

Gradient corrections to the local-density approximation for trapped superfluid Fermi gases

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Two species superfluid Fermi gas is investigated on the BCS side up to the Feshbach resonance. Using the Greens's function technique gradient corrections are calculated to the generalized Thomas-Fermi theory including Cooper pairing. Their relative magnitude is found to be measured by the small parameter $(d/R_{\text{TF}})^4$, where d is the oscillator length of the trap potential and R_{TF} is the radial extension of the density n in the Thomas-Fermi approximation. In particular, at the Feshbach resonance the universal corrections to the local density approximation are calculated and a universal prefactor $\kappa_W = 7/27$ is derived for the von Weizsäcker-type correction $\kappa_W(\hbar^2/2m)(\nabla^2 n^{1/2}/n^{1/2})$.

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I. INTRODUCTION

Fermi gases below the degeneracy temperature have been the subject of intensive research in the last years both experimentally and theoretically (see for reviews [1,2]). Particular interest has been devoted to the possible superfluid state whose creation and properties have been studied for both negative and positive values of s -wave scattering lengths a , characterizing the interaction between the particles. At the Feshbach resonance [3–7] a becomes infinity and certain universal behavior shows up. An important aspect of the problem is that the gas is trapped and thereby is inhomogeneous. When the energy gap function exceeds the level spacing near the Fermi sea a local density approximation (LDA) is applicable. As a simplest approach in its spirit neglecting the space gradients of the density and the gap function the Thomas-Fermi theory was generalized to include superfluid pair correlation results [8], when the system is treated in the generalized Hartree-Fock method [9]. Since the Thomas-Fermi approximation is widely used in case of trapped gases it is desirable to investigate systematically the corrections to it, even if they are expected to be small for large particle numbers, except in the surface region (here the gradient corrections make explicitly visible the limits of the usual LDA results). For particle numbers, however, which are treated in Monte Carlo simulations the Thomas-Fermi theory needs corrections. More importantly, it makes it possible to extend the concept of universality at unitarity [10]. In particular, we derive in this paper a universal prefactor for the von Weizsäcker-type correction to

the generalized Thomas-Fermi theory (for a review of the von Weizsäcker correction in normal systems, see [11]).

In the present paper gradient corrections are calculated up to second order at zero temperature. Baranov [12] studied the gradient corrections even at finite temperatures in cases when Eilenberger's equations [13] are applicable. That approach is different from ours, which is free from this restriction. The applied technique here is based upon the equation of motion as expressed in terms of the Green's functions. The method has been developed first to the electron gas of the atoms, which is, of course, a normal system [14]. It has been generalized to a superfluid state somewhat later independently for superconductors in a slowly varying magnetic field [15] and for nuclei [8]. The latter work is most closely related to the present one. The resulting expressions are rather cumbersome, but considerably simplified at unitarity. To evaluate them we choose the mean-field BCS (MF-BCS) model introduced by Leggett, Eagles, Nozières, and Schmitt-Rink [16–18], which neglects the self-consistent Hartree-type terms. We start, however, from the generalized Hartree-Fock (GHF) model [9] to present the results in a more complete form for future use. The Hamiltonian is

$$H = \sum_{\sigma} \int d^3r \psi_{\sigma}^{+}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U_{\text{ext}}(\mathbf{r}) - \mu \right) \psi_{\sigma}(\mathbf{r}) + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r d^3r' \psi_{\sigma}^{+}(\mathbf{r}) \psi_{\sigma'}^{+}(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}), \quad (1)$$

where $U_{\text{ext}}(\mathbf{r})$ is the trapping potential, μ is the chemical potential, $v(\mathbf{r} - \mathbf{r}')$ describes the interaction, and σ stands for the internal degrees of freedoms. We assume two equally populated hyperfine states and $\sigma = \uparrow, \downarrow$ will be termed as spin.

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In the GHF approximation the Hamiltonian simplifies to

$$\begin{aligned}
H_{\text{mf}} = & \sum_{\sigma} \int d^3r \psi_{\sigma}^{+}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U_{\text{ext}}(\mathbf{r}) - \mu \right) \psi_{\sigma}(\mathbf{r}) \\
& + \sum_{\sigma, \sigma'} \int d^3r d^3r' v(\mathbf{r}, \mathbf{r}') h_{\sigma, \sigma}(\mathbf{r}, \mathbf{r}') \psi_{\sigma}^{+}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \\
& - \sum_{\sigma, \sigma'} \int d^3r d^3r' v(\mathbf{r}, \mathbf{r}') h_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r}') \psi_{\sigma}^{+}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \\
& + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r d^3r' v(\mathbf{r}, \mathbf{r}') \\
& \times (\chi_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r}') \psi_{\sigma}^{+}(\mathbf{r}) \psi_{\sigma'}^{+}(\mathbf{r}') + \text{H.c.}). \tag{2}
\end{aligned}$$

Here,

$$\begin{aligned}
n(\mathbf{r})_{\text{tot}} &= \sum_{\sigma} n_{\sigma}(\mathbf{r}) = 2n(\mathbf{r}), \\
n_{\sigma}(\mathbf{r}) &= h_{\sigma, \sigma}(\mathbf{r}, \mathbf{r}), \\
h_{\sigma', \sigma}(\mathbf{r}', \mathbf{r}) &= \langle \psi_{\sigma'}^{+}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \rangle. \tag{3}
\end{aligned}$$

The first line in (2) contains the one-particle term of (1), the second line is the Hartree term, the third is the Fock term, and, furthermore, the Cooper pairing is represented by the last line, where

$$\chi_{\sigma', \sigma}(\mathbf{r}', \mathbf{r}) = \langle \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r}) \rangle. \tag{4}$$

The correlation functions χ and h have to be determined self-consistently.

