. The Laplace transform of $f(x)$ is defined by

$$\mathcal{L}(f) \equiv h(s) = \int_0^\infty e^{-sx} f(x) dx \tag{14}$$

where the integration is convergent in the half-plane $\text{Re}(s) > c_1$. $h(s)$ is an analytic function of s in the domain $\text{Re}(s) > c_1$. The inverse Laplace transform is given by

$$f(x) = \mathcal{L}^{-1}h(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{sx} h(s) ds \quad x > 0 \tag{15}$$

and

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{sx} h(s) ds = 0 \quad x < 0 \tag{16}$$

where $c > c_1$.

Proof. In equation (7), Taylor expanding $1/[e^{\beta(E_i-\mu)} + 1]$, we obtain

$$\begin{aligned} \rho(\vec{r}) &= g \sum_{n=0}^{\infty} (-1)^n \sum_i |\psi_i(\vec{r})|^2 e^{n\beta(E_i-\mu)} \Theta(-E_i + \mu) \\ &\quad + g \sum_{n=1}^{\infty} (-1)^{n+1} \sum_i |\psi_i(\vec{r})|^2 e^{-n\beta(E_i-\mu)} \Theta(E_i - \mu) \end{aligned} \tag{17}$$

where $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$.

From equation (6) we obtain

$$\begin{aligned} C(d; \vec{r}, \vec{r}; \beta') &= \sum_i |\psi_i(\vec{r})|^2 e^{-\beta' E_i} = \int_{E_0}^{\infty} dE D(E) |\psi_E(\vec{r})|^2 e^{-\beta' E} \\ &= \mathcal{L}_{\beta'} [D(E) |\psi_E(\vec{r})|^2] \end{aligned} \tag{18}$$

where $D(E)$ is the state density. Applying an inverse Laplace transform to equation (18) gives

$$D(E) |\psi_E(\vec{r})|^2 = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta' e^{\beta' E} C(d; \vec{r}, \vec{r}; \beta') = \mathcal{L}_E^{-1} C(d; \vec{r}, \vec{r}; \beta') \tag{19}$$

so that

$$\begin{aligned} \sum_i |\psi_i(\vec{r})|^2 e^{n\beta(E_i-\mu)} \Theta(-E_i + \mu) &= |\psi_0(\vec{r})|^2 e^{n\beta(E_0-\mu)} + \int_{E_0}^{\mu} dE D(E) |\psi_E(\vec{r})|^2 e^{n\beta(E-\mu)} \\ &= |\psi_0(\vec{r})|^2 e^{n\beta(E_0-\mu)} + \int_{E_0}^{\mu} dE e^{n\beta(E-\mu)} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta' e^{\beta' E} C(d; \vec{r}, \vec{r}; \beta') \\ &= |\psi_0(\vec{r})|^2 e^{n\beta(E_0-\mu)} - e^{n\beta(E_0-\mu)} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta' e^{\beta' E_0} C(d; \vec{r}, \vec{r}; \beta') \frac{1}{\beta' + n\beta} \\ &\quad + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta' e^{\beta' \mu} C(d; \vec{r}, \vec{r}; \beta') \frac{1}{\beta' + n\beta} = \mathcal{L}_{\mu}^{-1} \left[C(d; \vec{r}, \vec{r}; \beta') \frac{1}{\beta' + n\beta} \right] \end{aligned} \tag{20}$$

and

$$\begin{aligned} \sum_i |\psi_i(\vec{r})|^2 e^{-n\beta(E_i-\mu)} \Theta(E_i - \mu) &= \int_{\mu}^{\infty} dE e^{-n\beta(E-\mu)} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta' e^{\beta' E} C(d; \vec{r}, \vec{r}; \beta') \\ &= -\mathcal{L}_{\mu}^{-1} \left[\frac{C(d; \vec{r}, \vec{r}; \beta')}{\beta' - n\beta} \right] \Big|_{\text{Re}(\beta' - n\beta) < 0} \end{aligned} \tag{21}$$

where $E_0 = \hbar\omega d/2$ and $\psi_0(\vec{r}) = (m\omega/\pi\hbar)^{d/4} \exp(-m\omega r^2/2\hbar)$ are the energy and wavefunction of the ground state, respectively. By arriving at equation (20), we use the relation

$$|\psi_0(\vec{r})|^2 = \mathcal{L}_{E_0}^{-1} \left[C(d; \vec{r}, \vec{r}; \beta') \frac{1}{\beta' + n\beta} \right]. \tag{22}$$

