Scattering Hypervolume of Spin-Polarized Fermions

Zipeng Wang and Shina Tan

1International Center for Quantum Materials, Peking University, Beijing 100871, China
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We analyze the collision of three identical spin-polarized fermions at zero collision energy, assuming arbitrary finite-range potentials, and define the corresponding three-body scattering hypervolume $D_F$. The scattering hypervolume $D$ was first defined for identical bosons in 2008 by one of us. It is the three-body analog of the two-body scattering length. We solve the three-body Schrödinger equation asymptotically when the three fermions are far apart or one pair and the third fermion are far apart, deriving two asymptotic expansions of the wave function. Unlike the case of bosons for which $D$ has the dimension of length to the fourth power, here the $D_F$ we define has the dimension of length to the eighth power. We then analyze the interaction energy of three such fermions with momenta $\hbar k_1$, $\hbar k_2$, and $\hbar k_3$ in a large periodic cubic box. The energy shift due to $D_F$ is proportional to $D_F/\Omega^2$, where $\Omega$ is the volume of the box. We also calculate the shifts of energy and pressure of spin-polarized Fermi gases due to a nonzero $D_F$ and the three-body recombination rate of spin-polarized ultracold atomic Fermi gases at finite temperatures.

I. INTRODUCTION

When electrically neutral particles collide with small energies, such that the de Broglie wave lengths are large compared to the range of interaction, their effective interactions can be characterized by a small number of parameters such as the two-body $s$-wave scattering length. For identical spin-polarized fermions, however, the $s$-wave collision is forbidden due to the Pauli exclusion principle, and the low-energy effective interaction is dominated by the $p$-wave scattering volume $a_p$. All the two-body effective parameters for the interaction can be extracted from the wave functions for the two-body collision at energies equal to or close to zero, outside of the physical range of the interaction potential [1]. The $p$-wave scattering volume $a_p$, for example, can be extracted from the wave function of the two fermions colliding at zero incoming kinetic energy:

$$\phi^{(1, m)}(s) = \left(\frac{s}{3} - \frac{a_p}{s^2}\right) \sqrt{\frac{4\pi}{3}} Y_1^m(s), \quad s > r_e, \quad (1)$$

where $s$ is the spatial vector extending from one fermion to the other, $r_e$ is the range of the interaction potential, $Y_1^m(s)$ is the spherical harmonic ($m = -l, -l+1, \ldots, l$ is the magnetic quantum number).

The effective three-body interaction at small collision energies can also be described by some effective parameters, such as the scattering hypervolume $D$ which was first defined for three identical bosons by one of us [1]. It is the three-body analog of the two-body $s$-wave scattering length $a$, and is a fundamental parameter determining the effective strength of three-body interactions at small collision energies. $D$ affects the energies of dilute Bose-Einstein condensates [1]. The three-body recombination [2,8] rate is proportional to the imaginary part of $D$ [9,10]. $D$ determines the effective three-body coupling constant in the effective-field theoretical description of low energy particles [11,8,11]. The value of $D$ has been numerically computed for identical bosons interacting with hard-sphere [1], Gaussian [9], square-well [12] and Lennard-Jones [13] potentials. Recently, the definition of scattering hypervolume is generalized to three particles with unequal masses [14], two identical bosons and a particle with a different mass [15], and three identical spin-1 bosons [16]. In these three-body systems, the dimensions of the corresponding scattering hypervolumes are all [length]$^4$.

Can we also define a scattering hypervolume for three identical fermions in the same spin state? In this paper, we study the zero energy collision of three spin-polarized fermions with total orbital angular momentum $L = 1$, assuming arbitrary finite-range potentials. We solve the three-body Schrödinger equation asymptotically and get two expansions for the three-body wave function $\Psi$, one of which is applicable when all the three fermions are far away from each other and is named 111 expansion, the other of which is applicable when two fermions are held at a fixed distance and the third fermion is far away from the two and is named 21 expansion. The new scattering hypervolume $D_F$ is the dominant three-body parameter in these expansions. The dimension of $D_F$ is [length]$^8$. The parameter $D_F$ is applicable only if the thermal de Broglie wavelengths of the fermions are much larger than $r_e$, namely if the temperature $T \ll T_e$, where

$$T_e \equiv \frac{\hbar^2}{2M_F r_e^2 k_B}. \quad (2)$$

Here $\hbar$ is Planck’s constant over $2\pi$, $M_F$ is the mass of each fermion, and $k_B$ is the Boltzmann constant.

In Section II of this paper, we derive the 111 expansion and the 21 expansion for the collision of three identical spin-polarized fermions at zero energy. We assume that the fermions are electrically neutral, and the interaction potentials are finite-ranged, vanishing beyond a certain range $r_e$. In this paper we will expand the three-body...
wave function $\Psi$ to the order $B^{-6}$ in the 111 expansion and to the order $R^{-7}$ in the 21 expansion, which are the orders at which the three-body scattering hypervolume $D_F$ first appears. Here $B$ is the hyperradius, defined as the square root of a half of the sum of the squares of the three interfermionic distances; see Eq. (3) below. $R$ is the distance between the center of mass of the two fermions held at a fixed distance and the third fermion which is far away from the two; see Eq. (7) below.

In Section [III] we calculate the shift of the energy of three fermions in a large periodic cubic box due to a nonzero $D_F$. We then further calculate the shifts of energy and pressure caused by $D_F$ for a homogeneous spin-polarized Fermi gas at finite temperatures.

In Section [IV] we derive the formula for the three-body recombination rate in spin-polarized ultracold atomic Fermi gases. We find that in an intermediate temperature regime $T_F \ll T \ll T_c$, where $T_F$ is the Fermi temperature, $dn/dt$ is proportional to $n^3T^2$, in agreement with Refs. [17–19], while at low temperatures, $T \ll T_F$, $dn/dt$ is proportional to $n^{13/3}$.

II. ASYMPTOTICS OF THE THREE-BODY WAVE FUNCTION

We consider identical spin-polarized fermions with mass $M_F$ each. We assume that the interactions among these fermions are finite-ranged and depend only on the interparticle distances, and thus they are invariant under translation, rotation and Galilean transformations.

If the three fermions collide with zero energy, the three-body wave function $\Psi$ satisfies the Schrödinger equation:

\[
\left[-\frac{\hbar^2}{2M_F}(\nabla_1^2 + \nabla_2^2 + \nabla_3^2) + V(s_1) + V(s_2) + V(s_3) + V_{123}(s_1, s_2, s_3)\right] \Psi(r_1, r_2, r_3) = 0,
\]

where $r_i$ is the position vector of the $i$th fermion, and

\[
s_i \equiv r_j - r_k.
\]

In the above equation and in the following, $(i, j, k) = (1, 2, 3), (2, 3, 1), \text{ or } (3, 1, 2)$. $V(s_i)$ is the interaction potential between the $j$th fermion and the $k$th fermion, and $V_{123}(s_1, s_2, s_3)$ is the three-body potential. We assume the total momentum of three fermions is zero (which means we study the problem in the center-of-mass frame), and thus $\Psi$ is translationally invariant:

\[
\Psi(r_1 + \delta r, r_2 + \delta r, r_3 + \delta r) = \Psi(r_1, r_2, r_3)
\]

for any $\delta r$.

Equations (3) and (5) do not uniquely determine the wave function for the zero energy collision. We need to also specify the asymptotic behaviour of $\Psi$ when the three fermions are far apart. The leading-order term in $\Psi$ when $s_1, s_2, s_3$ go to infinity simultaneously, $\Psi_0$, should satisfying the Laplace equation $(\nabla_1^2 + \nabla_2^2 + \nabla_3^2)\Psi_0 = 0$, and scale like $B^0$ at large $B$, where

\[
B \equiv \sqrt{(s_1^2 + s_2^2 + s_3^2)/2}
\]

is the hyperradius. The most important three-body wave function for zero-energy collisions, for purposes of understanding ultracold collisions, should be the one with the minimum value of $p$. The larger the value of $p$, the less likely it is for the three particles to come to the range of interaction within which they can interact. (For this same reason, in the study of two-body ultracold collisions of identical fermions, the $p$-wave collision is usually the most important one.) One can easily show that the minimum value of $p$ for three identical spin-polarized fermions in three spatial dimensions is 2. There are only three linearly independent three-body wave functions for the zero-energy collision with $p = 2$, and they all have total orbital angular momentum quantum number $L = 1$, and they form an irreducible representation of the rotational group, and can be distinguished using the magnetic quantum number $M = -1, 0, 1$. These three-body wave functions are denoted as $\Psi_1^M$.

For later use, we define the Jacobi coordinates [18–20] used in this paper. $s_i$ has been defined in Eq. (1). We define $R_i$ as the vector extending from the center of mass of the $j$th fermion and the $k$th fermion to the $i$th fermion:

\[
R_i \equiv r_i - (r_j + r_k)/2.
\]

We also define three hyperangles:

\[
\theta_i \equiv \arctan \frac{2R_i}{\sqrt{3}s_i},
\]

$s_i, R_i, \theta_i$ and $B$ satisfy the following relations:

\[
s_i = \frac{2}{\sqrt{3}} B \cos \theta_i, \quad R_i = B \sin \theta_i.
\]

The $s_i, R_i, B$, and $\theta_i$ defined above are the same as the corresponding variables defined for identical bosons in Ref. [1].

