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The ground-state energy of an attractive Fermi gas along the Bardeen–Cooper–Schrieffer-unitarity crossover

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Abstract

The ratio $f(x)$ of the ground-state energy of an attractive Fermi gas to that of the noninteracting Fermi gas is a smooth and continuous function of $x = k_F a$ in the Bardeen–Cooper–Schrieffer (BCS)-unitarity crossover regime $-\infty < x \leqslant 0$. Here $k_F\hbar$ is the Fermi momentum, $\hbar$ is the Planck constant and a is the s-wave scattering length. The respective coefficients of the perturbation expansions of $f(x)$ in the BCS regime and in the unitary regime are expected to be related to each other. Unitary Fermi gases are expected to exhibit universal behaviors. So $f(-\infty)$ is universal and is only a function of the universal coefficients of the perturbation expansion of $f(x)$ in the BCS regime. Using these facts, we extend the perturbation expansion of $f(x)$ in the BCS regime to the BCS-unitarity crossover regime. $f(-\infty)$ is predicted to be 0.400 98 (0.422 94) for the Bose (Fermi) function, which are in good agreement with the quantum Monte Carlo results and the experimental results.

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1. Introduction

Recent experiments on two-component ultracold atomic Fermi gases near a Feshbach resonance have realized the crossover from a Bose–Einstein condensate (BEC) to a Bardeen–Cooper–Schrieffer (BCS) superfluid [1–16]. In these systems the interaction strength can be varied over a very wide range by magnetically tuning the two-body scattering length. For a dilute spin-1/2 Fermi gas with the interparticle distance much larger than the interaction range r_0, the interaction is predominantly determined by the s-wave scattering length a [3]. The physically relevant coupling parameter is $k_F a$. Here $k_F\hbar$ is the Fermi momentum and $\hbar$ is the Planck constant. For $a > 0$, fermionic atoms with opposite spins can form bound bosonic molecules. At a sufficiently low temperature, these bosonic molecules can condense. The molecular BEC state for $a > 0$ can be adiabatically converted into an ultracold Fermi gas with $a < 0$. For $a < 0$, at a sufficiently low temperature, fermionic atoms with opposite spins can form pairs and these pairs can condense. For $0 < -k_F a \ll 1$, standard BCS theory is expected to apply.

Of particular interest is the unitary limit $k_F a \to \pm\infty$. The details of the microscopic interaction include the two-body collisions (the two-body s-wave scattering length a, the interaction range r_0, etc), the three-body collisions and the more-body collisions. Let the characteristic length of the n-body collision be R_n ($n \geqslant 3$). At unitarity $a \to \pm\infty$, we have $\lim_{a\to\pm\infty} r_0/a = 0$ and $\lim_{a\to\pm\infty} R_n/a = 0$, which implies that the details of the microscopic interaction are lost. Hence unitary Fermi gases with any attractive short-range two-body interaction are expected to exhibit universal behaviors, which is the universality hypothesis [1, 2]. Although no rigorous proof of the universality hypothesis exists, the quantum Monte Carlo calculations [9–11] and the experimental results [12–16] all support this hypothesis. The universality hypothesis asserts that the only relevant physical parameter for the ground state is k_F and the ratio C of the ground-state energy of a unitary Fermi gas to that of the noninteracting Fermi gas is a universal quantity. There are many analytical, numerical and experimental researches for the determination of C. The Padé approximations [1/1] and [2/2] predict $C = 0.326, 0.568$, respectively [4, 5]. Here the Padé approximation $[L/M]$ is defined by

$$[L/M] = \frac{W_0 + W_1 x + \cdots + W_L x^L}{1 + V_1 x + \cdots + V_M x^M}, \tag{1}$$

where $W_0, W_1, \ldots, W_L$ and $V_1, \ldots, V_M$ are the coefficients.

The ϵ expansion [6] predicts $C = 0.475$. The mean-field BCS theory [7] predicts $C = 0.59$. The recent mean-field calculation considering quantum fluctuations [8] predicts $C = 0.40$. The most reliable estimates are the quantum Monte Carlo results: $C = 0.44 \pm 0.01$ [9], 0.42 ± 0.01 [10], 0.40 ± 0.01 [11]. The four recent experimental results are $C = 0.36 \pm 0.15$ [13], 0.51 ± 0.04 [14], 0.46 ± 0.05 [15] and $0.46^{+0.05}_{-0.12}$ [16]. In this paper, we will propose a new approach to the present problem.