□

Theorem 3. For $\mu > E_0$, $e(\vec{r})$ is given by

$$e(\vec{r}) = -g \sum_{n=0}^{\infty} (-1)^n \mathcal{L}_{\mu}^{-1} \left[\frac{1}{\beta' + n\beta} \frac{\partial C(d; \vec{r}, \vec{r}; \beta')}{\partial \beta'} \right] - g \sum_{n=1}^{\infty} (-1)^n \mathcal{L}_{\mu}^{-1} \left[\frac{1}{\beta' - n\beta} \frac{\partial C(d; \vec{r}, \vec{r}; \beta')}{\partial \beta'} \right] \Big|_{\text{Re}(\beta' - n\beta) < 0}. \tag{23}$$

Proof. Making use of

$$-\frac{\partial C(d; \vec{r}, \vec{r}; \beta')}{\partial \beta'} = \sum_i |\psi_i(\vec{r})|^2 E_i e^{-\beta' E_i} \tag{24}$$

and

$$E_0 |\psi_0(\vec{r})|^2 = -\mathcal{L}_{E_0}^{-1} \left[\frac{1}{\beta' + n\beta} \frac{\partial C(d; \vec{r}, \vec{r}; \beta')}{\partial \beta'} \right] \tag{25}$$

and following the same procedure as in the proof of theorem 1, we obtain the result. \square

3. The inverse Laplace transform

The above inverse Laplace transforms are obtained using the following lemmas.

Lemma 1. For $\beta > 0$, $C(d; \vec{r}, \vec{r}; \beta)$ may be expanded as a power series in $e^{-\beta \hbar \omega}$,

$$C(d; \vec{r}, \vec{r}; \beta) = |\psi_0(\vec{r})|^2 \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \times \sum_{k=0}^{\infty} \frac{\Gamma(d/2 + k)}{k! \Gamma(d/2)} [e^{\beta \hbar \omega(-j-2k-d/2)} + e^{\beta \hbar \omega(-j-1-2k-d/2)}] \tag{26}$$

where the Laguerre polynomials are defined by

$$L_n^\alpha(x) = \frac{1}{n!} e^x x^{-\alpha} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha}) = \sum_{m=0}^n (-1)^m \binom{n+\alpha}{n-m} \frac{x^m}{m!} \tag{27}$$

with

$$\binom{p}{n} = \frac{p(p-1)\cdots(p-n+1)}{n!} \quad \binom{p}{0} = 1 \tag{28}$$

$$L_n(x) \equiv L_n^0(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n} (e^{-x} x^n) = \sum_{m=0}^n (-1)^m \binom{n}{n-m} \frac{x^m}{m!} \tag{29}$$

and $L_0^\alpha(x) = 1$.

In order to evaluate the inverse Laplace transforms in equations (13) and (23), we need the analytical continuation of $C(d; \vec{r}, \vec{r}; \beta)$ from the smaller region $\beta > 0$ to the larger region $\text{Re}(\beta) > 0$. This is fulfilled using the Weierstrass analytical continuation method and the power series representation of $C(d; \vec{r}, \vec{r}; \beta)$. In this way, we obtain, for example,

$$\mathcal{L}_{\mu}^{-1} \left[\frac{C(d; \vec{r}, \vec{r}; \beta')}{\beta' + n\beta} \right] = |\psi_0(\vec{r})|^2 \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \times \sum_{k=0}^{\infty} \frac{\Gamma(d/2 + k)}{k! \Gamma(d/2)} \mathcal{L}_{\mu}^{-1} \left[\frac{e^{\beta \hbar \omega(-j-2k-d/2)} + e^{\beta \hbar \omega(-j-1-2k-d/2)}}{\beta' + n\beta} \right]. \tag{30}$$