A. Two-body special functions

We define the two-body special functions $\phi^{l, m}(s), f^{l, m}(s), g^{l, m}(s), \ldots$, for the collision of two particles with orbital angular momentum quantum number $l$ and magnetic quantum number $m$ along the $z$ direction [1] [13]:

\[
\bar{H}\phi^{l, m} = 0,
\]

\[
\bar{H}f^{l, m} = \phi^{l, m},
\]

\[
\bar{H}g^{l, m} = f^{l, m},
\]

\[
\ldots
\]
where $h^2 \tilde{H}/M_F$ is the two-body Hamiltonian for the collision of two fermions in the center-of-mass frame, and

$$\tilde{H} \equiv -\nabla_s^2 + \frac{M_F}{h^2} V(s).$$  \hspace{1cm} (11)

For identical spin-polarized fermions, $l$ must be odd due to Pauli principle. We use symbols $p, f, h, \cdots$ to represent $l = 1, 3, 5, \cdots$.

Given the two-body special functions $\phi_{(l,m)}$, $f_{(l,m)}$, $g_{(l,m)}$, $\cdots$, we can express the wave function for the collision of two particles at any small nonzero energy $E = h^2 k^2 / M_F$ as an infinite series in $k^2$ \[1\] \[13\

$$\phi_k^{(l,m)}(s) = \phi_{(l,m)}(s) + k^2 f_{(l,m)}(s) + k^4 g_{(l,m)}(s) + \cdots.$$  \hspace{1cm} (12)

To complete the definition of $\phi_{(l,m)}$, we need to specify its overall amplitude. Since the potential $V(s)$ vanishes beyond a finite range $r_c$, $\phi_{(l,m)}$ takes a simple form at $s > r_c$:

$$\phi_{(l,m)}(s) = \left[ \frac{s^l}{(2l+1)!!} \right] \sqrt{\frac{4\pi}{2l+1}} Y_l^m(s),$$  \hspace{1cm} (13)

where $Y_l^m$ is the spherical harmonic, and $a_l$ is the two-body $l$-wave scattering volume (with dimension $[l^2]$). We have fixed the overall amplitude of $\phi_{(l,m)}$ by specifying the coefficient of the term $s^l$.

The solution to the equation $\tilde{H} f_{(l,m)} = \phi_{(l,m)}$ is not unique, because if $f_{(l,m)}$ satisfies this equation, then $f_{(l,m)} + (\text{arbitrary coefficient}) \times \phi_{(l,m)}$ also satisfies this equation. To complete the definition of $f_{(l,m)}$, we specify that in the expansion of $f_{(l,m)}(s)$ at $s > r_c$ we do not have the term $\propto s^{-l-1}$ (if such a term exists, we can add a suitable coefficient times $\phi_{(l,m)}(s)$ to $f_{(l,m)}(s)$ to cancel this term). Then at $s > r_c$ we have the following analytical formula for $f_{(l,m)}(s)$:

$$f_{(l,m)}(s) = \left[ -\frac{s^{l+2}}{2(2l+3)!!} - \frac{a_l r_c s^l}{2(2l+1)!!} \right] \sqrt{\frac{4\pi}{2l+1}} Y_l^m(s).$$  \hspace{1cm} (14)

For brevity we do not show the explicit formula for $g_{(l,m)}$ as it is not used in this paper.

The two-body special functions will appear in the 21 expansions of the three-body wave functions at zero collision energy.

If the magnetic quantum number $m = 0$, these two-body functions we have defined here are the same as the special functions defined in Ref. [14] if one sets $\mathbf{n} = \mathbf{2}$ in Ref. [14].

One can show [1] [13] that $a_l$, which first appears in Eq. (4) is the two-body $l$-wave scattering volume, $r_l$ which first appears in Eq. (14) is the two-body $l$-wave effective range, and they are related to the scattering phase shift $\delta_l(k)$ in the well-known effective range expansion [21] [22]:

$$k^{2l+1} \cot \delta_l(k) = -\frac{1}{a_l} + \frac{1}{2} r_l k^2 + O(k^4).$$  \hspace{1cm} (15)

**B. 111 expansion and 21 expansion**

As in our previous works [1] [14], we derive two asymptotic expansions for the three-body wave function $\Psi^M_1$. When the three fermions are all far apart from each other, such that the pairwise distances $s_1$, $s_2$, $s_3$ go to infinity simultaneously for any fixed ratio $s_1 : s_2 : s_3$, we expand $\Psi^M_1$ in powers of $1/R$, and this expansion is called the 111 expansion. When one fermion (the i-th fermion) is far away from the other two (the j-th and the k-th fermions), but the two fermions (j and k) are held at a fixed distance $s_i$, we expand $\Psi^M_1$ in powers of $1/R_i$, and this is called the 21 expansion. The two expansions are

$$\Psi^M_1 = \sum_{p=-2}^{\infty} T^{(-p)}(r_1, r_2, r_3),$$  \hspace{1cm} (16a)

$$\Psi^M_1 = \sum_{q=-1}^{\infty} S^{(-q)}(R, s),$$  \hspace{1cm} (16b)

where $T^{(-p)}$ scales as $R^p$, $S^{(-q)}$ scales as $R^{-q}$. Without loss of generality, here we suppose the Jacobi coordinates $s = s_1$, and $R = R_1$.

$T^{(-p)}$ satisfies the free Schrödinger equation outside of the interaction range:

$$-\frac{h^2}{2M_F} \left( \nabla_q^2 + \nabla_s^2 + \nabla_R^2 \right) T^{(-p)} = 0.$$  \hspace{1cm} (17)

If one fermion is far away from the other two, Eq. (3) becomes

$$\left[ -\frac{h^2}{2M_F} \nabla_s^2 + V(s) - \frac{3h^2}{4M_F} \nabla_R \right] \Psi^M_1 = 0.$$  \hspace{1cm} (18)

Therefore, $S^{(-q)}$ satisfies the following equations,

$$\tilde{H} S^{(1)} = 0, \quad \tilde{H} S^{(0)} = 0,$$

$$\tilde{H} S^{(-q)} = \frac{3}{4} \nabla_R S^{(-q+2)} \quad (q \geq 1).$$  \hspace{1cm} (19)

If $s \ll R$, we can further expand $T^{(-p)}$ as

$$T^{(-p)} = \sum_i t^{(i,-p-i)},$$  \hspace{1cm} (20)

where $t^{(i-j)}$ scales like $R^i s^j$. If $s \gg r_c$, we can further expand $S^{(-q)}$ as

$$S^{(-q)} = \sum_j t^{(-q,j)}.$$  \hspace{1cm} (21)

Because the three-body wave function $\Psi^M_1$ may be expanded as $\sum_q S^{(-q)}$ at $R \to \infty$, and may also be expanded as $\sum_q S^{(-q)}$ at $R \to \infty$, the $t^{(i-j)}$ in the above two expansions should be the same. In fact the wave function has a double expansion $\Psi^M_1 = \sum_{i,j} t^{(i,j)}$ in the region $r_c \ll s \ll R$. 


We show the points at which \( t^{(i,j)} \neq 0 \) on the \((i,j)\) plane in Fig. 1. \( T^{(-p)} \) corresponds to the straight line with slope equal to \(-1\) and intercept equal to \(-p\). \( S^{(-q)} \) corresponds to the vertical line \( i = -q \). Therefore, all the points \( t^{(i,j)} \) satisfying \( i + j = -p \) are on the line corresponding to \( T^{(-p)} \), and all the points \( t^{(-q,j)} \) are on the line of \( S^{(-q)} \).

![Diagram](image)

**FIG. 1.** Diagram of the points representing \( t^{(i,j)} \) on the \((i,j)\) plane. Each point with coordinates \((i, j)\) represents \( t^{(i,j)} \) which scales like \( R^s s^j \). Thick dots represent those points at which \( t^{(i,j)} \neq 0 \). Each nonzero term \( T^{(-p)} \) in the 111-expansion is represented by a red dashed line satisfying the equation \( i + j = -p \). For \( s > r_e \), the term \( S^{(-q)} \) in the 21-expansion is represented by the vertical blue line satisfying the equation \( i = -q \). We have not derived the expressions for \( T^{(-2)} \), \( T^{(-3)} \), \( T^{(-4)} \) etc, and so the red dashed lines corresponding to them are not shown.

To derive the two expansions, we start from the leading-order term in the 111 expansion (which fixes the overall amplitude of \( \Psi_1^M \)):

\[
T^{(2)} = Q_1^M(s \times \mathbf{R}), \quad M = -1, 0, 1,
\]

where \( Q_L^M(\mathbf{u}) \) is the harmonic polynomial,

\[
Q_L^M(\mathbf{u}) \equiv \sqrt{\frac{4\pi}{2L + 1}} u^{L} Y_M^L(\hat{\mathbf{u}}).
\]

More explicitly, for \( M = 0 \),

\[
T^{(2)} = A_z,
\]

and for \( M = \pm 1 \),

\[
T^{(2)} = -\frac{M}{\sqrt{2}} (A_x + i M A_y),
\]

where

\[
\mathbf{A} = \mathbf{s} \times \mathbf{R} = -(\mathbf{r}_1 \times \mathbf{r}_2 + \mathbf{r}_2 \times \mathbf{r}_3 + \mathbf{r}_3 \times \mathbf{r}_1)
\]

is a vector perpendicular to the plane of the triangle formed by the three fermions, and \( \mathbf{A} \) is equal to twice the area of such triangle. One can check the leading-order term \( T^{(2)} \) satisfies the free Schrödinger equation. It is also translationally invariant, and is antisymmetric under the exchange of the fermions. \( T^{(2)} = t^{(1,1)} \) is denoted by the point with coordinates \((1, 1)\) in Fig. 1.