2. Basic approach

The ground-state energy E_0 of a spin-1/2 dilute Fermi gas with attractive short-range two-body potential is a function of $k_F a$,

$$E_0 = N \frac{3}{10} \frac{\hbar^2 k_F^2}{m} f(k_F a), \tag{2}$$

where $k_F = (3\pi^2 N/V)^{1/3}$, m is the mass of a fermion, N is the number of fermions and V is the volume of the system. For a dilute Fermi gas, only the two-body collisions are important. Since the ground-state energy is low, usually only the s-wave scattering is important, which is completely determined by the scattering length a. So $f(x)$ depends predominantly on $x = k_F a$. Of course, $f(x)$ also depends weakly on $k_F r_0$ and $k_F R_n$ ($n \geqslant 3$). Therefore $f(x)$ is an almost universal function of x and is weakly dependent on the details of the microscopic interaction. Although $f(x)$ is not known, $f(x)$ must satisfy some conditions.

In the BCS regime $0 < -x \ll 1$, the superfluid contribution to the ground-state energy is exponentially small and is negligible [1]. Hence $f(x)$ is essentially identical to the perturbation series of a dilute spin-1/2 Fermi gas with repulsive short-range two-body potential [17, 18], with $x < 0$, i.e.,

$$f(x) = 1 + \sum_{j=1}^{\infty} b_j x^j, \qquad 0 \leqslant -x \ll 1. \tag{3}$$

where $b_1 = 10/9\pi$ and $b_2 = 4(11 - 2\ln 2)/21\pi^2$ [17] are independent of the details of the interaction potential and hence are universal, b_j $(j \geqslant 3)$ are not universal and are dependent on the details of the interaction potential [1]. For an attractive zero-range square-well potential, Baker [4] obtained $b_3 = 0.030\,4667$ and $b_4 = -0.062\,0133$.

For dilute Bose gases with short-range repulsive potential, there are also non-universal effects [19–22],

$$E_0 = N\frac{2\pi\hbar^2}{m}\rho a[1 + A_1(\rho a^3)^{1/2} + A_2\rho a^3\ln(\rho a^3) + A_3\rho a^3 + \cdots], \qquad \rho a^3 \ll 1 \tag{4}$$

where $\rho = N/V$, $A_1 = 128/15\sqrt{\pi}$ and $A_2 = 8(4\pi/3 - \sqrt{3})$ are universal, A_3 and higher coefficients are not universal.

Equation (4) is a low-density expansion of a repulsive Bose gas. The first term was obtained by Lenz [19]. The second term was obtained by Lee *et al* [20]. The third term was obtained by Wu [21]. Hugenholtz and Pines [22] showed that the coefficients of the higher-order terms are not universal and are dependent on the details of the potential.

Let us explain why b_1, b_2, A_1 and A_2 are universal numbers while higher coefficients are not universal numbers. The reason is that for dilute Fermi and Bose gases, only the two-body collisions are important. Since the ground-state energy is low, usually only the s-wave scattering is important, which is completely determined by the scattering length a. So the low-order terms depend only on $(N/V)^{1/3}a$. Hence b_1, b_2, A_1 and A_2 are universal numbers. However, the higher-order terms not only depend on $(N/V)^{1/3}a$, but also depend on $(N/V)^{1/3}r_0$ and $(N/V)^{1/3}R_n$ $(n \geqslant 3)$. So b_j and A_j $(j \geqslant 3)$ are not universal numbers.

In the unitary regime $-x \gg 1$, $1/x$ is small. Therefore $f(x)$ is expected to be expanded as a power series in $1/x$, i.e.,

$$f(x) = C + \sum_{j=1}^{\infty}\frac{C_j}{x^j}, \qquad -x \gg 1. \tag{5}$$

where C and C_j are constants. The universality hypothesis asserts that $C = f(-\infty)$ is a universal quantity.

In the unitary regime $-x \gg 1$, the ϵ expansion [23] gives $f(x) = 0.475 - 0.884/x - 0.833/x^2$, which supports the perturbation expansion equation (5).