We shall consider the special case when the interaction can be approximated by a contact potential,

$$v(\mathbf{r}, \mathbf{r}') = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r} - \mathbf{r}') \equiv g\delta(\mathbf{r} - \mathbf{r}'). \tag{5}$$

In case of contact interaction the first three lines of the Hamiltonian (2) can be safely joined together as follows:

$$\begin{aligned}
H_{\text{mf}} = & \sum_{\sigma} \int d^3r \psi_{\sigma}^{+}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}) - \mu \right) \psi_{\sigma}(\mathbf{r}) \\
& + \frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r d^3r' v(\mathbf{r}, \mathbf{r}') \\
& \times (\chi_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r}') \psi_{\sigma}^{+}(\mathbf{r}) \psi_{\sigma'}^{+}(\mathbf{r}') + \text{H.c.}), \tag{6}
\end{aligned}$$

where

$$U(\mathbf{r}) = U_{\text{ext}}(\mathbf{r}) + gn(\mathbf{r}), \tag{7}$$

but we keep the fourth line of (2) as it is, because $\chi_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r})$ is not a well-defined object.

The paper is organized as follows. In Sec. II we present the equations for the Green's functions, while in Sec. III their perturbation series are presented. The self-consistent scheme for the density and the gap function is worked out in Sec. IV up to second order in \hbar to the local density approximation, which can be regarded as a generalized Thomas-Fermi theory. In the second part of the paper the MF-BCS model is applied. In Sec. V the second-order corrections are evaluated perturbatively in the case of a general external potential. Section VI is devoted to the problems of the unitary gas, in particular, the prefactor of the von Weizsäcker-type correction

is calculated. In Sec. VII the trap potential is assumed to be an isotropic harmonic one to make some features more visible. Section VIII contains the discussion of the results.

II. FORMULATION

The gradient expansion can be best derived using the one-particle normal,

$$G_{\sigma, \sigma'}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = -i \langle T \psi_{\sigma}(\mathbf{r}_1, t_1) \psi_{\sigma'}^{+}(\mathbf{r}_2, t_2) \rangle, \tag{8}$$

and the anomalous,

$$F_{\sigma, \sigma'}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = -i \langle T \psi_{\sigma}^{+}(\mathbf{r}_1, t_1) \psi_{\sigma'}^{+}(\mathbf{r}_2, t_2) \rangle, \tag{9}$$

Green's functions [8, 15].

If the Hamiltonian is time independent, which is the case we want to discuss, the Green's functions depend on the combination $t_1 - t_2$ not separately on t_1 and t_2 [i.e., $G_{\sigma, \sigma'}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) \equiv G_{\sigma, \sigma'}(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$, and similarly for F]. Correlation functions (4) and (3) can be calculated from G and F by the limiting procedures,

$$h_{\sigma', \sigma}(\mathbf{r}', \mathbf{r}) = -i \lim_{\varepsilon \rightarrow 0} G_{\sigma', \sigma}(\mathbf{r}', \mathbf{r}, \varepsilon), \tag{10}$$

$$\chi_{\sigma', \sigma}(\mathbf{r}', \mathbf{r}) = -i \lim_{\varepsilon \rightarrow 0} F_{\sigma', \sigma}^{*}(\mathbf{r}', \mathbf{r}, -\varepsilon). \tag{11}$$

We consider the problem of singlet Cooper pairing. In that case the nonvanishing elements of the Green's functions can be chosen to be $G_{\uparrow\uparrow} = G_{\downarrow\downarrow}$ and $F_{\downarrow\downarrow} = -F_{\uparrow\uparrow}$, respectively [19]. For practical purposes let us introduce the functions,

$$v(\mathbf{r}_1, \mathbf{r}_2) = \left(-\frac{\hbar^2}{2m} \nabla_1^2 + U(\mathbf{r}_1) - \mu \right) \delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{12}$$

$$\Delta_{\sigma\sigma'}(\mathbf{r}_1, \mathbf{r}_2) = v(\mathbf{r}_1 - \mathbf{r}_2) \chi_{\sigma\sigma'}(\mathbf{r}_1, \mathbf{r}_2). \tag{13}$$

Then, the time evolutions of the two Green's functions can be written as

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t_1} G_{\uparrow\uparrow}(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) &= \hbar\delta(t_1 - t_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\
&+ \int d^3r v(\mathbf{r}_1, \mathbf{r}) G_{\uparrow\uparrow}(\mathbf{r}, \mathbf{r}_2, t_1 - t_2) \\
&+ \int d^3r \Delta_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}) F_{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}_2, t_1 - t_2), \tag{14}
\end{aligned}$$

and

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t_1} F_{\downarrow\uparrow}(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2) &= - \int d^3r \Delta_{\downarrow\uparrow}^{*}(\mathbf{r}_1, \mathbf{r}) G_{\uparrow\uparrow}(\mathbf{r}, \mathbf{r}_2, t_1 - t_2) \\
&- \int d^3r v(\mathbf{r}_1, \mathbf{r}) F_{\downarrow\uparrow}(\mathbf{r}, \mathbf{r}_2, t_1 - t_2). \tag{15}
\end{aligned}$$

The symbol “*” denotes complex conjugation. Let us take the Fourier transform with respect to time of the Green's functions as

$$G_{\uparrow\uparrow}(\mathbf{r}_1, \mathbf{r}_2, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G_{\uparrow\uparrow}(\mathbf{r}_1, \mathbf{r}_2, t) \tag{16}$$

(and similarly for F). Next we transform quantities like $A(\mathbf{r}_1, \mathbf{r}_2)$ in Eqs. (14) and (15) to mixed

position-momentum representation by introducing $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and taking the Fourier transform with respect to \mathbf{r} :

$$A(\mathbf{R}, \mathbf{p}) = \int d^3k e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} A(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2). \quad (17)$$

