THE LOGARITHMIC TERM IN THE GROUND STATE ENERGY OF A HARD CORE FERMI GAS*,**

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The logarithmic term $\sim c^4 \ln c$ ($c = k_F r_c$, k_F — Fermi momentum, r_c — hard core radius) in the expression for the ground state energy of a hard core Fermi gas is derived, without the usual cut off procedure. The reaction matrix method is used, with sufficiently exact expressions for the relevant matrix elements.

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1. Introduction

The expansion of the ground state energy E of an infinite system of fermions interacting with a hard core two body potential in powers of the parameter $c = k_F r_c$ (k_F is the Fermi momentum in units of $\hbar$, r_c is the hard core radius) has been investigated by a number of authors [1–15]. The first three terms of this expansion are well established. Beyond the c^3 approximation the divergent integrals appear [7–9, 12, 13]. Cutting off the upper limits of the divergent integrals somewhat arbitrarily [7, 8, 13] or introducing the cut off function under the divergent integral [9, 12], one gets the logarithmic term $\sim c^4 \ln c$.

The aim of this paper is to obtain the logarithmic term in a natural way without the cut off procedure. We will use the method of perturbation expansion of E in terms of the Brueckner reaction matrix K. The method is described in detail by Bishop in [13], hereafter referred to as B.

The expansion of E in powers of c is obtained in B by expanding in powers of c each K-matrix element in the formula for energy. Computing in this way the term proportional to c^4 in the energy series, one obtains integrals logarithmically divergent when the powers

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of the momenta in the K-matrices expansions in numerators sufficiently overtake the energy denominators.

In this paper we do not expand the K-matrix elements. Instead, we use the sufficiently exact solution of the K-matrix equation and obtain convergent integrals which are then expanded in powers of c. Actually, a possibility of such a derivation was mentioned in B.

The present paper is organized as follows. In Section 2 we show that to obtain the logarithmic term it is sufficient to solve the K-matrix equation for S wave only, with neglected Pauli operator, and with neglecting dependence on the hole momenta. We also exemplify the difference between our approach and that of B. In Section 3 we compute the total contribution $\sim c^4 \ln c$ to the ground state energy per particle. In the Appendix expressions for the elements of the free reaction matrix $K^0(z)$ with negative argument z are derived.

2. *The solution of the K-matrix equation*

The K-matrix is defined by the equation:

$$(\boldsymbol{p}_1'\boldsymbol{p}_2'|K(z)\,|\boldsymbol{p}_1\boldsymbol{p}_2) = (\boldsymbol{p}_1'\boldsymbol{p}_2'|v|\boldsymbol{p}_1\boldsymbol{p}_2)$$

$$+\sum_{\boldsymbol{k}_1\boldsymbol{k}_2} (\boldsymbol{p}_1'\boldsymbol{p}_2'|v|\boldsymbol{k}_1\boldsymbol{k}_2)\,\frac{1}{z-\varepsilon(k_1)-\varepsilon(k_2)}\,(\boldsymbol{k}_1\boldsymbol{k}_2|K(z)\,|\boldsymbol{p}_1\boldsymbol{p}_2), \tag{1}$$

where states denoted by $|\boldsymbol{p}_i)$ are plane waves normalized in volume Ω, v is the hard core two body interaction, $\varepsilon(p) = p^2/(2M)$ is the kinetic energy of the $\boldsymbol{p}$ state, M is the mass of a particle. From now on we shall denote by $\boldsymbol{m}_i$ the hole momenta for which $|\boldsymbol{m}_i| \leqslant k_F$, by $\boldsymbol{k}_i$ the particle momenta for which $|\boldsymbol{k}_i| > k_F$, and by $\boldsymbol{p}_i$ any momenta.

If we introduce the relative and center-of-mass momenta

$$\boldsymbol{p} = (\boldsymbol{p}_1-\boldsymbol{p}_2)/2, \qquad \boldsymbol{P} = \boldsymbol{p}_1+\boldsymbol{p}_2, \tag{2}$$

we have

$$(\boldsymbol{p}_1'\boldsymbol{p}_2'|K|\boldsymbol{p}_1\boldsymbol{p}_2) = (\delta_{\boldsymbol{P}\boldsymbol{P}'}/\Omega)\,\langle \boldsymbol{p}'|K_{\boldsymbol{P}}|\boldsymbol{p}\rangle, \tag{3}$$

where $\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \exp(i\boldsymbol{p}\boldsymbol{r})$.