The BCS–BEC crossover of a Fermi gas with attractive short-range two-body interaction is smooth. $f(x)$ is a smooth and continuous function of x in the BCS-unitarity crossover regime $-\infty < x \leqslant 0$. The perturbation expansions of $f(x)$ in the BCS regime and in the unitary regime are different portions of a single continuous curve. So the coefficients C and $C_1, C_2, \ldots, C_j, \ldots$ of the perturbation expansion of $f(x)$ in the unitary regime are expected to be related to the coefficients $b_1, b_2, \ldots, b_n, \ldots$ of the perturbation expansion of $f(x)$ in the BCS regime, i.e., $C = C(b_1, b_2, \ldots, b_n, \ldots)$ and $C_j = C_j(b_1, b_2, \ldots, b_n, \ldots)$. However, b_1, b_2 and C are universal quantities. So C is independent of the non-universal quantities b_n $(n \geqslant 3)$ and is only dependent on b_1 and b_2, i.e., $C = C(b_1, b_2)$, which is the universality condition.

In order to extend the perturbation expansion equation (3) in the BCS regime to the BCS-unitarity crossover regime, let us construct a function that can be expanded as a power series in x for small x and in $1/x$ for large x, respectively, i.e.,

$$\Phi_\theta(\alpha x) = \int_0^\infty y^{\theta-1}G(y)e^{\alpha xy}\,dy, \qquad -\infty < x \leqslant 0, \qquad \alpha > 0, \theta \geqslant 1 \tag{6}$$

with

$$\Phi_\theta(\alpha x) = \sum_{j=0}^{\infty}\frac{\Phi_{\theta+j}(0)}{j!}(\alpha x)^j, \qquad 0 < -\alpha x \ll 1 \tag{7}$$

$$\Phi_\theta(\alpha x) = \sum_{j=0}^{\infty} \frac{\Gamma(\theta + j)G^{(j)}(0)}{j!} \frac{1}{(-\alpha x)^{\theta+j}}, \qquad -\alpha x \gg 1 \tag{8}$$

where $G(y)$ is not known. For $0 < y \ll 1$, $G(y)$ is required to be expanded as a power series in y, i.e., $G(y) = \sum_{j=0}^{\infty} G^{(j)}(0)y^j/j!$, with $G^{(j)}(0) \neq 0$. For $y \gg 1$, $G(y)$ is required to be so small that the integral $\int_0^\infty y^{\theta-1}G(y)\mathrm{d}y = \Phi_\theta(0)$ is convergent.

Here it is necessary that Φ_θ should include a parameter α. The role played by α is that through α, the respective coefficients of the two expansions of $\Phi_\theta(\alpha x)$ for small x and for large x are related to each other.

In equation (3), we replace b_j by $\sum_{n=j}^{\infty} A_{nj}\Phi_n(\alpha x)$, which gives

$$f(x) = 1 + \sum_{j=1}^{\infty} x^j \sum_{n=j}^{\infty} A_{nj}\Phi_n(\alpha x), \qquad -\infty < x \leqslant 0 \tag{9}$$

with

$$b_1 = \sum_{n=1}^{\infty} A_{n1}\Phi_n(0), \qquad b_2 = \sum_{n=1}^{\infty}(A_{n+1,2} + \alpha A_{n1})\Phi_{n+1}(0), \tag{10}$$

$$C = \sum_{n=1}^{\infty} A_{nn}(n-1)!G(0)\frac{1}{(-\alpha)^n}. \tag{11}$$

where A_{nj} are constants.

Substituting equation (10) into the universality condition $C = C(b_1, b_2)$, we obtain $C = C(\{A_{n1}, A_{n2}\})$. Equation (11) gives $C = C(\{A_{nn}\})$. Comparing the resulting two equations, we obtain $C = C(A_{11}, A_{22})$, $A_{n1} = 0$, $(n \geqslant 2)$, $A_{n2} = 0$, $(n \geqslant 3)$, $A_{nn} = 0$, $(n \geqslant 3)$ and

$$f(x) = 1 + A_{11}x\Phi_1(\alpha x) + A_{22}x^2\Phi_2(\alpha x) + \sum_{j=3}^{\infty} x^j \sum_{n=j+1}^{\infty} A_{nj}\Phi_n(\alpha x). \tag{12}$$