We use the term phase space for the (\mathbf{R}, \mathbf{p}) space in the following. If a quantity $C(\mathbf{r}_1, \mathbf{r}_2)$ is given by

$$C(\mathbf{r}_1, \mathbf{r}_2) = \int d^3r A(\mathbf{r}_1, \mathbf{r}) B(\mathbf{r}, \mathbf{r}_2), \quad (18)$$

then Baraff and Borowitz [14,20] showed that the corresponding relation in position-momentum space can be expressed as

$$C(\mathbf{R}, \mathbf{p}) = \Theta[A(\mathbf{R}, \mathbf{p}), B(\mathbf{R}, \mathbf{p})], \quad (19)$$

where Θ is a bilinear operator acting on two phase space functions as [21]

$$\begin{aligned} & \Theta[A(\mathbf{R}, \mathbf{p}), B(\mathbf{R}, \mathbf{p})] \\ &= \lim_{\substack{\mathbf{R}' \rightarrow \mathbf{R} \\ \mathbf{p}' \rightarrow \mathbf{p}}} \exp \left[\frac{i\hbar}{2} \sum_{i=1}^3 \left(\frac{\partial}{\partial R_i} \frac{\partial}{\partial p'_i} - \frac{\partial}{\partial R'_i} \frac{\partial}{\partial p_i} \right) \right] A(\mathbf{R}, \mathbf{p}) B(\mathbf{R}', \mathbf{p}'). \end{aligned} \quad (20)$$

Equations (14) and (15) in the $\mathbf{R}, \mathbf{p}, \omega$ representation can be written in the compact forms,

$$\hbar = \hbar\omega G - \Theta[v, G] - \Theta[\Delta, F], \quad (21)$$

$$0 = \hbar\omega F + \Theta[v, F] - \Theta[\Delta^*, G], \quad (22)$$

where $G \equiv G_{\uparrow\uparrow}(\mathbf{R}, \mathbf{p}, \omega)$, $F \equiv F_{\downarrow\uparrow}(\mathbf{R}, \mathbf{p}, \omega)$, $\Delta \equiv \Delta_{\uparrow\downarrow}(\mathbf{R}, \mathbf{p})$, $v \equiv v(\mathbf{R}, \mathbf{p})$, respectively. In deriving Eqs. (21) and (22) we used the properties,

$$\Delta_{\sigma\sigma'}(\mathbf{r}_1, \mathbf{r}_2) = -\Delta_{\sigma'\sigma}(\mathbf{r}_2, \mathbf{r}_1),$$

$$\Delta_{\downarrow\uparrow}(\mathbf{R}, -\mathbf{p}) = \Delta_{\uparrow\downarrow}(\mathbf{R}, \mathbf{p}),$$

which can be proven from the definition of Δ [Eq. (13)]. The ω -independent functions v and Δ in the mixed representation are

$$v(\mathbf{R}, \mathbf{p}) = \frac{p^2}{2m} + U(\mathbf{R}) - \mu, \quad (23)$$

and

$$\Delta(\mathbf{R}, \mathbf{p}) = \int d^3r e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} v(\mathbf{r}) \chi(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2). \quad (24)$$

Green's function are useful for calculating physical quantities such as the density $n(\mathbf{R}) \equiv n_{\uparrow}(\mathbf{R})$, or the equal-time expectation values $h(\mathbf{R}, \mathbf{p}) \equiv h_{\uparrow\uparrow}(\mathbf{R}, \mathbf{p})$ and $\chi(\mathbf{R}, \mathbf{p}) \equiv \chi_{\uparrow\downarrow}(\mathbf{R}, \mathbf{p})$ [defined in Eqs. (3) and (4)]. From Eqs. (10) and (11) it follows that

$$n(\mathbf{R}) = \int \frac{d^3p}{(2\pi\hbar)^3} h(\mathbf{R}, \mathbf{p}), \quad (25)$$

$$h(\mathbf{R}, \mathbf{p}) = -i \int \frac{d\omega}{2\pi} G(\mathbf{R}, \mathbf{p}, \omega) e^{i\omega\varepsilon}, \quad (26)$$

$$\chi(\mathbf{R}, \mathbf{p})^* = -i \int \frac{d\omega}{2\pi} F(\mathbf{R}, \mathbf{p}, \omega) e^{i\omega\varepsilon}, \quad (27)$$

where ε is an infinitesimally small positive regularization parameter.

The widely used interaction potential (5) leads to divergence in the gap equation, which requires some special care. Due to the δ interaction $\Delta(\mathbf{R}, \mathbf{p})$ is momentum independent. In that case, the self-consistent equation for the local gap $\Delta(\mathbf{R})$ has to be regularized. It means that we should take the regularized part F_{reg} of F by which the self-consistent gap equation,

$$\Delta(\mathbf{R})^* = \frac{4\pi\hbar^2 a}{im} \int \frac{d^3p}{(2\pi\hbar)^3} \int \frac{d\omega}{2\pi} F_{\text{reg}}(\mathbf{R}, \mathbf{p}, \omega) e^{i\omega\varepsilon}, \quad (28)$$

provides a finite value for $\Delta(\mathbf{R})$ [22,23].

III. PERTURBATION SERIES FOR G AND F

In this section we shall construct a formal solution of Eqs. (21) and (22) supposing that the functions v and Δ are known. The bilinear operator Θ as defined in Eq. (20) can be expanded as a formal series of \hbar :

$$\Theta[K_1, K_2] = \sum_{j=0}^{\infty} \hbar^j \Theta_j[K_1, K_2]. \quad (29)$$

The first two operators Θ_0 and Θ_1 are simply

$$\Theta_0[K_1, K_2] = K_1 K_2, \quad (30)$$

$$\Theta_1[K_1, K_2] = \frac{i}{2} \{K_1, K_2\},$$

where $\{\dots\}$ is a usual Poisson bracket. For higher order terms in the series (29) it is useful to treat derivatives according to the phase space variables on equal footing by the definition,

$$\{\partial_i\}_{i=1}^6 \equiv \left(\frac{\partial}{\partial R_1}, \frac{\partial}{\partial R_2}, \frac{\partial}{\partial R_3}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \frac{\partial}{\partial p_3} \right). \quad (31)$$