In the relative and c.m. momenta Eq. (1) takes the form

$$\langle \boldsymbol{p}'|K_{\boldsymbol{P}}(z)\,|\boldsymbol{p}\rangle = \langle \boldsymbol{p}'|v|\boldsymbol{p}\rangle + \int \frac{d\boldsymbol{k}}{(2\pi)^3}\,\langle \boldsymbol{p}'|v|\boldsymbol{k}\rangle\,\frac{Q(\boldsymbol{P},\boldsymbol{k})}{z-\varepsilon(P)/2-2\varepsilon(k)}\,\langle \boldsymbol{k}|K_{\boldsymbol{P}}(z)\,|\boldsymbol{p}\rangle, \tag{4}$$

where Q is the exclusion principle operator:

$$Q(\boldsymbol{P},\boldsymbol{k}) = \begin{cases} 1 \text{ for } \frac{1}{2}|\boldsymbol{P}\pm\boldsymbol{k}| > k_F, \\ 0 \text{ otherwise.} \end{cases} \tag{5}$$

To solve Eq. (4) we consider the matrix K^0, defined by the equation

$$\langle \boldsymbol{p}'|K_P^0(z)\,|\boldsymbol{p}\rangle = \langle \boldsymbol{p}'|v|\boldsymbol{p}\rangle + \int \frac{d\boldsymbol{k}}{(2\pi)^3}\,\langle \boldsymbol{p}'|v|\boldsymbol{k}\rangle\,\frac{1}{z-\varepsilon(P)/2-2\varepsilon(k)}\,\langle \boldsymbol{k}|K_P^0(z)\,|\boldsymbol{p}\rangle, \tag{6}$$

where the principal value of the integral over $\boldsymbol{k}$ is taken.

From Eq. (4) and (6) we obtain:

$$\langle p'|K_P(z)\,|p\rangle = \langle p'|K_P^0(z)\,|p\rangle$$

$$+\int \frac{dk}{(2\pi)^3}\langle p'|K_P^0(z)\,|k\rangle \frac{Q(P,k)-1}{z-\varepsilon(P)/2-2\varepsilon(k)}\langle k|K_P(z)\,|p\rangle. \tag{7}$$

Solving Eq. (7) by iteration we get:

$$\langle p'|K_P(z)\,|p\rangle = \langle p'|K_P^0(z)\,|p\rangle$$

$$+\int \frac{dk}{(2\pi)^3}\langle p'|K_P^0(z)\,|k\rangle \frac{Q(P,k)-1}{z-\varepsilon(P)/2-2\varepsilon(k)}\langle k|K_P^0(z)\,|p\rangle + \dots \tag{8}$$

To obtain the logarithmic term $\sim c^4 \ln c$ it is sufficient to consider diagrams of the third and fourth order in K-matrix. So we need the K-matrix expression exact to second order in parameter c. Since the contribution from P-wave in the K-matrix expansion is of the third order in c, we may confine ourselves to the S-wave solution for the K-matrix.

If the K-matrix element $\langle p'|K_P(z)|p\rangle$ is on the energy shell, it means $z = 2\varepsilon(p) + \varepsilon(P)/2$, K^0 is the free space reaction matrix and does not depend on the center of mass momentum. In this case we may write (see e.g. B)

$$\langle p'|K^0|p\rangle = \frac{4\pi}{Mk_F}\frac{\sin(p'c/k_F)}{p'/k_F} + O(c^3). \tag{9}$$

We will also need the solution for the off-shell $K^0(z)$ matrix elements with negative argument z. As it is shown in the Appendix, for $z < 0$ the K^0-matrix element exact to the second order in c has the form

$$\langle p'|K_P^0(z)\,|p\rangle = \frac{4\pi}{Mk_F}\frac{\sin(p'c/k_F)}{p'/k_F}(1+bc)+O(c^3), \tag{10}$$

where

$$b^2 = \frac{1}{k_F^2}(-Mz+P^2/4). \tag{11}$$

Let us consider the third order K-matrix diagram shown in Fig. 1. (One of the diagrams which contributes to the logarithmic term.)