It is reasonable to require that $f(x)$ satisfy the condition of the uniqueness of the solution, i.e., the coefficients $A_{11}, A_{22}, A_{43}, \ldots$ in equation (12) as well as C and $C_1, C_2, \ldots, C_j, \ldots$ be uniquely determined by the coefficients $b_1, b_2, \ldots, b_n, \ldots$. This gives

$$A_{nj} = 0 \qquad (n \neq 2j-2), \qquad C = C(b_1, b_2), \qquad C_n = C_n(b_1, b_2, \ldots, b_{n+2}),$$

$$f(x) = 1 + A_{11}x\Phi_1(\alpha x) + A_{22}x^2\Phi_2(\alpha x) + \sum_{j=3}^{\infty} A_{2j-2,j}x^j\Phi_{2j-2}(\alpha x), \tag{13}$$

$$A_{11} = \frac{b_1}{\Phi_1(0)}, \qquad A_{22} = \frac{b_2}{\Phi_2(0)} - \frac{b_1\alpha}{\Phi_1(0)}, \qquad C = 1 - \frac{2b_1G(0)}{\Phi_1(0)\alpha} + \frac{b_2G(0)}{\Phi_2(0)\alpha^2}.$$

Since the ground-state energy is an absolute minimum, the parameter α is determined by the minimum condition $\partial C/\partial\alpha = 0$, which gives

$$\alpha = \frac{\Phi_1(0)b_2}{\Phi_2(0)b_1}, \qquad A_{22} = 0, \qquad C = 1 - \frac{G(0)\Phi_2(0)b_1^2}{[\Phi_1(0)]^2b_2}, \tag{14}$$

$$f(x) = 1 + A_{11}x\Phi_1(\alpha x) + \sum_{j=3}^{\infty} A_{2j-2,j}x^j\Phi_{2j-2}(\alpha x), \tag{15}$$

with

$$f(x) = 1 + A_{11}\Phi_1(0)x + A_{11}\alpha\Phi_2(0)x^2 + \sum_{n=3}^{\infty}\left[\frac{A_{11}\alpha^{n-1}}{(n-1)!}\Phi_n(0) + \sum_{j=3}^{n}\frac{A_{2j-2,j}\alpha^{n-j}}{(n-j)!}\Phi_{n+j-2}(0)\right]x^n, \qquad 0 < -x \ll 1 \tag{16}$$

$$f(x) = 1 - \frac{A_{11}G(0)}{\alpha} + \sum_{n=1}^{\infty}\left[\frac{A_{11}G^{(n)}(0)}{(-\alpha)^{1+n}} + \sum_{j=3}^{n+2}\frac{A_{2j-2,j}}{(n+2-j)!(-\alpha)^{n+j}}\Gamma(n+j)G^{(n+2-j)}(0)\right]\frac{1}{x^n}, \qquad -x \gg 1. \tag{17}$$

From the above we see that through replacing b_j in equation (3) by $\sum_{n=j}^{\infty} A_{nj}\Phi_n(\alpha x)$, we extend the small-$x$ expansion of $f(x)$ in the BCS regime to the BCS-unitarity crossover regime. Indeed, the replacement leads to equation (15) with the two expansion equations (16) and (17), which are the required results.

3. Predictions and comparison

3.1. Determination of $G(y)$

$G(y)$ is not known. There exists an infinity of possible functions of $G(y)$ that satisfy the requirements stated. In order to find some hints to determine $G(y)$, let us recall that for a solid, the phonon frequency distribution function $g(\omega)$ can be expanded as a power series in ω^2 for small frequency ω [24, 25], i.e.,

$$g(\omega) = \sum_{j=1}^{\infty}\eta_j\omega^{2j}, \qquad \omega \sim 0 \tag{18}$$

where η_j are constants. At a sufficiently low temperature, the energy $E(T)$ of a solid (an ideal Bose gas of phonons) is given by

$$E(T) = E(0) + \sum_{j=1}^{\infty}\eta_j\hbar\left(\frac{k_BT}{\hbar}\right)^{2j+2}\int_0^{\infty}\frac{y^{2j+1}}{\mathrm{e}^y - 1}\,\mathrm{d}y, \qquad T \sim 0\ \mathrm{K}, \tag{19}$$

where k_B is the Boltzmann constant and T is the absolute temperature.