We then first derive \( S^{(1)} \), and then derive \( T^{(1)} \), and then derive \( S^{(0)} \), and then derive \( T^{(0)} \), and so on, all the way until \( S^{(-7)} \). At every step, we require the 111 expansion and the 21 expansion to be consistent in the region \( r_e < s < R \). See Appendices A and B for more details.

Our resultant 111 expansion is

\[
\Psi_1^M = Q_1^M(s \times \mathbf{R}) \left[ 1 - 3a_p \sum_{i=1}^{3} \frac{1}{s_i^3} + \frac{36a_p^2}{\pi} \sum_{i=1}^{3} \left( \frac{\theta_i - \frac{1}{4} \sin 4\theta_i}{R_i^2 s_i^3} \right) - \frac{9\sqrt{3} D_F}{4\pi^3 B^8} \right] + O(B^{-7}),
\]

where \( D_F \) is the three-body scattering hypervolume of identical spin-polarized fermions, and it appears at the order of \( B^{-6} \). We have chosen the coefficient \(-9\sqrt{3}/4\pi^3\) in front of \( D_F \) to simplify the formula for the energy shift of three identical fermions in a large periodic volume due to the three-body parameter; see Sec. IIIA for details.
Our resultant 21 expansion is

\[
\Psi_1^M = 6i \sqrt{\frac{2\pi}{3}} \left[ R - \frac{6a_p}{R^2} + \frac{12a_p^2}{R^5} \left( 8 - \frac{9\sqrt{3}}{\pi} \right) - \frac{\xi}{R^7} \right] \sum_m C_{1,M-m;1,m}^{1,M} \phi^{(1,m)}(\mathbf{R}) + \text{O}(R^{-8}),
\]

where

\[
C_{i_1,i_2,m_1,i_2,m_2}^{J,M} = \langle i_1, m_1; i_2, m_2 | J, M \rangle
\]

is the Clebsch-Gordan coefficient, and \( \xi \) is a parameter related to \( D_F \),

\[
\xi = \frac{9\sqrt{3}D_F}{4\pi^3} - 81a_p^3 r_p \left( 8 - \frac{9\sqrt{3}}{\pi} \right). \tag{30}
\]

### III. ENERGY SHIFTS AND THERMODYNAMIC PROPERTIES

In this section, we study the energy shifts of \( N \) identical spin-polarized fermions caused by the scattering hypervolume \( D_F \) in a periodic box. Using this result we derive the thermodynamic properties, including the energy and the pressure, of the spin-polarized Fermi gas due to a nonzero \( D_F \).

#### A. Three fermions in a cubic box

In this subsection, for the sake of simplicity we assume that the fermions have vanishing or negligible two-body interactions but have a nonzero three-body scattering hypervolume \( D_F \), and the 111 expansion for the zero-energy three-body wave function in Eq. (27) is simplified as

\[
\Psi_1^M = Q_1^M (s \times \mathbf{R}) \left( 1 - \frac{9\sqrt{3}D_F}{4\pi^3 B^3} \right) + \text{O}(B^{-7}). \tag{31}
\]

For purposes of calculating the energy shifts due to a nonzero \( D_F \), we can replace the true interaction potential \( V(s_1) + V(s_2) + V(s_3) + V_{123}(s_1, s_2, s_3) \), which in general has a complicated dependence on the interparticle distances, by a three-body pseudopotential \( V_{ps} \). We use the following pseudopotential:

\[
V_{ps} = \frac{\hbar^2 D_F}{6 M_F} \left\{ \left[ \nabla_s \nabla_R - (\nabla_s \cdot \nabla_R) \right] \delta(s) \delta(R) \right\} \Lambda, \tag{32}
\]

where \( \Lambda \) is a projection operator which, when acting on the \( \text{O}(B^{-6}) \) term in the three-body wave function, yields zero. The operator \( \Lambda \) is an analog of the operator \( \frac{\delta}{\delta R} \) in the two-body pseudopotential for \( s \)-wave two-body collisions in Refs. [23, 24]. One can check the pseudopotential in Eq. (32) is symmetric under the interchange of the three fermions. The coefficient on the right hand side of Eq. (32) has been chosen such that

\[
\left[ -\frac{\hbar^2}{2M_F} \left( \nabla_1^2 + \nabla_2^2 + \nabla_3^2 \right) + V_p \right] \Psi_1^M \simeq 0. \tag{33}
\]

We now consider three fermions in a large periodic cubic box with volume \( \Omega \). Their momenta are \( \hbar \mathbf{k}_1, \hbar \mathbf{k}_2 \) and \( \hbar \mathbf{k}_3 \) in the absence of interactions. When we introduce interactions that give rise to a nonzero \( D_F \), the energy eigenvalue of the three-body state is shifted by the following amount at first order in the perturbation:

\[
\mathcal{E}_{k_1,k_2,k_3} = \int d^3r_1 d^3r_2 d^3r_3 |\Psi_{k_1,k_2,k_3}|^2 V_{ps}, \tag{34}
\]

where \( \Psi_{k_1,k_2,k_3} \) is the normalized unperturbed wave function and it can be written as a Slater determinant:

\[
\Psi_{k_1,k_2,k_3} = \frac{1}{\sqrt{6\Omega^{3/2}}} \begin{bmatrix} e^{ik_1 \cdot r_1} e^{ik_2 \cdot r_2} e^{ik_3 \cdot r_3} \\ e^{ik_1 \cdot r_1} e^{ik_2 \cdot r_2} e^{ik_3 \cdot r_3} \\ e^{ik_1 \cdot r_1} e^{ik_2 \cdot r_2} e^{ik_3 \cdot r_3} \end{bmatrix}. \tag{35}
\]

We get

\[
\mathcal{E}_{k_1,k_2,k_3} = \frac{\hbar^2 D_F}{3 M_F \Omega} (k_1 \times k_2 + k_2 \times k_3 + k_3 \times k_1)^2. \tag{36}
\]

Note that \(|k_1 \times k_2 + k_2 \times k_3 + k_3 \times k_1| \) is twice the area of the \( k \)-space triangle whose vertices are \( k_1, k_2, k_3 \).

Note that Eq. (33) is only satisfied approximately. In particular, if we take into account the \( \text{O}(B^{-7}) \) corrections in the asymptotic expansion of the wave function in Eq. (31), Eq. (33) is violated. So the three-body pseudopotential in Eq. (32) is only an approximate description of the effective three-body interaction. However,
we believe that this does not affect our leading-order result for the energy shift in Eq. (36). In Appendix C we show another calculation, using Gauss's theorem, without resorting to the pseudopotential, that also gives rise to Eq. (36).

If there are two-body interactions, the shift of the energy of the three particles will also contain terms due to the two-body parameters including \( a_p, r_p, \gamma_f \) etc.; nevertheless, the shift due to \( D_F \) in Eq. (36) is still valid. If \( a_p \neq 0 \), the leading-order shift of the three-body energy due to \( a_p \) is the sum of contributions from the three pairs of fermions. To quickly derive this shift, we may write down the \( p \)-wave pseudopotential

\[
V^{2\text{-body}}_{ps} = \frac{6\pi\hbar^2 a_p}{M_F} \left[ \nabla^2 \delta(s) \right] \Lambda, \tag{37}
\]

where \( s \) is the pair distance, and \( \Lambda \) is the operator that annihilates the singular term that is \( \propto s^{-2} \) in the two-body wave function \( \phi^{(1,m)}(s) \). The coefficient in this pseudopotential is chosen such that the two-body wave function \( \phi^{(1,m)}(s) \) satisfies the Schrödinger equation \( -\frac{\hbar^2}{2M_F} \nabla^2 \phi^{(1,m)}(s) = 0 \). The pseudopotential that we write in Eq. (37) is similar to those given in Refs. 25 32 but is of a simpler form. Taking the expectation value of the pseudopotential in Eq. (37) in the unperturbed three-body state, we derive the leading-order shift of the three-body energy due to a nonzero \( a_p \):

\[
\epsilon^{2\text{-body}}_{k_1,k_2,k_3} = \frac{6\pi\hbar^2 a_p}{M_F \Omega} \left[ (k_1-k_2)^2 + (k_2-k_3)^2 + (k_3-k_1)^2 \right]. \tag{38}
\]

**B. Energy shift of many fermions and thermodynamic consequences**

We generalize the energy shift in Eq. (36) to \( N \) fermions in the periodic volume \( \Omega \). The number density of the fermions is \( \rho = N/\Omega \). We define the Fermi wave number \( k_F = \sqrt{2\rho n}\sqrt{\frac{3}{\pi}} \), the Fermi energy \( \epsilon_F = \hbar^2 k_F^2/2M_F \), and the Fermi temperature \( T_F = \epsilon_F/k_B \). We assume that the density is low such that the average interparticle distance \( n^{-1/3} \gg r_e \).