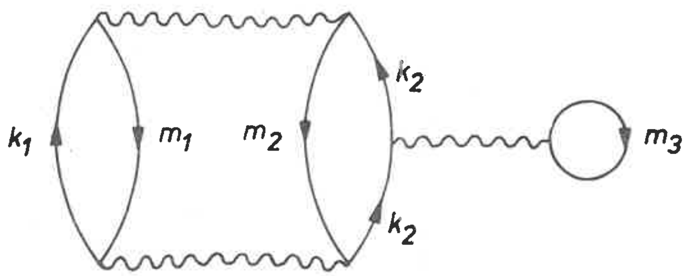

Fig. 1. The third order K-matrix diagram corresponding to expression (12)

The contribution to the energy per particle from this diagram is

$$\frac{\Delta E}{N} = \frac{6\pi^2 v^2}{k_F^3} \sum_{\substack{m_1 m_2 m_3 \\ k_1 k_2}} \frac{|(\boldsymbol{k}_1 \boldsymbol{k}_2 | K(\varepsilon(m_1)+\varepsilon(m_2)) | \boldsymbol{m}_1 \boldsymbol{m}_2)|^2}{[\varepsilon(m_1)+\varepsilon(m_2)-\varepsilon(k_1)-\varepsilon(k_2)]^2}$$

$$\times (\boldsymbol{k}_2 \boldsymbol{m}_3 | K(\varepsilon(m_1)+\varepsilon(m_2)+\varepsilon(m_3)-\varepsilon(k_1)) | \boldsymbol{k}_2 \boldsymbol{m}_3), \tag{12}$$

where v is the number of spin and isospin degrees of freedom per particle. Using Eq. (3) we may express Eq. (12) as follows:

$$\frac{\Delta E}{N} = \int d\boldsymbol{m}_1 d\boldsymbol{m}_2 d\boldsymbol{m}_3 \int d\boldsymbol{k}_1 F(\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3, \boldsymbol{k}_1), \tag{13}$$

where

$$F(\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3, \boldsymbol{k}_1) = \frac{6\pi^2 v^2}{(2\pi)^{12} k_F^3} \frac{|\langle(\boldsymbol{k}_1-\boldsymbol{k}_2)/2 | K_{\boldsymbol{m}_1+\boldsymbol{m}_2}(\varepsilon(m_1)+\varepsilon(m_2)) | (\boldsymbol{m}_1-\boldsymbol{m}_2)/2\rangle|^2}{[\varepsilon(m_1)+\varepsilon(m_2)-\varepsilon(k_1)-\varepsilon(k_2)]^2}$$

$$\times \langle(\boldsymbol{k}_2-\boldsymbol{m}_3)/2 | K_{\boldsymbol{k}_2+\boldsymbol{m}_3}(\varepsilon(m_1)+\varepsilon(m_2)+\varepsilon(m_3)-\varepsilon(k_1)) | (\boldsymbol{k}_2-\boldsymbol{m}_3)/2\rangle, \tag{14}$$

$$\boldsymbol{k}_2 = \boldsymbol{m}_1+\boldsymbol{m}_2-\boldsymbol{k}_1. \tag{15}$$

To calculate the logarithmic term we can equate the hole momenta to zero in the expression under the integral in Eq. (12). To see this we transform Eq. (13) as follows:

$$\frac{\Delta E}{N} = (\tfrac{4}{3}\pi k_F^3)^3 4\pi \int_{k_F}^{\infty} k_1^2 F(\boldsymbol{m}_1 = 0, \boldsymbol{m}_2 = 0, \boldsymbol{m}_3 = 0, \boldsymbol{k}_1) dk_1$$

$$+\int d\boldsymbol{m}_1 d\boldsymbol{m}_2 d\boldsymbol{m}_3 \int d\boldsymbol{k}_1 F(\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3, \boldsymbol{k}_1) - F(\boldsymbol{m}_1 = 0, \boldsymbol{m}_2 = 0, \boldsymbol{m}_3 = 0, \boldsymbol{k}_1). \tag{16}$$

Confining ourselves to the first term of iterative solution for the K-matrix (Eq. (8)) and using Eq. (9) and (10) we see that

$$\{F(\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3, \boldsymbol{k}_1) - F(\boldsymbol{m}_1 = 0, \boldsymbol{m}_2 = 0, \boldsymbol{m}_3 = 0, \boldsymbol{k}_1)\} \xrightarrow[|\boldsymbol{k}_1| \to \infty]{} 0. \tag{17}$$

(The on-shell K^0-matrix elements exact to c^2 from Eq. (9) do not depend on the hole momenta, the argument z of the off-shell K^0-matrix element becomes negative for $|\boldsymbol{k}_1| \gg k_F$ so we may use Eq. (10).) Since the divergences come from high momenta values ($\gg k_F$) the logarithmic term comes from the first integral on the r.h.s. of Eq. (16) only. Denoting this term by $(\Delta E)'/N$ we have

$$\frac{(\Delta E)'}{N} = \frac{6\pi^2 v^2}{(2\pi)^{12} k_F^3} (\tfrac{4}{3}\pi k_F^3)^3 4\pi M^2$$

$$\times \int_{k_F}^{\infty} \frac{dk_1}{k_1^2} \langle \boldsymbol{k}_1 | K^0(0) | 0\rangle^2 \langle -\boldsymbol{k}_1/2 | K_{-\boldsymbol{k}_1}(-k_1^2/(2M)) | -\boldsymbol{k}_1/2\rangle. \tag{18}$$