At a sufficiently low temperature, the energy $E(T)$ of an ideal spin-1/2 Fermi gas [26] is given by

$$E(T) = \frac{3}{5}N\mu\left[1 + \sum_{j=0}^{\infty}w_j\left(\frac{k_BT}{\mu}\right)^{2j+2}\int_0^{\infty}\frac{y^{2j+1}}{\mathrm{e}^y + 1}\,\mathrm{d}y\right], \qquad T \ll \mu/k_B, \tag{20}$$

where $w_j = [5/(2j+1)!]\prod_{i=0}^{j-1}(3/2 - i)$ and μ is the chemical potential.

We see that the coefficients of the low-temperature expansions of the energies of a solid (an ideal Bose gas of phonons) and of an ideal Fermi gas are proportional to the Bose integral $\int_0^{\infty} y^{z-1}(\mathrm{e}^y - 1)^{-1}\,\mathrm{d}y = \Gamma(z)\zeta(z)$ and the Fermi integral $\int_0^{\infty} y^{z-1}(\mathrm{e}^y + 1)^{-1}\,\mathrm{d}y = (1 - 2^{1-z})\Gamma(z)\zeta(z)$, respectively. The coefficients of the small-x expansion equation (16) of

$f(x)$ are linear combinations of $\Phi_\theta(0)$. There are remarkable similarities between the small-x expansion of $f(x)$ and the low-temperature expansions. Hence it is expected that the best approximation of $\Phi_\theta(0)$ should be the Bose or Fermi integral, i.e., the best approximation of $G(y)$ should be either the Bose function $G(y) = y/(\mathrm{e}^y - 1)$ or the Fermi function $G(y) = 1/(\mathrm{e}^y + 1)$.

Here we draw an analogy between the small-x expansion of $f(x)$ and the low-temperature expansions of the energies of solids (ideal Bose gases of phonons) and of ideal Fermi gases. The reason is that the low-temperature expansions involve the Riemann ζ function, which is one of the fundamental functions in nature. It is expected that the best approximation of $\Phi_\theta(\alpha x)$ should also involve the Riemann ζ function.

3.2. Bose function

For the Bose function, we obtain

$$\begin{aligned} &\Phi_\theta(\alpha x) = \Gamma(\theta+1)\zeta(\theta+1, 1-\alpha x), \qquad \alpha = \frac{\pi(11 - 2\ln 2)}{70\zeta(3)} = 0.358\,937, \\ &A_{11} = \frac{20}{3\pi^3} = 0.215\,01, \qquad C = 1 - \frac{1400\zeta(3)}{3\pi^4(11-2\ln 2)} = 0.400\,98, \end{aligned} \tag{21}$$

where $\zeta(t, s)$ is the Riemann ζ function [27]

$$\zeta(t, s) = \frac{1}{\Gamma(t)} \int_0^\infty \frac{y^{t-1}\mathrm{e}^{-(s-1)y}}{\mathrm{e}^y - 1}\,\mathrm{d}y = \sum_{j=0}^{\infty} \frac{1}{(j+s)^t}, \qquad t > 1, s > 0. \tag{22}$$

Using Baker's results $b_3 = 0.030\,4667$ and $b_4 = -0.062\,0133$ [4], we obtain

$$\begin{aligned} f(x) = 1 &+ 0.215\,01x\zeta(2, 1 - 0.358\,937x) \\ &- 0.057\,3593x^3\zeta(5, 1 - 0.358\,937x) + 0.001\,4614x^4\zeta(7, 1 - 0.358\,937x) \\ &+ \sum_{j=5}^{\infty} A_{2j-2,j}\Gamma(2j-1)x^j\zeta(2j-1, 1 - 0.358\,937x). \end{aligned} \tag{23}$$

3.3. Fermi function

For the Fermi function, we obtain

$$\begin{aligned} &\Phi_\theta(\alpha x) = \Gamma(\theta)[\zeta(\theta, 1-\alpha x) - 2^{1-\theta}\zeta(\theta, 1 - \alpha x/2)], \\ &A_{11} = \frac{10}{9\pi \ln 2} = 0.510\,249, \qquad \alpha = \frac{72(11-2\ln 2)\ln 2}{35\pi^3} = 0.442\,111, \\ &C = 1 - \frac{175\pi^2}{648(11 - 2\ln 2)(\ln 2)^2} = 0.422\,94. \end{aligned}$$