We also need an antisymmetric metric $g^{\alpha\beta}$, where $g^{14} = g^{25} = g^{36} = -g^{41} = -g^{52} = -g^{63} = 1$ and all the other elements are zero. The metrics reflect the symplectic structure of the phase space. For example,

$$\Theta_2[K_1, K_2] = -\frac{1}{8} g^{\alpha\beta} g^{\gamma\delta} (\partial_\alpha \partial_\gamma K_1) (\partial_\beta \partial_\delta K_2). \quad (32)$$

Expressions for higher order Θ_j 's can be derived similarly in a straightforward manner. Let us write now the normal and the anomalous Green's functions G and F as a formal power series in \hbar :

$$G(\mathbf{R}, \mathbf{p}, \omega) = \hbar \sum_{j=0}^{\infty} \hbar^j G_j(\mathbf{R}, \mathbf{p}, \omega), \quad (33)$$

$$F(\mathbf{R}, \mathbf{p}, \omega) = \hbar \sum_{j=0}^{\infty} \hbar^j F_j(\mathbf{R}, \mathbf{p}, \omega). \quad (34)$$

If we write

$$\Omega = \hbar\omega, \quad (35)$$

and treat this quantity as an $o(\hbar^0)$ term then we get from (21) and (22) in different orders of \hbar the following equations,

$$(\Omega - v)G_j - \Delta F_j = Q_j, \quad (36)$$

$$-\Delta^* G_j + (\Omega + v)F_j = P_j, \quad (37)$$

with

$$Q_0 = 1, \quad (38)$$

$$P_0 = 0, \quad (39)$$

and for $j \geq 1$,

$$Q_j = \sum_{k=1}^j (\Theta_k[v, G_{j-k}] + \Theta_k[\Delta, F_{j-k}]), \quad (40)$$

$$P_j = \sum_{k=1}^j (\Theta_k[\Delta^*, G_{j-k}] - \Theta_k[v, F_{j-k}]). \quad (41)$$

It is clear from this structure that Q_j and P_j for fixed j are given in terms of lower order corrections of G and F . Solutions to (36) and (37) are

$$G_j = \frac{1}{\Omega^2 - E^2} [(\Omega + v)Q_j + \Delta P_j], \quad (42)$$

$$F_j = \frac{1}{\Omega^2 - E^2} [(\Omega - v)P_j + \Delta^* Q_j], \quad (43)$$

where

$$E = E(\mathbf{R}, \mathbf{p}) = \sqrt{v^2(\mathbf{R}, \mathbf{p}) + |\Delta(\mathbf{R}, \mathbf{p})|^2}. \quad (44)$$

Using Equations (38)–(44) one can calculate corrections to G and F up to arbitrary large orders.

Up to now, we have not addressed the question of the correct pole structure of G and F . This requires one to introduce infinitesimal imaginary parts in the denominators of G and F . This step can be easily performed if we write the corrections as partial fractions in Ω with Ω independent numerators and choose $i\delta$ accordingly to

$$G_j = \sum_k \left[\frac{A_{j,k}(\mathbf{R}, \mathbf{p})}{(\hbar\omega - E + i\delta)^k} + \frac{B_{j,k}(\mathbf{R}, \mathbf{p})}{(\hbar\omega + E - i\delta)^k} \right], \quad (45)$$

$$F_j = \sum_k \left[\frac{C_{j,k}(\mathbf{R}, \mathbf{p})}{(\hbar\omega - E + i\delta)^k} + \frac{D_{j,k}(\mathbf{R}, \mathbf{p})}{(\hbar\omega + E - i\delta)^k} \right]. \quad (46)$$

The zeroth order coefficients are

$$A_{0,1} = \frac{1}{2} \left(1 + \frac{v}{E} \right), \quad B_{0,1} = \frac{1}{2} \left(1 - \frac{v}{E} \right), \quad (47)$$

and

$$C_{0,1} = -D_{0,1} = \frac{\Delta^*}{2E}. \quad (48)$$

All the other coefficients are zero. Nonvanishing first-order corrections involve Poisson brackets in the combinations of

$$\begin{aligned} A_{1,1} &= -\frac{i}{8E^3} (\Delta^* \{v, \Delta\} - \Delta \{v, \Delta^*\} + v \{\Delta, \Delta^*\}) \\ &= -B_{1,1}, \end{aligned} \quad (49)$$

$$A_{1,2} = EB_{1,1} + \frac{i}{8E} \{\Delta, \Delta^*\}, \quad B_{1,2} = EB_{1,1} - \frac{i}{8E} \{\Delta, \Delta^*\}. \quad (50)$$

See also Ref. [8]. It is important to note that for real Δ the first-order correction G_1 to the normal Green's function is

identically zero. Coefficients of F_1 are nonzero even for real Δ as can be seen from

$$C_{1,2} = -D_{1,2} = -\frac{i}{4E} \{v, \Delta^*\}. \quad (51)$$

There are no first-order poles of (46) for $j = 1$, consequently,

$$C_{1,1} = D_{1,1} = 0. \quad (52)$$

Higher than first-order coefficients require tedious calculations. Here we do not give explicitly the second-order coefficient functions in the numerators of Eqs. (45) and (46). Instead, we sketch the structure of these corrections. G_2 and F_2 involve $k = 1, \dots, 4$ and the coefficient functions for real Δ are linear combinations of ten (usual and) generalized Poisson brackets $\{\Delta; v, v\}$, $\{\Delta, \Delta\}_+$, $\{\Delta; \Delta, \Delta\}$, $\{\Delta; v, \Delta\}$, $\{v; \Delta, \Delta\}$, $\{v, \Delta\}_+^2$, $\{v, v\}_+$, $\{v; v, v\}$, $\{v; \Delta, v\}$, $\{v, \Delta\}_+$. The first generalized Poisson bracket is defined as

$$\{A, B\}_+ = g^{\alpha\beta} g^{\gamma\delta} (\partial_\alpha \partial_\gamma A) (\partial_\beta \partial_\delta B), \quad (53)$$

and is symmetric if one makes the changement $A \leftrightarrow B$. The second generalized Poisson bracket acts on three phase space quantities as

$$\{A; B, C\} = g^{\alpha\beta} g^{\gamma\delta} (\partial_\alpha \partial_\gamma A) (\partial_\beta B) (\partial_\delta C). \quad (54)$$