1. **Adiabatic shifts of energy and pressure in the thermodynamic limit**

Starting from a many-body state at a finite temperature \( T \), if we introduce a nonzero \( D_F \) adiabatically, the energy shift at first order in \( D_F \) is equal to the sum of the contributions from all the triples of fermions, namely

\[
\Delta E = \frac{1}{6} \sum_{k_1,k_2,k_3} \epsilon_{k_1,k_2,k_3} n_{k_1} n_{k_2} n_{k_3}, \tag{39}
\]

where \( n_k = (1 + e^{\beta(\epsilon_k - \mu)})^{-1} \) is the Fermi-Dirac distribution function, \( \beta = 1/k_B T \), \( \epsilon_k = \hbar^2 k^2/2M_F \) is the kinetic energy of a fermion with linear momentum \( \hbar k \), and \( \mu \) is the chemical potential. The summation over \( k \) can be replaced by a continuous integral \( \sum_k = \Omega \int d^3k/(2\pi)^3 \) in the thermodynamic limit. Carrying out the integral, we get

\[
\Delta E(T) = \frac{N\hbar^2 D_F}{36\pi^4 M_F} k_F^{10} \cdot \left( \frac{9\pi}{64} \right) \tilde{T}^5 [f_{5/2}(e^\beta\mu)]^2, \tag{40}
\]

where \( \tilde{T} = T/T_F \), and the function \( f_{5/2}(z) \) is defined as

\[
f_{5/2}(z) \equiv -\text{Li}_5(-z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \frac{z^4}{4} + \cdots. \tag{41}
\]

The chemical potential \( \mu \) is determined by the number of fermions,

\[
\mu = \Omega \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1} \tag{42}
\]

which is equivalent to

\[
1 = 3\sqrt{\pi} \tilde{T}^{1/2} f_{3/2}(e^\beta\tilde{T}), \tag{43}
\]

where \( \tilde{\mu} = \mu/\epsilon_F \).

In the low temperature limit, \( T \ll T_F \),

\[
\Delta E(T) = \frac{N\hbar^2 D_F}{36\pi^4 M_F} k_F^{10} \cdot \left[ \frac{1}{25} + \frac{\pi^2}{30} \tilde{T}^2 + O(\tilde{T}^4) \right]. \tag{44}
\]

In particular, at absolute zero temperature,

\[
\Delta E(0) = \frac{N\hbar^2 D_F}{900\pi^4 M_F} k_F^{10}, \tag{45}
\]

and the ground state energy of the Fermi gas is

\[
E = \frac{3}{5} \epsilon_F N \left( 1 + \frac{D_F k_F^6}{270\pi^4} + \cdots \right). \tag{46}
\]

If there are two-body interactions, the total ground state energy should contain terms that depend on the two-body parameters such as \( a_p, r_p, \gamma_f \), but the term due to \( D_F \) remains the same as in the above formula to leading order in \( D_F \).

In an intermediate temperature regime, \( T_F \ll T \ll T_c \),

\[
\Delta E(T) = \frac{N\hbar^2 D_F}{36\pi^4 M_F} k_F^{10} \left[ \frac{1}{4} \frac{1}{\tilde{T}^2} + \frac{\sqrt{T}}{6\sqrt{2\pi}} + O(\tilde{T}^{-1}) \right]. \tag{47}
\]

If \( T \) is comparable to or higher than \( T_c \), the de Broglie wave lengths of the fermions will be comparable to or shorter than the range \( r_e \) of interparticle interaction potentials, and we can no longer use the effective parameter \( D_F \) to describe the system. See Fig. 2 for \( \Delta E \) as a function of the initial temperature.

The pressure of the spin-polarized Fermi gas changes by the following amount due to the adiabatic introduction of \( D_F \):

\[
\Delta p(T) = - \left( \frac{\partial \Delta E}{\partial \Omega} \right)_{s,N} = \frac{10\Delta E}{3\Omega} = \frac{5\hbar^2 D_F}{54\pi^4 M_F} \cdot \left( \frac{9\pi}{64} \right) \tilde{T}^5 \left[ f_{5/2}(e^\beta\mu) \right]^2. \tag{48}
\]
The subscripts $S, N$ in Eq. (48) mean that we keep the entropy $S$ and the particle number $N$ fixed when taking the partial derivative. See Fig. 3 for $\Delta \rho$ as a function of the initial temperature. In particular, at zero temperature

$$\Delta \rho(0) = \frac{n\hbar^2 D_F}{270\pi^4 M_F} k_F^{10}. \quad (49)$$

2. Isothermal shifts of energy and pressure in the thermodynamic limit

If the interaction is introduced adiabatically, the temperature will increase (if $D_F > 0$) or decrease (if $D_F < 0$). The change of temperature is

$$\Delta T = \left( \frac{\partial \Delta E}{\partial S} \right)_{N, \Omega}.$$ \quad (50)

Therefore, if we introduce $D_F$ isothermally, the energy shift $\Delta E'$ should be approximately

$$\Delta E' = \Delta E - C \Delta T = \left( 1 - T^2 \frac{\partial}{\partial T} \right) \Delta E,$$ \quad (51)

where $C$ is the heat capacity of the noninteracting Fermi gas at constant volume. In the low temperature limit, $T \ll T_F$,

$$\Delta E'(T) = \frac{Nh^2 D_F}{36\pi^4 M_F} k_F^{10} \left[ \frac{1}{25} - \frac{25}{30} T^2 + O(T^4) \right]. \quad (52)$$

In an intermediate temperature regime, $T_F \ll T \ll T_c$,

$$\Delta E'(T) = \frac{Nh^2 D_F}{36\pi^4 M_F} k_F^{10} \left[ - \frac{1}{4} T^2 + \frac{\sqrt{T}}{12\sqrt{2\pi}} + O(T^{-1}) \right]. \quad (53)$$

According to Eqs. (52) and (53), $\Delta E'$ changes sign as we increase the temperature. Therefore, there is a critical temperature $T_c$ at which $\Delta E' = 0$. We find

$$T_c \approx 0.377 T_F. \quad (54)$$

The pressure of the spin-polarized Fermi gas changes by the following amount due to the isothermal introduction of $D_F$:

$$\Delta p' = \Delta p - \frac{2C \Delta T}{3\Omega} = \left( 1 - \frac{1}{5} T^2 \frac{\partial}{\partial T} \right) \Delta p.$$ \quad (55)

In the low temperature limit, $T \ll T_F$,

$$\Delta p' = \frac{5n\hbar^2 D_F}{54\pi^4 M_F} k_F^{10} \left[ \frac{1}{25} + \frac{25}{50} T^2 + O(T^4) \right]. \quad (56)$$

In an intermediate temperature regime, $T_F \ll T \ll T_c$,

$$\Delta p' = \frac{5n\hbar^2 D_F}{54\pi^4 M_F} k_F^{10} \left[ \frac{3}{20} T^2 + \frac{3\sqrt{T}}{20\sqrt{2\pi}} + O(T^{-1}) \right]. \quad (57)$$

The energy shift and the pressure change as functions of temperature are shown in Fig. 2 and Fig. 3 respectively.

IV. THE THREE-BODY RECOMBINATION RATE

If the collision of the three particles is purely elastic, $D_F$ is a real number. But if the two-body interactions support bound states, then the three-body collisions are usually not purely elastic, three-body recombination [2] [8] will occur, and $D_F$ will acquire some negative imaginary part. The three-body recombination rate constant is proportional to the imaginary part of $D_F$ [9] [10].

Within a short time $\Delta t$, the probability that no recombination occurs is $\exp(-2|\text{Im} E|\Delta t/h) \approx 1 - 2|\text{Im} E|\Delta t/h$. 
Then the probability that one recombination event occurs is $2\left|\text{Im}E_\Delta/\hbar\right|$. Since each recombination event causes the loss of three low-energy atoms, the change of the number of remaining low-energy atoms in the short time $dt$ is

$$dN = \frac{1}{6} \sum_{k_1k_2k_3} 3 \cdot 2\frac{dt}{\hbar} |\text{Im}E_{k_1k_2k_3}| n_{k_1} n_{k_2} n_{k_3}. \quad (58)$$

This leads to

$$\frac{dn}{dt} = -L_3 n^3, \quad (59)$$

and the three-body recombination rate constant $L_3$ is

$$L_3 = 6(6\pi^2)^{4/3} \left(\frac{9\pi}{64}\right)^{2/3} \left(1 + \frac{5\pi^2}{6} \frac{\hbar}{M_F} |\text{Im}D_F| n^{4/3}. \quad (60)$$

$L_3$ now in general depends on the density $n$ and the temperature $T$.