Proof. Making use of the mathematical identity [17]

$$(1 - z)^{-\alpha-1} \exp\left[x \frac{z}{z-1}\right] = \sum_{n=0}^{\infty} L_n^\alpha(x) z^n \quad |z| < 1 \tag{31}$$

we obtain

$$\exp[-x \tanh(y/2)] = e^{-x} \sum_{j=0}^{\infty} (-1)^j L_j(2x) [e^{-jy} + e^{-(j+1)y}]. \tag{32}$$

Using equation (32) and the mathematical identity [17]

$$(1 - z)^{-p} = \sum_{k=0}^{\infty} \frac{\Gamma(p+k)}{k! \Gamma(p)} z^k \quad p > 0 \quad |z| < 1 \tag{33}$$

we obtain the desired result. □

Lemma 2.

$$\mathcal{L}_\mu^{-1} \left[\frac{A(\beta')}{\beta' - n\beta} \right] \Big|_{\text{Re}(\beta' - n\beta) < 0} = \mathcal{L}_\mu^{-1} \left[\frac{A(\beta')}{\beta' - n\beta} \right] \Big|_{\text{Re}(\beta' - n\beta) > 0} - e^{n\beta\mu} A(n\beta) \tag{34}$$

where $A(\beta') = C(d; \vec{r}, \vec{r}; \beta')$ or $\frac{\partial}{\partial \beta'} C(d; \vec{r}, \vec{r}; \beta')$.

These results are evident using the residue theorem.

Lemma 3. For real constants a and b , we have

$$\mathcal{L}_\lambda^{-1} \left[\frac{e^{a\beta'}}{\beta' - b} \right] \Big|_{\text{Re}(\beta' - b) > 0} = e^{b(\lambda+a)} \Theta(\lambda + a). \tag{35}$$

This result is evident using the residue theorem and equation (16).

4. Formulae of particle and energy densities

Collecting the above results, we obtain

Theorem 5. For $\mu > E_0$, we have

$$\begin{aligned} \rho(\vec{r}) &= g |\psi_0(\vec{r})|^2 \sum_{n=0}^{\infty} (-1)^n \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \\ &\times \sum_{k=0}^{\infty} \frac{\Gamma(d/2+k)}{k! \Gamma(d/2)} [e^{-n\beta\hbar\omega(\mu/\hbar\omega - j - 2k - d/2)} \Theta(\mu/\hbar\omega - j - 2k - d/2) \\ &- (1 - \delta_{n,0}) e^{-n\beta\hbar\omega(-\mu/\hbar\omega + j + 2k + d/2)} \Theta(-\mu/\hbar\omega + j + 2k + d/2) \\ &+ (j \rightarrow j + 1)] \end{aligned} \tag{36}$$

and

$$\begin{aligned} e(\vec{r}) &= -g\hbar\omega |\psi_0(\vec{r})|^2 \sum_{n=0}^{\infty} (-1)^n \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \sum_{k=0}^{\infty} \frac{\Gamma(d/2+k)}{k! \Gamma(d/2)} \\ &\times [(-j - 2k - d/2) e^{-n\beta\hbar\omega(\mu/\hbar\omega - j - 2k - d/2)} \Theta(\mu/\hbar\omega - j - 2k - d/2) \\ &- (1 - \delta_{n,0})(-j - 2k - d/2) e^{-n\beta\hbar\omega(-\mu/\hbar\omega + j + 2k + d/2)} \\ &\times \Theta(-\mu/\hbar\omega + j + 2k + d/2) + (j \rightarrow j + 1)] \end{aligned} \tag{37}$$

where

$$\sum_{n,j,k} [f(n, j, k) + (j \rightarrow j + 1)] \equiv \sum_{n,j,k} [f(n, j, k) + f(n, j + 1, k)]. \tag{38}$$