IV. GRADIENT EXPANSION OF PHYSICAL QUANTITIES

In the previous section we have seen that the one particle Green's function G can be written as a formal power series in \hbar , where the correction terms G_j in (33) are given by the partial fraction series (45). Performing the ω integral in Eq. (26) it is easy to see that only the first-order poles located on the upper half of the complex omega plane give contributions to $h(\mathbf{R}, \mathbf{p})$. Correspondingly, by Eq. (25) the density $n(\mathbf{R})$ has the expansion,

$$n(\mathbf{R}) = \sum_{j=0}^{\infty} \hbar^j \int \frac{d^3 p}{(2\pi\hbar)^3} B_{j,1}(\mathbf{R}, \mathbf{p}) \equiv \sum_{j=0}^{\infty} \hbar^j g_j(\mathbf{R}). \quad (55)$$

Similarly, Eqs. (34), (46), (27), and (24) lead to

$$\begin{aligned} \Delta(\mathbf{R}, \mathbf{p}) &\equiv \sum_{j=0}^{\infty} \hbar^j f_j(\mathbf{R}, \mathbf{p}) = \sum_{j=0}^{\infty} \hbar^j \int d^3 r e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} v(\mathbf{r}) \\ &\times \int \frac{d^3 q}{(2\pi\hbar)^3} e^{-i\mathbf{q}\cdot\mathbf{r}/\hbar} D_{j,1}(\mathbf{R}, \mathbf{q}). \end{aligned} \quad (56)$$

Calculating the first few $g_j(\mathbf{R})$'s and $f_j(\mathbf{R}, \mathbf{p})$'s, it can be seen that the \mathbf{R} dependence enters in g_j and f_j through the quantities $U(\mathbf{R})$ and $\Delta(\mathbf{R}, \mathbf{p})$ and through the spatial derivatives of order $\leq j$ of $U(\mathbf{R})$ and $\Delta(\mathbf{R}, \mathbf{p})$. For $j = 0$ there are no spatial derivatives [see Eqs. (47) and (48)]. For $j = 1$ the Poisson brackets in (49) bring the dependence also on gradients of $U(\mathbf{R})$ and $\Delta(\mathbf{R}, \mathbf{p})$ into $B_{1,1}$, and correspondingly into $g_1(\mathbf{R})$ for complex Δ . $B_{1,1}$ vanishes if Δ real, and we consider in the following only this case. Here we write the $j = 2$ results

expressed in terms of the generalized Poisson brackets,

$$\begin{aligned}
B_{2,1}(\mathbf{R}, \mathbf{p}) &= -\frac{2v^3\Delta - 3v\Delta^3}{16E^7} \{\Delta; v, v\} - \frac{3\Delta^2 v}{32E^5} \{v, v\}_+ \\
&\quad - \frac{2v\Delta^3 - 3v\Delta^2}{16E^7} \{\Delta; \Delta, \Delta\} - \frac{3v^2\Delta^2 - v^4 - \Delta^4}{8E^7} \{\Delta; v, \Delta\} \\
&\quad - \frac{\Delta^4 - 4v^2\Delta^2}{16E^7} \{v; v, v\} - \frac{v(2v^2 - 3\Delta^2)\Delta}{8E^7} \{v; \Delta, v\} \\
&\quad - \frac{5v^2\Delta^2}{16E^7} \{v; \Delta, \Delta\} + \frac{(2v^2 - \Delta^2)\Delta}{16E^5} \{v, \Delta\}_+ \\
&\quad + \frac{v^3 + v\Delta^2}{16E^7} \{v, \Delta\}^2 - \frac{v^3 - 2v\Delta^2}{32E^5} \{\Delta, \Delta\}_+, \quad (57)
\end{aligned}$$

$$\begin{aligned}
D_{2,1}(\mathbf{R}, \mathbf{p}) &= \frac{(3\Delta^3 - 2v^2)v\Delta}{16E^7} \{v; v, v\} - \frac{3v^2\Delta}{32E^5} \{\Delta, \Delta\}_+ \\
&\quad - \frac{(\Delta^2 - 2v^2)\Delta}{32E^5} \{v, v\}_+ - \frac{v(2\Delta^2 - 3v^2)\Delta}{8E^7} \{\Delta; \Delta, v\} \\
&\quad - \frac{v(2\Delta^2 - 3v^2)\Delta}{16E^7} \{v; \Delta, \Delta\} - \frac{v(v^2 - 2\Delta^2)}{16E^5} \{v, \Delta\}_+ \\
&\quad - \frac{5v^2\Delta^2}{16E^7} \{\Delta; v, v\} + \frac{v^4 + \Delta^4 - 3v^2\Delta^2}{8E^7} \{v; \Delta, v\} \\
&\quad - \frac{v^4 - 4v^2\Delta^2}{16E^7} \{\Delta; \Delta, \Delta\} + \frac{\Delta}{16E^5} \{v, \Delta\}^2. \quad (58)
\end{aligned}$$