In the low temperature limit, $T \ll T_F$, we have

$$L_3 \approx \frac{6(6\pi^2)^{4/3}}{25} \left(1 + \frac{5\pi^2}{6} \frac{\hbar}{M_F} |\text{Im}D_F| n^{4/3}. \quad (61)$$

In this limit, $dn/dt$ is proportional to $n^\alpha$ where $\alpha = 13/3 = 4.333\cdots$. In particular, at absolute zero temperature,

$$L_3 = \frac{6}{25} \frac{\hbar|\text{Im}D_F|}{M_F} k_B^2. \quad (62)$$

In an intermediate temperature regime, $T_F \ll T \ll T_c$, we find that

$$L_3 = \frac{6M_F}{\hbar^3} |\text{Im}D_F| (k_B T)^2. \quad (63)$$

and $L_3$ is approximately independent of $n$, and is proportional to $T^2$. It was predicted that $L_3 \propto T^2$ according to the Wigner threshold law [17]. Our Eq. (63) is consistent with this prediction. In Refs. [18, 19] the quadratic dependence of $L_3$ on the temperature was experimentally confirmed for ultracold $^6\text{Li}$ atoms in the $|F = 1/2, m_F = 1/2\rangle$ state. In Ref. [19] it was reported that $L_3 = (3.55 \pm 0.22) \times 10^{-23} \times T^2 \text{cm}^6/\text{s} (T \text{ in units of Kelvin})$ at $T \sim 100 - 300\mu\text{K}$ for $^6\text{Li}$ atoms in a magnetic field of 1G (far away from the $p$-wave Feshbach resonance located at 15G). Using this result in Ref. [19] we find that the order of magnitude of $|\text{Im}D_F|$ for these fermionic atoms in such magnetic field is about $-(125a_0)^8$, where $a_0$ is the Bohr radius.

In the intermediate temperature regime, $T_F \ll T \ll T_c$, the characteristic thermal de Broglie wavelength $\lambda$ of the fermions is shorter than the average interfermionic distance. Hence the orbital angular momentum quantum number for three colliding fermions may easily exceed 1. One may wonder why the three-body recombination rate is still dominated by the parameter $D_F$ which refers to the $L = 1$ collisions only. We can resolve this paradox by noting that in this temperature regime $\lambda$ is still much larger than the range $r_c$ of the interaction potentials. In the many-body wave function, when three fermions come to a spatial region whose size is much smaller than the average interfermionic distance but much larger than $r_c$, the many-body wave function is approximately factorized as a 3-fermion Slater determinant [analogous to the one shown in Eq. (57)], times a function that depends on the positions of the other fermions and the position of the center of mass of the three nearby fermions, and when the three fermions come to distances smaller than $\lambda$ this 3-fermion Slater determinant may be further approximated by Eq. (53) and Eq. (54) which in fact correspond to a collision with orbital angular momentum quantum number $L = 1$. When the three fermions come to even smaller distances, the three-body wave function acquires correction terms due to the interactions, and can be approximately described by the 111 expansion we have derived. Therefore, the rate of three-body recombination events, which can occur only if three fermions come within the range of interaction, is dominated by the parameter $D_F$ we have defined.

Ref. [33] considered spin-polarized fermionic atoms near a $p$-wave Feshbach resonance. It was shown that when the two-body scattering volume $a_p$ is positive and large, such that there is a shallow two-body $p$-wave bound state, the three-body recombination rate constant diverges as $a_p^{5/2}$ [33]:

$$L_3 \approx \frac{9\hbar}{25M_F} (48\pi)^2 \left(\frac{a_p^5}{-3r_p/2}\right)^{1/2} k_F^2. \quad (64)$$

at $T \ll T_F$. Comparing this result with Eq. (61) we infer that near such a $p$-wave Feshbach resonance, on the $a_p > 0$ side,

$$\text{Im}D_F \approx -\frac{3}{2} (48\pi)^2 \left(\frac{a_p^5}{-3r_p/2}\right)^{1/2}. \quad (65)$$

Note that the $a_{\text{res}}$ in Ref. [33] is equal to $(-r_p/2)$ in our paper, and is positive.

V. SUMMARY AND DISCUSSION

We have defined the three-body scattering hypervolume $D_F$ for identical spin-polarized fermions by considering the collision of three such fermions at zero energy. We solved the three-body Schrödinger equation asymptotically at large interparticle distances and expanded the three-body wave function in powers of $1/B$ when the pairwise distances go to infinity simultaneously (here $B$ is the three-body hyperradius), and expanded the same wave function in powers of $1/R$ when two fermions are held at a fixed distance and the third fermion is far away from the two (here $R$ is the distance between this third fermion and the center of mass of the other two fermions). In the expansion in powers of $1/B$, the parameter $D_F$...
first appears at the order $1/B^2$. In the expansion in powers of $1/R$, the parameter $D_F$ first appears at the order $1/R^7$. For any given microscopic interaction potentials, one can solve the three-body Schrödinger equation numerically and match the solution to these expansions to compute $D_F$.

The three-body scattering hypervolume we have defined in this paper plays a fundamental role in three-body, four-body, . . . , and many-body physics for ultracold Fermi gases. Although usually the two-body $p$-wave scattering volume is the dominant parameter for the effective interactions in spin-polarized ultracold Fermi gases, and $D_F$ serves as a small correction, $D_F$ may become the dominant parameter if $a_p$ happens to be zero or tiny or is tuned to zero, or if the system is near a three-body resonance close to zero energy. If the system is near a three-body resonance close to zero energy, $D_F$ may be anomalously large.

In the second part of this paper we computed the energy shift of three fermions in a large periodic volume due to $D_F$. From this result we computed the energy shift of many fermions in the thermodynamic limit due to $D_F$. We also computed the shift of pressure due to $D_F$. The energy shift and the pressure shift are related. We computed the two shifts in two scenarios as functions of temperatures: either introducing the three-body parameter adiabatically or introducing it isothermally. For isothermal introduction of $D_F$, we found that the shift of energy changes sign at temperature $T \approx 0.377T_F$, where $T_F$ is the Fermi temperature. The energy and pressure shifts could be experimentally detected in trapped ultracold atomic Fermi gases. In particular, $D_F$ will cause a small change of the atomic cloud size and small changes of the collective mode frequencies.

If the two-body interactions are sufficiently attractive such that there are two-body bound states, $D_F$ will acquire some negative imaginary part related to the three-body recombination processes. We computed the three-body recombination rate constant $L_3$ in terms of $\text{Im} \, D_F$ as functions of temperature. In particular, we found that at low temperatures ($T \ll T_F$) $L_3 \propto n^{4/3}$. These results could be verified in future experiments concerning ultracold atomic Fermi gases.

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**Appendix A: Derivation of the 111 expansion and the 21 expansion for $L = 1$, $M = 0$**

We consider the collision of three identical spin-polarized fermions with orbital angular momentum $L = 1$. The magnetic quantum number $M$ can be $-1$, 0, and 1. Here we first derive the 111 expansion and the 21 expansion for $M = 0$.

We expand the three-body wave function in two forms:

\[
\Psi = \sum_{p=-2}^{\infty} \mathcal{T}^{(-p)}(r_1, r_2, r_3), \quad (A1a)
\]

\[
\Psi = \sum_{q=-1}^{\infty} S^{(-q)}(R, s), \quad (A1b)
\]

where $\mathcal{T}^{(-p)}$ scales as $B^{-p}$, $S^{(-q)}$ scales as $R^{-q}$. The hyperradius $B$ and the vectors $R$ and $s$ are already defined in the main text.

If $s \ll R$, we can further expand $\mathcal{T}^{(-p)}$ as

\[
\mathcal{T}^{(-p)} = \sum_i t^{(i,-p-i)},
\]

where $t^{(i,j)}$ scales as $R^i s^j$. If $s \gg r_\epsilon$, we can expand $S^{(-q)}$ as

\[
S^{(-q)} = \sum_j t^{(-q,j)}. \quad (A3)
\]

Because the three-body wave function $\Psi_0^n$ may be expanded as $\sum_p \mathcal{T}^{(-p)}$ at $B \to \infty$, and may also be expanded as $\sum_q S^{(-q)}$ at $R \to \infty$, the $t^{(i,j)}$ in the above two expansions should be the same. In fact the wave function has a double expansion $\Psi = \sum_{i,j} t^{(i,j)}$ in the region $r_\epsilon \ll s \ll R$.

**Step 1.** We start from the leading-order term in the 111 expansion:

\[
\mathcal{T}^{(2)} = Q_1^0(s \times R) = s_x R_y - s_y R_x = t^{(1,1)}, \quad (A4)
\]

and this indicates that $S^{(1)}$ is nonzero, but $S^{(2)}$, $S^{(3)}$, $S^{(4)}$, . . . are zero. Consequently

\[
t^{(i,j)} = 0, \quad \text{if } i \geq 2. \quad (A5)
\]

Expanding $\mathcal{T}^{(2)}$ at $s \ll R$, we find that

\[
t^{(0,2)} = t^{(-1,3)} = t^{(-2,4)} = t^{(-3,5)} = \ldots = 0. \quad (A6)
\]

Since $\mathcal{T}^{(3)}$, $\mathcal{T}^{(4)}$, $\mathcal{T}^{(5)}$, . . . are zero, we have

\[
t^{(i,j)} = 0, \quad \text{if } i + j \geq 3. \quad (A7)
\]

**Step 2.** At $s \gg r_\epsilon$ we expand $S^{(1)}$ as

\[
S^{(1)} = t^{(1,1)} + \sum_{j \leq 0} t^{(1,j)}. \quad (A8)
\]

$S^{(1)}$ also satisfies

\[
\tilde{H} S^{(1)} = 0, \quad (A9)
\]

where $\tilde{H}$ is proportional to the two-body Hamiltonian, and has been defined in the main text. Therefore, we have

\[
S^{(1)} = R \sum_{l,m} c_m \phi^{(l,m)}(s). \quad (A10)
\]
Here $l$ must be equal to 1, because $\phi^{(l,m)}$ contributes a term proportional to $s^l$, and thus $S^{(l)}$ contains a term scaling as $R^ls^l$. On the other hand, the leading order term on the right hand side of Eq. (A8) is $t^{(1,1)}$ which scales as $R^1s^1$.