Using Baker's results $b_3 = 0.030\,4667$ and $b_4 = -0.062\,0133$ [4], we obtain

$$\begin{aligned} f(x) = 1 &+ 0.510\,249x\Phi_1(0.442\,111x) - 0.010\,4622x^3\Phi_4(0.442\,111x) \\ &+ 0.000\,035\,0405x^4\Phi_6(0.442\,111x) + \sum_{j=5}^{\infty} A_{2j-2,j}x^j\Phi_{2j-2}(0.442\,111x). \end{aligned} \tag{25}$$

Table 1. The ground-state energy $f(k_F a)$ in units of $N3k_F^2/10m$.

$k_F a$	MC1	MC2	$(23)_{(2)}$	$(25)_{(2)}$	$(23)_{(3)}$	$(25)_{(3)}$	$(23)_{(4)}$	$(25)_{(4)}$
$-1/6$	0.94(1)		0.9458	0.9458	0.9460	0.9460	0.9460	0.9460
$-1/4$	0.92(1)		0.9219	0.9219	0.9225	0.9225	0.9225	0.9225
$-1/2$	0.87(1)		0.8604	0.8604	0.8637	0.8637	0.8638	0.8638
-1	0.79(2)		0.7705	0.7706	0.7838	0.7837	0.7840	0.7842
-2.5	0.72(3)	0.65	0.6295	0.6311	0.6720	0.6729	0.6726	0.6747
-5	0.62(3)	0.56	0.5385	0.5434	0.5947	0.5995	0.5955	0.6015
-10		0.48	0.4768	0.4867	0.5257	0.5355	0.5262	0.5367
$-\infty$	0.42(1)	0.40	0.400 98	0.422 94	0.400 98	0.422 94	0.400 98	0.422 94

3.4. Predictions and comparison

The quantum Monte Carlo results [10] (MC1) and [11] (MC2) are listed in table 1. The first two, three and four terms of equations (23) and (25) are represented by $(23)_{(2)}$, $(23)_{(3)}$, $(23)_{(4)}$, $(25)_{(2)}$, $(25)_{(3)}$ and $(25)_{(4)}$, respectively and are listed in table 1. We see that the main contributions to $f(x)$ come from the first two terms, which reflects the fact that $f(x)$ is predominantly dependent on $x = k_F a$ and is an almost universal function of x. The third term makes a little contribution to $f(x)$ and the fourth term makes almost no contribution to $f(x)$, which reflects the fact that $f(x)$ also depends weakly on the details of the microscopic interaction. Hence almost all the contributions to $f(x)$ come from the first three terms. The predictions of the Bose function and of the Fermi function are very close to each other and are in good agreement with the simulation results. Furthermore, the higher-order approximations are in better agreement with the simulation results than the lower-order approximations.

4. Conclusion

The BCS–BEC crossover of a Fermi gas with attractive short-range two-body potential is smooth. The ratio $f(x)$ of the ground-state energy to that of the noninteracting Fermi gas is a smooth and continuous function of $x = k_F a$ in the BCS-unitarity crossover regime $-\infty < x \leqslant 0$. So the respective coefficients of the perturbation expansions of $f(x)$ in the BCS regime and in the unitary regime are expected to be related to each other. At unitarity, the details of the microscopic interaction are lost. Unitary Fermi gases are expected to exhibit universal behaviors. Hence $f(-\infty)$ is universal and is only a function of the universal coefficients of the perturbation expansion of $f(x)$ in the BCS regime. Using these facts, we extend the perturbation expansion of $f(x)$ in the BCS regime to the BCS-unitarity crossover regime. The resulting expansion of $f(x)$ in the BCS regime is analogous to the low-temperature expansions of the energies of solids (ideal Bose gases of phonons) and of ideal Fermi gases, which involve the Bose and Fermi integrals, respectively. It is natural to expect that the best approximation of $f(x)$ should involve the Bose or Fermi integral. $f(-\infty)$ is predicted to be 0.40098(0.42294) for the Bose (Fermi) function, which are in good agreement with the quantum Monte Carlo results and the experimental results.

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