It is sufficient to take in Eq. (18) the expression (9) or (10) for only one of the K-matrix elements and expand the remaining matrix elements in powers of c to the c^2 term to obtain the following convergent integral:

$$\frac{(\Delta E)'}{N} = \frac{4\sqrt{3}\,v^2 k_F^2 c^4}{9\pi^3 M} \int_{k_F}^{\infty} \frac{dk_1}{k_1} \frac{\sin(k_1 c/k_F)}{k_1 c/k_F} + \dots \tag{19}$$

By dots we indicated the part of $\Delta E'/N$ which does not lead to the logarithmic term. The integral in Eq. (19) gives in a natural way the logarithmic term

$$\int_c^{\infty} \frac{\sin x}{x^2}\, dx = \frac{\sin c}{c} - \mathrm{Ci}\, c = 1 - \gamma - \ln c + \frac{c^2}{12} + \dots, \tag{20}$$

where γ is the Euler constant.

If we expand the function under integral in Eq. (19) in powers of c we obtain the expression used in B which gives the logarithmic divergence. (Because the Maclaurin expansion of sin is valid only for finite values of argument, we must not compute the improper integral on the l.h.s. of Eq. (20) term by term.)

From Eq. (18) we see that the logarithmic term appears because the expansion of the product of the three K-matrix elements contains a term linear in k_1. This term derives from the expansion of the part proportional to b of the r.h.s. of Eq. (10) and is proportional to c^2. So from the second iterative term of solution of the K-matrix equation (8) we get the logarithmic term $\sim c^5 \ln c$. We conclude that to obtain the term $\sim c^4 \ln c$ we can neglect the Pauli principle in the K-matrix equation, it means we can replace the K-matrix by the K^0-matrix.

3. The total logarithmic term from the third and fourth order K-matrix diagrams

Third order diagrams fall into two separate classes: those containing four hole lines and those containing three hole lines as shown in B. Whith the hole momenta being neglected, each diagram with three hole lines contributes an identical amount to logarithmic term as diagram in Fig. 1, apart from the trivial difference of spin and isospin traces. The sum of these contributions is

$$\varepsilon_3 = -(v-1)(v-2)\frac{8\sqrt{3}\,k_F^2}{9\pi^3 M} c^4 \ln c. \tag{21}$$

In calculating contribution to the energy from diagrams with four hole lines, we may take all K-matrix elements on the energy shell. In this way we calculate contribution from the entire class of four hole lines diagrams as shown, e.g., in Fig. 2.

This diagram does not give the logarithmic term because the expansion of the product of three K-matrices, each of which is on the energy shell, cannot contain a term linear in particle momentum and we get the convergent integral $\int dk_1/k_1^2$.

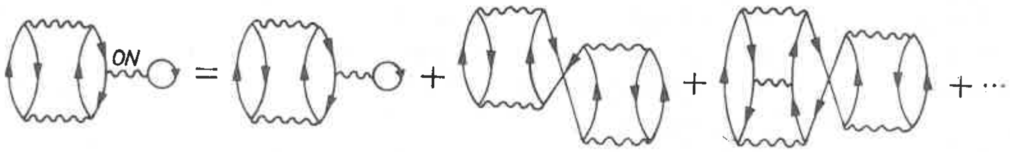

Fig. 2. The hole self energy diagram with the on-energy-shell K-matrix

In the case of the fourth order diagrams in K we need the K-matrix elements exact to the first order in the parameter c only. In agreement with Eq. (9) and (10), we have

$$\langle p'|K_P(z)\,|p\rangle = \frac{4\pi}{Mk_F}\,\frac{\sin(p'c/k_F)}{p'/k_F} + O(c^2). \tag{22}$$

The logarithmic term $\sim c^4 \ln c$ comes from the fourth order diagrams containing the minimal number of hole lines, namely three, as shown in B. To obtain convergent integrals it is sufficient to express one of the four K-matrix elements in the formula for energy with the help of Eq. (22) and other remaining elements by $4\pi c/(Mk_F)$. The logarithmic term from all fourth order diagrams is

$$\varepsilon_4 = (\nu-1)(\nu-2)\,\frac{32k_F^2}{27M\pi^2}\,c^4 \ln c. \tag{23}$$