For the δ interaction Eq. (56) simplifies; $f_j(\mathbf{p}, \mathbf{R})$ has no momentum dependence:

$$\begin{aligned}
\Delta(\mathbf{R}) &\equiv \sum_{j=0}^{\infty} \hbar^j f_j(\mathbf{R}) \\
&= \frac{4\pi\hbar^2 a}{m} \sum_{j=0}^{\infty} \hbar^j \int \frac{d^3 p}{(2\pi\hbar)^3} D_{j,1}^{\text{reg}}(\mathbf{R}, \mathbf{p}), \quad (59)
\end{aligned}$$

where $D_{j,1}^{\text{reg}}$ denotes the regularized part of $D_{j,1}$, which can be obtained from Eq. (56) if the pseudopotential is used for the interaction. Equations (55) and (59) can be solved perturbatively whose formal solutions become of the form,

$$n(\mathbf{R}) = \sum_{j=0}^{\infty} \hbar^j n_j(\mathbf{R}), \quad (60)$$

$$\Delta(\mathbf{R}) = \sum_{j=0}^{\infty} \hbar^j \Delta_j(\mathbf{R}). \quad (61)$$

It is important to stress that on the right-hand sides of Eqs. (55) and (59) all the quantities g_j and f_j depend on the total $\Delta(\mathbf{R})$ and $U(\mathbf{R})$, thus $n_j \neq g_j$ and $\Delta_j \neq f_j$.

A. Local density approximation

The leading order $j = 0$ approximation in Eqs. (55) and (59) are equivalent to the LDA. In that approximation one has to solve the equations,

$$n_0(\mathbf{R}) = g_0(U_0(\mathbf{R}), \Delta_0(\mathbf{R})), \quad (62)$$

$$\Delta_0(\mathbf{R}) = f_0(U_0(\mathbf{R}), \Delta_0(\mathbf{R})). \quad (63)$$

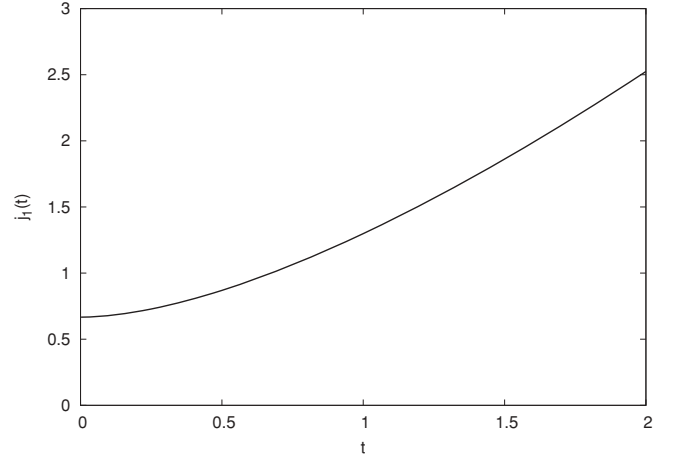


FIG. 1. The dimensionless function $j_1(t)$ defined in Eq. (A4).

The Hartree-Fock terms in $U(\mathbf{R})$ are density dependent. By the notation U_0 in that case we mean that they are evaluated using $n_0(\mathbf{R})$. If the Hartree-Fock terms are neglected $U_0 = U_{\text{ext}}$ and $U_j = 0$ for $j > 0$. Let us introduce the local chemical potential α by

$$\alpha(\mathbf{R}) = \mu - U(\mathbf{R}). \quad (64)$$

The quantity $v(\mathbf{R}, \mathbf{p})$ defined in Eq. (23) is simply $v(\mathbf{R}, \mathbf{p}) = p^2/2m - \alpha(\mathbf{R})$. The phase space quantity $E(\mathbf{R}, \mathbf{p})$ in Eq. (44) with real $\Delta(\mathbf{R})$ is equal to $E(\mathbf{R}, \mathbf{p}) = \sqrt{v^2(\mathbf{R}, \mathbf{p}) + \Delta(\mathbf{R})^2}$. The g_0 function occurring in (62) can be calculated from (55) and (47) and it is given by

$$g_0(U(\mathbf{R}), \Delta(\mathbf{R})) = \frac{1}{2} \int \frac{d^3 p}{(2\pi\hbar)^3} \left(1 - \frac{v(\mathbf{R}, \mathbf{p})}{E(\mathbf{R}, \mathbf{p})} \right). \quad (65)$$

The momentum integrals can be performed analytically,

$$g_0(U(\mathbf{R}), \Delta(\mathbf{R})) = \frac{1}{4\pi^2} \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{3/2} j_1 \left(\frac{\Delta(\mathbf{R})}{\alpha(\mathbf{R})} \right), \quad (66)$$

where we have used the dimensionless function $j_1(x)$ (see Appendix A and Fig. 1). The f_0 function in (63) can be calculated in a similar way:

$$f_0(U(\mathbf{R}), \Delta(\mathbf{R})) = -\frac{\Delta(\mathbf{R})}{2} g \int \frac{d^3 p}{(2\pi\hbar)^3} \left[\frac{1}{E(\mathbf{R}, \mathbf{p})} - \frac{2m}{p^2} \right]. \quad (67)$$

The second term in the integrand ensures a finite value for the momentum integral (i.e., $D_{0,1}$ is regularized with this term subtracted). The momentum integral in Eq. (67) can be written in terms of complete elliptic functions (see Appendix A) and can be expressed for negative scattering length as

$$f_0(U(\mathbf{R}), \Delta(\mathbf{R})) = \Delta(\mathbf{R}) \frac{2}{\pi} |a| \sqrt{\frac{2m\alpha(\mathbf{R})}{\hbar^2}} i_1 \left(\frac{\Delta(\mathbf{R})}{\alpha(\mathbf{R})} \right), \quad (68)$$

where the dimensionless function $i_1(x)$, depicted in Fig. 2, is defined by Eq. (A3). The overall constant chemical potential μ is fixed by