Expanding Eq. (A10) at $s \gg r_e$ to the order $s^1$, and using Eq. (13), we get

$$t^{(1,1)} = R \sum_m c_m s \frac{4\pi}{3} Y^m_l(\hat{s}) .$$  \hfill (A11)

Comparing this result with Eq. (A4), we find

$$c_{-1} = -\frac{3i}{\sqrt{2}R} (R_x + iR_y), \quad c_0 = 0, \quad c_1 = -\frac{3i}{\sqrt{2}R} (R_x - iR_y).$$  \hfill (A12a, A12b, A12c)

Therefore,

$$S^{(1)} = -\frac{3i}{\sqrt{2}} (R_x + iR_y) \phi^{(1,-1)}(s) + \frac{3i}{\sqrt{2}} (R_x - iR_y) \phi^{(1,1)}(s).$$  \hfill (A13)

The above result can be expressed in terms of the Clebsch-Gordan coefficients as

$$S^{(1)} = 6i \sqrt{\frac{2\pi}{3}} R \sum_m C_{1,-m;1,m}^0 Y_{-m}^1(R) \phi^{(1,m)}(s).$$  \hfill (A14)

Expanding $S^{(1)}$ at $s > r_e$, we get

$$t^{(1,0)} = 0, \quad t^{(1,-1)} = 0, \quad t^{(1,-2)} = -\frac{3a_p}{s^3} (s_x R_y - s_y R_x), \quad t^{(1,j)} = 0, \quad j \leq -3.$$  \hfill (A15a, A15b, A15c, A15d)

**Step 3.** At $s \ll R$ we expand $T^{(1)}$ as

$$T^{(1)} = t^{(1,0)} + t^{(0,1)} + t^{(1,-2)} + \ldots = t^{(0,1)} + t^{(-1,2)} + \ldots.$$  \hfill (A16)

So $T^{(1)}$ goes to zero at $s \to 0$. So Eq. (17) may be written as $(\nabla^2_1 + \nabla^2_2 + \nabla^2_3) T^{(1)} = 0$ for $p = -1$, and $T^{(1)}$ should satisfy this partial differential equation even at $s_i = 0$. Thus $T^{(1)}$ must be a harmonic polynomial. But we do not have any nontrivial harmonic polynomial of degree 1 that also satisfies the fermionic antisymmetry. We are therefore forced to take

$$T^{(1)} = 0.$$  \hfill (A17)

So

$$t^{(i,j)} = 0, \quad \text{if } i + j = 1.$$  \hfill (A18)

**Step 4.** At $s \gg r_e$ we expand $S^{(0)}$ as

$$S^{(0)} = t^{(0,2)} + t^{(0,1)} + O(s^0) = O(s^0).$$ \hfill (A19)

Combining this with the equation $\tilde{H} S^{(0)} = 0$, we get

$$S^{(0)} = 0.$$  \hfill (A20)

So

$$t^{(0,j)} = 0.$$  \hfill (A21)

**Step 5.** At $s \ll R$ we expand $T^{(0)}$ as

$$T^{(0)} = t^{(1,-1)} + t^{(0,0)} + t^{(-1,1)} + t^{(-2,2)} + \ldots = t^{(-1,1)} + t^{(-2,2)} + \ldots.$$  \hfill (A22)

So $T^{(0)}$ goes to zero at $s \to 0$. So Eq. (17) may be written as $(\nabla^2_1 + \nabla^2_2 + \nabla^2_3) T^{(0)} = 0$ for $p = 0$, and $T^{(0)}$ should satisfy this partial differential equation even at $s_i = 0$. Thus $T^{(0)}$ must be a harmonic polynomial. But we do not have any nontrivial harmonic polynomial of degree 0 that also satisfies the fermionic antisymmetry. We are therefore forced to take

$$T^{(0)} = 0.$$  \hfill (A23)

So

$$t^{(i,j)} = 0, \quad \text{if } i + j = 0.$$  \hfill (A24)

**Step 6.** At $s \gg r_e$ we expand $S^{(-1)}$ as

$$S^{(-1)} = t^{(-1,3)} + t^{(-1,2)} + t^{(-1,1)} + O(s^0) = O(s^0).$$ \hfill (A25)

Combining this with the equation

$$\tilde{H} S^{(-1)} = \frac{3}{4} \nabla^2 R S^{(1)} = 0,$$ \hfill (A26)

we get

$$S^{(-1)} = 0.$$ \hfill (A27)

So

$$t^{(-1,j)} = 0.$$ \hfill (A28)

**Step 7.** At $s \ll R$ we expand $T^{(-1)}$ as

$$T^{(-1)} = t^{(-1,-2)} + O(s^{-1}).$$ \hfill (A29)

$t^{(-1,-2)}$ is shown in Eq. (15c). $T^{(-1)}$ should satisfy the free Schrödinger equation outside of the interaction range, so $(-\nabla^2 - 3\nabla^2 R/4) T^{(-1)}$ should be equal to some Dirac delta functions that are nonzero at $s_i = 0$ only. $T^{(-1)}$ should also be antisymmetric under the interchange of the fermions. We have

$$-\nabla^2 t^{(-1,-2)} = 12\pi a_p [R_y \partial_x \delta(s) - R_x \partial_y \delta(s)],$$
so

\[
\left(-\nabla_s^2 - \frac{3}{4} \nabla_R^2\right) T_{s_1}^{(-1)} = 12\pi a_p [R_y \partial_y \delta(s) - R_x \partial_x \delta(s)],
\]

where \( T_{s_1}^{(-1)} \) is one term of the full \( T^{(-1)} \). Solving the above equation, we get

\[
T_{s_1}^{(-1)} = -\frac{3a_p}{s_1^3} (s_x R_y - s_y R_x).
\]  

(A31)

The full \( T^{(-1)} \) should also be antisymmetric under the interchange of the fermions, so

\[
T^{(-1)} = -3a_p (s_x R_y - s_y R_x) \left( \frac{1}{s_1^3} + \frac{1}{s_2^3} + \frac{1}{s_3^3} \right).
\]  

(A32)

If \( s \ll R \), we expand \( T^{(-1)} \) as \( \sum_{n+m=-1} t^{(n,m)} \), and get

\[
\begin{align*}
t^{(-2,1)} &= -6a_p (s_x R_y - s_y R_x) \frac{1}{R^3}, \\
t^{(-3,2)} &= 0, \\
t^{(-4,3)} &= 9a_p (s_x R_y - s_y R_x) \frac{(R^2 - 5R_y^2)s^2}{4R^2}, \\
t^{(-5,4)} &= 0, \\
t^{(-6,5)} &= -45a_p (s_x R_y - s_y R_x) \frac{(R^4 - 14R^2 R_y^2 + 21R_y^4)s^4}{64R^{11}}, \\
t^{(-7,6)} &= 0,
\end{align*}
\]

(A33a-d)

where \( R_s = R \cdot \hat{s} \). 

**Step 8.** At \( s \gg r_e \) we expand \( S^{(-2)} \) as

\[
S^{(-2)} = t^{(-2,1)} + t^{(-2,2)} + t^{(-2,3)} + \sum_{j \leq 0} t^{(-2,j)} = t^{(-2,1)} + \sum_{j \leq 0} t^{(-2,j)}.
\]  

(A34)

So we get

\[
S^{(-2)} = \frac{3}{4} \nabla_R^2 S^{(0)} = 0.
\]  

(A35)

Comparing this with Eq. (A33a), we find

\[
\begin{align*}
d_{-1} &= \frac{9\sqrt{2} a_p i}{R} (R_x + iR_y), \\
d_0 &= 0, \\
d_1 &= \frac{9\sqrt{2} a_p i}{R} (R_x - iR_y).
\end{align*}
\]  

(A38a-c)

Substituting these results into Eq. (A36), we get

\[
S^{(-2)} = \frac{9\sqrt{2} a_p i}{R^3} \left[ (R_x + iR_y)\phi^{(1,-1)}(s) + (R_x - iR_y)\phi^{(1,1)}(s) \right].
\]  

(A39)

This can be re-expressed in terms of the Clebsch-Gordan coefficients as

\[
S^{(-2)} = \frac{-36i a_p}{R^2} \sqrt{\frac{2\pi}{3}} \sum_m c_{1,m} a_{1,m} Y_{1}^{-(m)}(R) \phi^{(1,1)}(s).
\]  

(A40)

Expanding \( S^{(-2)} \) at \( s \gg r_e \), we find

\[
\begin{align*}
t^{(-2,0)} &= 0, \\
t^{(-2,-1)} &= 0, \\
t^{(-2,-2)} &= \frac{18a_p^2}{R^3 s^3} (s_x R_y - s_y R_x), \\
t^{(-2,j)} &= 0, \quad j \leq -3.
\end{align*}
\]  

(A41a-d)

**Step 9.** At \( s \ll R \) we expand \( T^{(-2)} \) as

\[
T^{(-2)} = t^{(1,-3)} + t^{(0,-2)} + O(s^{-1}) = O(s^{-1}).
\]  