Corollary. At absolute zero, equations (36) and (37) reduce to

$$\begin{aligned} \rho(\vec{r}) &= g|\psi_0(\vec{r})|^2 \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \sum_{k=0}^{\infty} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} \\ &\times [\Theta(\mu/\hbar\omega - j - 2k - d/2) + \Theta(\mu/\hbar\omega - j - 1 - 2k - d/2)] \end{aligned} \tag{39}$$

and

$$\begin{aligned} e(\vec{r}) &= -g\hbar\omega|\psi_0(\vec{r})|^2 \sum_{j=0}^{\infty} (-1)^j L_j(2m\omega r^2/\hbar) \sum_{k=0}^{\infty} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} \\ &\times [(-j - 2k - d/2)\Theta(\mu/\hbar\omega - j - 2k - d/2) \\ &+ (-j - 1 - 2k - d/2)\Theta(\mu/\hbar\omega - j - 1 - 2k - d/2)]. \end{aligned} \tag{40}$$

Let $\mu/\hbar\omega = M + d/2$, $M = 0, 1, 2, \dots$. Equations (39) and (40) reduce to

$$\begin{aligned} \rho(\vec{r}) &= g|\psi_0(\vec{r})|^2 \left[\sum_{k=0}^{\text{Int}(M/2)} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} (-1)^{M-2k} L_{M-2k}(2m\omega r^2/\hbar) \right. \\ &\left. + \sum_{k=0}^{\text{Int}[(M-1)/2]} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} \sum_{j=0}^{M-1-2k} 2(-1)^j L_j(2m\omega r^2/\hbar) \right] \end{aligned} \tag{41}$$

$$\begin{aligned} e(\vec{r}) &= g\hbar\omega|\psi_0(\vec{r})|^2 \left[(M + d/2) \sum_{k=0}^{\text{Int}(M/2)} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} (-1)^{M-2k} \right. \\ &\times L_{M-2k}(2m\omega r^2/\hbar) + \sum_{k=0}^{\text{Int}[(M-1)/2]} \frac{\Gamma(d/2+k)}{k!\Gamma(d/2)} \\ &\left. \times \sum_{j=0}^{M-1-2k} (2j + 1 + 4k + d)(-1)^j L_j(2m\omega r^2/\hbar) \right] \end{aligned} \tag{42}$$

where $\text{Int}(M/2)$ is the integer part of $M/2$.

Theorem 6. For any μ and hence for any temperature, the particle and energy densities are still given by equations (36) and (37).

This result is evident since, for $\mu < E_0$, equations (36) and (37) reduce to (11) and (12), respectively.

5. Conclusion

The explicit expressions of Hermite polynomials with order large enough are not available. Hence, the evaluation of the particle and energy densities for a noninteracting Fermi gas at any temperature in a d -dimensional harmonic trap by summing over Hermite polynomials is not feasible. We have used the Laplace transform method to obtain the analytical results. The

particle and energy densities are expressed by two special functions, i.e. the gamma function and the Laguerre polynomials. The obtained formulae are rapidly converging series that are valid in the weak and strong degenerate regimes, including the absolute zero limit. So it is convenient to carry out numerical calculations. The advantage of our method is that we make use of the simple expressions of the density matrix of a harmonic oscillator and, hence, avoid the tedious process of summing over Hermite polynomials.

Because of the Pauli exclusion principle, spin-polarized Fermi atoms in the same hyperfine sublevel do not interact through s-wave collisions. The noninteracting Fermi gas is a very good approximation to an ultracold spin-polarized Fermi gas. Therefore, these analytical expressions can be used for the comparison with the experimental results. Furthermore, these exact expressions are useful for the test of the local density approximation.

Acknowledgment

This research is supported by the Excellent Young Teachers Program of the Ministry of Education of China.

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