$$\frac{N}{2} = \int n_0(\mathbf{R}) d^3 R. \quad (69)$$

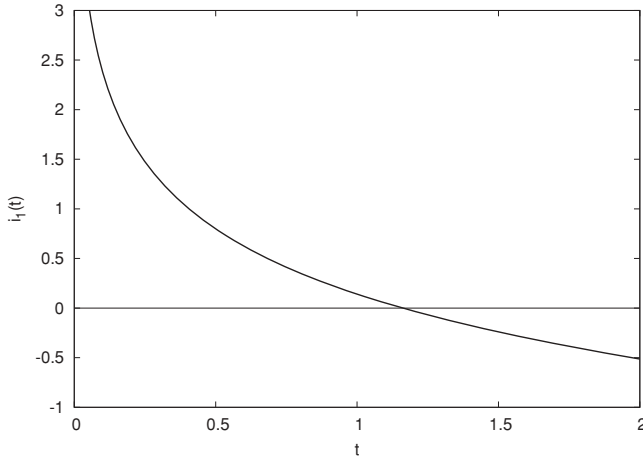


FIG. 2. The dimensionless function $i_1(t)$ defined in Eq. (A3).

Here N is the total particle number (including both hyperfine states). Solutions to Eqs. (62), (63), and (69) with g_0 and f_0 given by (66) and (68) are the solutions in leading order. Thus, the zeroth-order terms in the gradient expansion lead to the local density approximation. This corresponds to the Thomas-Fermi approach generalized to taking into account the pairing field $\Delta(\mathbf{r})$. In the following we shall calculate corrections to g_0 and f_0 .

B. $O(\hbar)$ order

We have shown that for real Δ the quantity $B_{1,1}$ is zero. Thus, $g_1(\mathbf{R}) = 0$ in Eq. (55). Due to the property (52) the regularized part of $D_{1,1}$ is also zero. It means there are no corrections to the density and to the gap equations in this $j = 1$ order.

C. $O(\hbar^2)$ order

The evaluations of the $j = 2$ second-order corrections $g_2(\mathbf{R})$, $f_2(\mathbf{R})$ are rather tedious. In the case of the momentum-independent gap and $v(\mathbf{R}, \mathbf{p})$ given by Eq. (23) nonvanishing generalized Poisson brackets are

$$\{v, \Delta\}^2 = \sum_{i,j=1}^3 \frac{p_i p_j}{m m} (\nabla \Delta)_i (\nabla \Delta)_j, \quad (70)$$

$$\{v, v\}_+ = \frac{2}{m} (\nabla^2 U), \quad \{v, \Delta\}_+ = \frac{1}{m} (\nabla^2 \Delta), \quad (71)$$

$$\{v; v, v\} = \frac{1}{m} (\nabla U)^2 + \sum_{i,j=1}^3 \left[\left(\frac{\partial^2 U}{\partial R_i \partial R_j} \right) \frac{p_i p_j}{m m} \right],$$

$$\{v; \Delta, v\} = \frac{1}{m} (\nabla \Delta) (\nabla U), \quad (72)$$

$$\{\Delta; v, v\} = \frac{1}{m^2} \sum_{i,j=1}^3 \left(\frac{\partial^2 \Delta}{\partial R_i \partial R_j} \right) p_i p_j,$$

$$\{v; \Delta, \Delta\} = \frac{1}{m} (\nabla \Delta)^2.$$

Note that the Laplace operator will be written as ∇^2 to avoid confusion with the gap. We gave a general expression for $B_{2,1}$

in Eq. (57) by which g_2 can be obtained by evaluating the momentum integrals. For the details, see Appendix A. The result is rather lengthy and can be presented in the following way. Let us define

$$A(\alpha) \equiv A(\alpha(\mathbf{R})) = \frac{(2m\alpha(\mathbf{R}))^{3/2}}{2\pi^2 \hbar^3}, \quad (73)$$

and the dimensionless combination t by

$$t \equiv t(\mathbf{R}) = \frac{\Delta(\mathbf{R})}{\alpha(\mathbf{R})}, \quad (74)$$

where $\alpha(\mathbf{R})$ is the local chemical potential (64). The second-order correction g_2 to the density Eq. (55) is

$$g_2(\mathbf{R}) = A(\alpha) \left[\frac{(\nabla^2 U)}{m\alpha^2} H_1(t) + \frac{(\nabla \Delta)(\nabla U)}{m\alpha^3} H_2(t) + \frac{(\nabla \Delta)^2}{m\alpha^3} H_3(t) + \frac{(\nabla^2 \Delta)}{m\alpha^2} H_4(t) + \frac{(\nabla U)^2}{m\alpha^3} H_5(t) \right]. \quad (75)$$

Functions $H_1(t), \dots, H_5(t)$ are given in Appendix B by Eq. (B1). The second-order corrections to the gap equation can be calculated using Eqs. (58) and (59). In second order the momentum integrals exist, consequently $D_{2,1}^{\text{reg}} = D_{2,1}$ (i.e., there is no need to regularize $D_{2,1}$). Proceeding as mentioned previously, the momentum integrals can be treated as in Appendix A. Second-order gradient correction f_2 to the gap Eq. (59) can be expressed as

$$f_2(\mathbf{R}) = g A(\alpha) \left[\frac{(\nabla^2 U)}{m\alpha^2} M_1(t) + \frac{(\nabla \Delta)(\nabla U)}{m\alpha^3} M_2(t) + \frac{(\nabla \Delta)^2}{m\alpha^3} M_3(t) + \frac{(\nabla^2 \Delta)}{m\alpha^2} M_4(t) + \frac{(\nabla U)^2}{m\alpha^3} M_5(t) \right], \quad (76)$$

where the functions $M_1(t), \dots, M_5(t)$ also can be found in Appendix B in Eq. (B2). From Eqs. (75) and (76) it is obvious that the second-order corrections to the density and to the gap equation involve the spatial derivatives of the external potential U_{ext} and the gap profile Δ . If the generalized Hartree-Fock approximation is considered, g_2 and f_2 will contain terms with the spatial derivatives of the density, too.