(A42)

So the solution to the equation \( \nabla_s^2 + \nabla_y^2 + \nabla_R^2 T^{(-1)} = 0 \) that is compatible with the above expansion is

\[
T^{(-2)} = 0.
\]  

(A43)

So

\[
t^{(i,j)} = 0, \quad \text{if } i + j = -2.
\]  

(A44)

**Step 10.** At \( s \gg r_e \) we expand \( S^{(-3)} \) as

\[
S^{(-3)} = \sum_{j \geq 5} t^{(-3,j)} = \sum_{j \leq 0} t^{(-3,j)}.
\]  

(A45)

Combining this with the equation

\[
\tilde{H} S^{(-3)} = \frac{3}{4} \nabla_R^2 S^{(-1)} = 0,
\]  

(A46)

we get

\[
S^{(-3)} = 0.
\]  

(A47)

So

\[
t^{(-3,j)} = 0.
\]  

(A48)
Step 11. At \( s \ll R \) we expand \( T^{(-3)} \) as
\[
T^{(-3)} = t^{(1,-4)} + t^{(0,-3)} + t^{(-1,-2)} + O(s^{-1}) = O(s^{-1}).
\] (A49)
So the solution to the equation \((\nabla_1^2 + \nabla_2^2 + \nabla_3^2)T^{(-3)} = 0\) that is compatible with the above expansion is
\[
T^{(-3)} = 0.
\] (A50)
So
\[
t^{(i,j)} = 0, \quad \text{if } i + j = -3. \tag{A51}
\]

Step 12. At \( s \gg r_e \) we expand \( S^{(-4)} \) as
\[
S^{(-4)} = \sum_{j \leq 6} t^{(-4,j)} = t^{(-4,3)} + \sum_{j \leq 0} t^{(-4,j)}.
\] (A52)
Combining this with the equation
\[
\tilde{H}S^{(-4)} = \frac{3}{4} \nabla_R S^{(-2)} = 0,
\] (A53)
we find
\[
S^{(-4)} = -\frac{630\sqrt{\pi} \pi_p}{R^4} \sum_m C_{3,-m;3,m} \psi_{-m}(\hat{R}) \phi^{(3,m)}(s).
\] (A54)
Expanding \( S^{(-4)} \) at \( s \gg r_e \), we get
\[
t^{(-4,0)} = 0, \tag{A55a}
\]
\[
t^{(-4,-1)} = 0, \tag{A55b}
\]
\[
t^{(-4,-2)} = 0. \tag{A55c}
\]

Step 13. At \( s \ll R \) we expand \( T^{(-4)} \) as
\[
T^{(-4)} = t^{(1,-5)} + t^{(0,-4)} + t^{(-1,-3)} + t^{(-2,-2)} + O(s^{-1})
\]= \[
= \frac{18a_p^2}{R^3 s^3} (s_x R_y - s_y R_x) + O(s^{-1}). \tag{A56}
\]
The solution to the equation \((\nabla^2_1 + \nabla_2^2 + \nabla_3^2)T^{(-4)} = 0\) that is compatible with the above expansion is
\[
T^{(-4)} = \frac{36a_p^2}{\pi} (s_x R_y - s_y R_x) \sum_{i=1}^{3} \frac{\theta_i - \frac{1}{4} \sin 4\theta_i}{R_i^3 s_i^3}. \tag{A57}
\]
Expanding \( T^{(-4)} \) at \( s \ll R \) as \( \sum_{i+j=-4} t^{(i,j)} \), we get
\[
t^{(-3,-1)} = 0, \tag{A58a}
\]
\[
t^{(-4,0)} = 0, \tag{A58b}
\]
\[
t^{(-5,1)} = \frac{12a_p^2}{\pi} (s_x R_y - s_y R_x) \frac{8\pi - 9\sqrt{3}}{R^6}, \tag{A58c}
\]
\[
t^{(-6,2)} = 0, \tag{A58d}
\]
\[
t^{(-7,3)} = \frac{9a_p^2}{5\pi} (s_x R_y - s_y R_x) \frac{[297\sqrt{3} - 200\pi] R^2}{(264\pi - 1080\sqrt{3}) R^2} \frac{s^2}{R^{10}}, \tag{A58e}
\]
\[
\ldots
\]

Step 14. At \( s \gg r_e \) we expand \( S^{(-5)} \) as
\[
S^{(-5)} = \sum_{j \leq 7} t^{(-5,j)}
\]
\[
= \frac{12a_p^2}{\pi} (s_x R_y - s_y R_x) \frac{8\pi - 9\sqrt{3}}{R^6} + \sum_{j \leq 0} t^{(-5,j)}.
\] (A59)
Combining this with the equation
\[
\tilde{H}S^{(-5)} = \frac{3}{4} \nabla_R S^{(-2)} = 0,
\] (A60)
we get
\[
S^{(-5)} = \frac{72(8 - \frac{9\sqrt{3}}{\pi} \pi_p)^2}{R^5} \sqrt{\frac{2\pi}{3}} \times \sum_m C_{1,-m;1,m} \psi_{-m}(\hat{R}) \phi^{(1,m)}(s).
\] (A61)
So
\[
t^{(-5,0)} = 0, \tag{A62a}
\]
\[
t^{(-5,-1)} = 0. \tag{A62b}
\]

Step 15. At \( s \ll R \) we expand \( T^{(-5)} \) as
\[
T^{(-5)} = \sum_{i \leq 1} t^{(i,-5-i)} = O(s^{-1}). \tag{A63}
\]
The solution to the equation \((\nabla^2_1 + \nabla_2^2 + \nabla_3^2)T^{(-5)} = 0\) that is compatible with the above expansion is
\[
T^{(-5)} = 0. \tag{A64}
\]
So
\[
t^{(i,j)} = 0, \quad \text{if } i + j = -5. \tag{A65}
\]

Step 16. At \( s \gg r_e \) we expand \( S^{(-6)} \) as
\[
S^{(-6)} = \sum_{j \leq 8} t^{(-6,j)} = t^{(-6,5)} + O(s^0). \tag{A66}
\]
Combining this with the equation
\[
\tilde{H}S^{(-6)} = \frac{3}{4} \nabla_R S^{(-2)} = 0,
\] (A67)
we get
\[
S^{(-6)} = -\frac{31185\sqrt{10\pi} \pi_p}{4 R^6} \times \sum_m C_{5,-m;5,m} \psi_{-m}(\hat{R}) \phi^{(5,m)}(s).
\] (A68)
So
\[
t^{(-6,0)} = 0. \tag{A69}
\]
Step 17. At \( s \ll R \) we expand \( \mathcal{T}^{(-6)} \) as
\[
\mathcal{T}^{(-6)} = \sum_{i \leq 1} t^{(i, -6 - i)} = O(s^{-1}).
\]

The solution to the equation \( (\nabla^2 + \nabla_x^2 + \nabla_y^2) \mathcal{T}^{(-6)} = 0 \) (for \( B > 0 \)) that is compatible with the above expansion is
\[
\mathcal{T}^{(-6)} = -\frac{9\sqrt{3}D_F}{4\pi^3B^8} (s_x R_y - s_y R_x).
\]

It satisfies
\[
\left( -\nabla_x^2 - \frac{3}{4} \nabla_R^2 \right) \mathcal{T}^{(-6)} = -D_F \left[ \frac{\partial^2(s) \partial^2(R)}{\partial s_x \partial R_y} - \frac{\partial^2(s) \partial^3(R)}{\partial s_y \partial R_x} \right].
\]

Expanding \( \mathcal{T}^{(-6)} \) at \( s \ll R \), we get
\[
\mathcal{T}^{(-7,1)} = -\frac{9\sqrt{3}D_F}{4\pi^3R^8} (s_x R_y - s_y R_x),
\]
(...

Step 18. At \( s \gg r_c \) we expand \( \mathcal{S}^{(-7)} \) as
\[
\mathcal{S}^{(-7)} = \sum_{j \geq 0} t^{(j, -7)} = t^{(-7,3)} + t^{(-7,1)} + O(s^0).
\]

Combining this with the equation
\[
\hat{H} \mathcal{S}^{(-7)} = \frac{3}{4} \nabla_R^2 \mathcal{S}^{(-5)}
\]
\[
= 324\frac{\sqrt{6\pi}(8 - \frac{9\sqrt{3}}{\pi})a_p^2}{R^3} \sum_m C_{1,-m,1,m}^{1,0}(\mathbf{R}) \phi^{(1,m)}(s),
\]
we get
\[
\mathcal{S}^{(-7)} = \frac{324\sqrt{6\pi}(8 - \frac{9\sqrt{3}}{\pi})a_p^2}{R^3} \sum_m C_{1,-m,1,m}^{1,0}(\mathbf{R}) f^{(1,m)}(s)
\]
\[
- \frac{6\xi}{R^7} \sqrt{\frac{2\pi}{3}} \sum_m C_{1,0,-m,1,m}^{1,0}(\mathbf{R}) \phi^{(1,m)}(s)
\]
\[
+ \frac{4032\sqrt{\pi}(16 - \frac{27\sqrt{3}}{\pi})a_p^2}{R^3} \sum_m C_{3,0,-m,3,m}^{1,0}(\mathbf{R}) \phi^{(3,m)}(s),
\]

where \( \xi \) is a parameter related to \( D_F \),
\[
\xi = \frac{9\sqrt{3}D_F}{4\pi^3} - 8a_p^3 r_p \left( 8 - \frac{9\sqrt{3}}{\pi} \right).
\]

We have thus derived the 111 expansion to the order \( B^{-6} \) and the 21 expansion to the order \( R^{-7} \).