The sum of Eq. (21) and (23) gives the total contribution to the logarithmic term

$$\varepsilon_{\log} = (\nu-1)(\nu-2)\,\frac{8k_F^2}{27M\pi^3}\,(4\pi-3\sqrt{3})c^4 \ln c. \tag{24}$$

Sufficiently exact expressions (9) or (10) for the K-matrix elements are also necessary for computing all terms $\sim c^4$ (not $\sim c^4 \ln c$) in the expansion of E. For example, we see that performing integration in Eq. (19) we obtain from Eq. (20) the term $\sim (1-\gamma)c^4$ which could not be obtained with the help of cut off procedure used in B.

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APPENDIX

Matrix elements of $K^0(z)$ for $z < 0$

The reaction matrix K^0 is defined by Eq. (6):

$$\langle p'|K_P^0(z)\,|p\rangle = \langle p'|v|p\rangle + \int \frac{dk}{(2\pi)^3}\,\frac{\langle p'|v|k\rangle\,\langle k|K_P^0(z)\,|p\rangle}{z-\varepsilon(P)/2-2\varepsilon(k)}\,. \tag{A1}$$

Eq. (A1) is equivalent to the differential equation

$$\left(\Delta + Mz - \frac{P^2}{4}\right)[\Psi_p^P(x) - e^{ipx}] = Mv(x)\Psi_p^P(x), \tag{A2}$$

where the two body wave function Ψ_p^P is introduced in the following way:

$$\langle p'|K_P^0|p\rangle = \langle p'|v|\Psi_p^P\rangle. \tag{A3}$$

For $z < 0$ function $\Psi_p^P(x)$ has the "healing property", i.e., it becomes asymptotically identical with $\langle x|p\rangle$.

We look for S wave solution of Eq. (A2) in the form:

$$\Psi_p^P(r) = \frac{u(r)}{r}, \tag{A4}$$

where

$$r = k_F|x|. \tag{A5}$$

Inserting Eq. (A4) into Eq. (A2) yields

$$\left(\frac{d^2}{dr^2} - b^2\right)\xi(r) = \frac{M}{k_F^2}u(r)v(r) \equiv w(r), \tag{A6}$$

where

$$\xi(r) = u(r) - \frac{\sin(\kappa r)}{\kappa}, \qquad \kappa = \frac{p}{k_F}, \tag{A7}$$

$$-b^2 = \frac{1}{k_F^2}\left(Mz - \frac{P^2}{4}\right). \tag{A8}$$

Since the wave function must vanish inside the infinite potential, the product $(M/k_F^2)u(r)v(r)$ can thus be written as:

$$w(r) = A\delta(r-c) + (b^2+\kappa^2)\frac{\sin \kappa r}{\kappa}\,\Theta(c-r). \tag{A9}$$

Here the first term gives a finite discontinuity in the slope of the wave function at the core boundary. The remaining term cannot contribute outside the core where the potential vanishes. Outside the hard core the solution of Eq. (A6) is given by

$$\xi(r) = e^{-b(r-c)} + e^{b(r-c)}, \qquad r > c. \tag{A10}$$

From the boundary conditions

$$\xi(c) = -\frac{\sin \kappa c}{\kappa}, \qquad \xi(r) \xrightarrow[r\to\infty]{} 0,$$

$$\xi'(c) = A - \cos \kappa c, \tag{A11}$$

we obtain

$$A = \cos \kappa c + b\frac{\sin \kappa c}{\kappa}. \tag{A12}$$

From Eq. (A2) we get for the S-wave:

$$\langle \boldsymbol{p}'| K_{\boldsymbol{P}}^0(z) |\boldsymbol{p}\rangle = \frac{4\pi}{k_F^3} \int_0^\infty v(r)u(r) \frac{\sin \kappa' r}{\kappa'} dr$$

$$= \frac{4\pi}{Mk_F} \left[A \frac{\sin \kappa' c}{\kappa'} + \int_0^c (b^2+\kappa^2) \frac{\sin \kappa r \sin \kappa' r}{\kappa\kappa'} dr. \right. \quad \text{(A13)}$$

Eq. (A13) exact to the second order in c may be written as:

$$\langle \boldsymbol{p}'| K_{\boldsymbol{P}}^0(z) |\boldsymbol{p}\rangle = \frac{4\pi}{Mk_F} \frac{\sin \kappa' c}{\kappa'} (1+bc). \quad \text{(A14)}$$

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