Appendix B: The 111 expansion and the 21 expansion for \( L = 1, M = \pm 1 \)

For the magnetic quantum number \( M = \pm 1 \), one can start from the leading order term
\[
\mathcal{T}^{(2)} = Q_1^{(1)}(s \times \mathbf{R}),
\]
and do the same type of step-by-step derivation as in the last section. The details of the derivation are similar. For brevity we do not show the details.

We can also use the ladder operators \( J_\pm \),
\[
J_\pm = J_x \pm iJ_y,
\]
where \( J_x \) and \( J_y \) are the projections of the total orbital angular momentum operator in the \( x \) and \( y \) directions, respectively. Applying the ladder operator \( J_+ \) or \( J_- \) to the 111 expansion and the 21 expansion for \( M = 0 \), we get the corresponding expansions for \( M = 1 \) or \( M = -1 \).

Appendix C: An alternative method for the derivation of the energy of three fermions in a large box

The wave function of three free fermions with momenta \( h\mathbf{k}_1, h\mathbf{k}_2, h\mathbf{k}_3 \) in a large periodic cubic box is
\[
\Psi_{k_1,k_2,k_3} = \frac{1}{\sqrt{6\Omega}^{3/2}} \begin{vmatrix}
  e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} & e^{i\mathbf{k}_1 \cdot \mathbf{r}_2} & e^{i\mathbf{k}_1 \cdot \mathbf{r}_3} \\
  e^{i\mathbf{k}_2 \cdot \mathbf{r}_1} & e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} & e^{i\mathbf{k}_2 \cdot \mathbf{r}_3} \\
  e^{i\mathbf{k}_3 \cdot \mathbf{r}_1} & e^{i\mathbf{k}_3 \cdot \mathbf{r}_2} & e^{i\mathbf{k}_3 \cdot \mathbf{r}_3}
\end{vmatrix}.
\]

We define the Jacobi momenta \( h\mathbf{q}, h\mathbf{p}, h\mathbf{k}_c \) such that
\[
k_1 = \frac{1}{3} \mathbf{k}_c + \frac{1}{2} \mathbf{q} + \mathbf{p},
\]
\[
k_2 = \frac{1}{3} \mathbf{k}_c + \frac{1}{2} \mathbf{q} - \mathbf{p},
\]
\[
k_3 = \frac{1}{3} \mathbf{k}_c - \mathbf{q}.
\]

\( h\mathbf{k}_c \) is the total momentum of three fermions. We extract the motion of the center of mass \( \mathbf{R}_c = (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)/3 \),
\[
\Psi_{k_1,k_2,k_3} = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}_c \cdot \mathbf{R}_c} \Phi_{\mathbf{q},\mathbf{p}}.
\]

Suppose that the typical momentum of each fermion is \( \sim 2\pi\hbar/\lambda \). For small hyperradii, \( B \ll \lambda \), we Taylor expand \( \Phi_{\mathbf{q},\mathbf{p}} \) and get
\[
\Phi_{\mathbf{q},\mathbf{p}} \approx \frac{3}{\sqrt{6\Omega}} (\mathbf{p} \times \mathbf{q}) \cdot (\mathbf{s}_3 \times \mathbf{R}_3).
\]

\( \Phi_{\mathbf{q},\mathbf{p}} \) is the wave function of the relative motion of three free fermions. If we introduce a small three-body \( D_F \) adiabatically, it is changed to
\[
\Phi_{\mathbf{q},\mathbf{p}} \approx \frac{3}{\sqrt{6\Omega}} (\mathbf{p} \times \mathbf{q}) \cdot (\mathbf{s}_3 \times \mathbf{R}_3) \left( 1 - \frac{9\sqrt{3}D_F}{4\pi^3B^8} \right).
\]
for \( r_c \ll B \ll \lambda \), where \( r_c \) is the range of interaction. The wave function satisfies the free Schrödinger equation outside of the range of interaction,

\[
- \frac{\hbar^2}{M_F} \nabla^2 \Phi_{q,p} = E \Phi_{q,p},
\]

(C6)

where \( \rho = (s, 2R/\sqrt{3}) \) is a six-dimensional vector, \( E \) is the energy of the relative motion, and \( B = \sqrt{3}\rho/2 \).

For large box sizes, we may compute the energy \( E \) approximately. We rewrite Eq. (C6) as

\[
- \frac{\hbar^2}{M_F} \nabla^2 \Phi_1 = E_1 \Phi_1,
\]

(C7a)

\[
- \frac{\hbar^2}{M_F} \nabla^2 \Phi_2 = E_2 \Phi_2,
\]

(C7b)

for two different interactions that yield two different three-body scattering hypervolumes, \( D_{F1} \) and \( D_{F2} \) respectively. Here we omit the subscript \( q,p \) for simplicity. Multiplying both sides of Eq. (C7a) by \( \Phi_2 \), multiplying both sides of Eq. (C7b) by \( \Phi_1 \), subtracting the two resultant equations, and taking six-dimensional integral over \( \rho \) for \( \rho > \rho_0 \) (where \( \rho_0 \) is any length scale satisfying \( r_c \ll \rho_0 \ll \lambda \)), we get

\[
- \frac{\hbar^2}{M_F} \int_{\rho > \rho_0} d^6 \rho \nabla \rho \cdot (\Phi_2 \nabla \rho \Phi_1 - \Phi_1 \nabla \rho \Phi_2) = (E_1 - E_2) \int_{\rho > \rho_0} d^6 \rho \Phi_1 \Phi_2.
\]

(C8)

In the region \( \rho > \rho_0 \), \( \Phi_1 \approx \Phi_2 \), and the right hand side of Eq. (C8) is

\[
(E_1 - E_2) \frac{8}{3\sqrt{3}} \int_{\rho > \rho_0} d^3 s d^3 R |\Phi|^2 \approx \frac{8}{3\sqrt{3}} (E_1 - E_2)
\]

(C9)

because the wave function for the relative motion is normalised, and the volume of the region \( \rho < \rho_0 \) is small and may be omitted in the integral. Applying Gauss’s divergence theorem to the left hand side of Eq. (C8), we get

\[
- \frac{\hbar^2}{M_F} \oint_{\rho = \rho_0} dS \cdot (\Phi_2 \nabla \rho \Phi_1 - \Phi_1 \nabla \rho \Phi_2) \simeq \frac{8}{3\sqrt{3}} (E_1 - E_2),
\]

(C10)

where \( S \) is the surface of the hypersphere with radius \( \rho = \rho_0 \), and \( dS \) points toward the center of the hypersphere.

To evaluate the integral on the surface, we parametrize the six coordinates \( \rho = (\rho^{(1)}, \rho^{(2)}, \rho^{(3)}, \rho^{(4)}, \rho^{(5)}, \rho^{(6)}) \) as

\[
\rho^{(1)} = \rho \cos \varphi_1,
\rho^{(2)} = \rho \sin \varphi_1 \cos \varphi_2,
\rho^{(3)} = \rho \sin \varphi_1 \sin \varphi_2 \cos \varphi_3,
\rho^{(4)} = \rho \sin \varphi_1 \sin \varphi_2 \sin \varphi_3 \cos \varphi_4,
\rho^{(5)} = \rho \sin \varphi_1 \sin \varphi_2 \sin \varphi_3 \sin \varphi_4 \cos \varphi_5,
\rho^{(6)} = \rho \sin \varphi_1 \sin \varphi_2 \sin \varphi_3 \sin \varphi_4 \sin \varphi_5,
\]

(C11a)

(C11b)

(C11c)

(C11d)

(C11e)

(C11f)

where \( 0 \leq \varphi_1, \cdots, \varphi_5 \leq \pi \), and \( 0 \leq \varphi_5 < 2\pi \). Here \( s = (\rho^{(1)}, \rho^{(2)}, \rho^{(3)}) \) and \( R = \sqrt{3}/2 (\rho^{(4)}, \rho^{(5)}, \rho^{(6)}) \). The surface element \( dS \) is

\[
dS = \rho^5 d\varphi_1 d\varphi_2 d\varphi_3 d\varphi_4 d\varphi_5 \sin^4 \varphi_1 \sin^3 \varphi_2 \sin^2 \varphi_3 \sin \varphi_4.
\]

(C12)

The minus sign in the above equation means that the direction of \( dS \) is towards the origin. Using the coordinates \( \rho, \varphi_1, \cdots, \varphi_5 \), we rewrite the wave function in Eq. (C5), and evaluate the integral on the hypersphere with radius \( \rho = \rho_0 \). We get

\[
E_2 - E_1 = \frac{3\hbar^2}{M_F \Omega^2} (D_{F2} - D_{F1}) (p \times q)^2
\]

\[
\simeq \frac{\hbar^2 (D_{F2} - D_{F1})}{3M_F \Omega^2} (k_1 \times k_2 + k_2 \times k_3 + k_3 \times k_1)^2.
\]

(C13)

This result agrees with Eq. (36).

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