In second-order approximation $n \approx n_0 + \hbar^2 n_2$, $\Delta \approx \Delta_0 + \hbar^2 \Delta_2$, $U \approx (U_{\text{ext}} + gn_0) + \hbar^2 gn_2$. Expanding both sides of Eqs. (55) and (59) up to second order in \hbar , the zeroth-order terms cancel. The second-order gradient corrections to density and the gap are the solution of the

$$\begin{pmatrix} 1 - \partial_1 g_0(U_0, \Delta_0) & -\partial_2 g_0(U_0, \Delta_0) \\ -\partial_1 f_0(U_0, \Delta_0) & 1 - \partial_2 f_0(U_0, \Delta_0) \end{pmatrix} \begin{pmatrix} n_2 \\ \Delta_2 \end{pmatrix} = \begin{pmatrix} g_2 \\ f_2 \end{pmatrix} \quad (77)$$

inhomogeneous linear equations (here ∂_1 and ∂_2 denote partial derivatives with respect to n_0 and Δ_0 , respectively).

The spatial derivatives of the density in Eqs. (75) and (76) are, however, missing if the MF-BCS model is considered, which neglects the Hartree-Fock terms in v . The density and the gap still get gradient corrections in the case of this model, which will be studied next.

V. SECOND-ORDER CORRECTIONS CALCULATED PERTURBATIVELY IN THE MF-BCS MODEL

In the MF-BCS model the quantity,

$$\alpha(\mathbf{R}) = \mu - U_{\text{ext}}(\mathbf{R}), \quad (78)$$

is density independent and it is advantageous to use t defined in (74) instead of Δ . We keep the density Eq. (55), but rewrite (59) as

$$t(\mathbf{R}) = \sum_{j=0}^{\infty} \tilde{f}_j \hbar^j, \quad \tilde{f}_j = f_j / \alpha. \quad (79)$$

\tilde{f}_1 vanishes as in the previously discussed general case. Similarly to (61) we are seeking the solution for $t(\mathbf{R})$ as a formal series in \hbar ,

$$t(\mathbf{R}) = \sum_{j=0}^{\infty} \hbar^j t_j(\mathbf{R}), \quad (80)$$

where t_1 is zero due $\tilde{f}_1 = 0$. The first \tilde{f}_0 is given by

$$\tilde{f}_0 = \frac{2}{\pi} |a| \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{1/2} t_1(t), \quad (81)$$

and \tilde{f}_2 can be obtained from Eq. (76) by dividing both sides by α . g_0 is still given by (66)

In the MF-BCS model the leading order LDA equations are

$$n_0(\mathbf{R}) = \frac{1}{4\pi^2} \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{3/2} j_1(t_0), \quad (82)$$

$$1 = \frac{2}{\pi} |a| \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{1/2} i_1(t_0). \quad (83)$$

For fixed chemical potential μ the $t_0(\mathbf{R})$ profile can be calculated from (83).

To obtain the second-order gradient corrections n_2 and t_2 we can approximate in the expressions (75) and (76) for g_2 and \tilde{f}_2 the quantity t by its zeroth-order value t_0 , because g_2 and \tilde{f}_2 are already of second order. Taking the gradient of the leading order gap Eq. (83) $\nabla \Delta(\mathbf{R})$ can be approximated as

$$(\nabla \Delta_0(\mathbf{R})) = -(\nabla U_{\text{ext}}(\mathbf{R})) T_1(t_0), \quad (84)$$

where the dimensionless function $T_1(t)$ is given by

$$T_1(t) = \frac{j_3(t)}{t i_3(t)}. \quad (85)$$

[See Appendix A for the definitions of $i_n(t)$ and $j_n(t)$.] Taking the divergence of the two sides of Eq. (84) $\nabla^2 \Delta_0(\mathbf{R})$ can be reduced to

$$\nabla^2 \Delta_0(\mathbf{R}) = -(\nabla^2 U_{\text{ext}}) T_1(t_0) + \frac{(\nabla U_{\text{ext}})^2}{\alpha} T_2(t_0), \quad (86)$$

where we have introduced another dimensionless t -dependent function $T_2(t)$. Explicitly:

$$T_2(t) = [t - T_1(t)] \times \frac{i_3(t)j_3(t) + 3t^2(j_5(t)i_3(t) - j_3(t)i_5(t))}{t^2 \cdot i_3^2(t)}. \quad (87)$$

Using Eqs. (84) and (86) in the expressions of the second-order corrections (75) and (76) and the results of Appendixes A and B the perturbatively calculated corrections are

$$g_2(\mathbf{R}) = \frac{A(\alpha)}{m\alpha^2} \left[\frac{(\nabla U_{\text{ext}})^2}{\alpha} P_1(t_0) + (\nabla^2 U_{\text{ext}}) Q_1(t_0) \right], \quad (88)$$

and

$$f_2(\mathbf{R}) = \frac{gA(\alpha)}{m\alpha^2} \left[\frac{(\nabla U_{\text{ext}})^2}{\alpha} P_2(t_0) + (\nabla^2 U_{\text{ext}}) Q_2(t_0) \right], \quad (89)$$

where $A(\alpha)$ is defined by (73). Explicit expressions for P_1 , Q_1 , P_2 , and Q_2 are given in Appendix B in Eqs. (B3)–(B6). Corrections (88) and (89) involve terms proportional to $(\nabla U_{\text{ext}})^2$ and $\nabla^2 U_{\text{ext}}$. We remind the reader that g is proportional to the scattering length a [see Eq. (5)].

Expanding both sides of Eq. (79) up to second order using $\tilde{f}_0(t) \approx \tilde{f}_0(t_0 + \hbar^2 t_2) \approx \tilde{f}_0(t_0) + \hbar^2 t_2 \tilde{f}'_0(t_0)$ the zeroth-order terms cancel, and t_2 can be expressed as

$$t_2 = -\frac{\tilde{f}_2}{t_0 i'_1(t_0)} \frac{1}{\frac{2|a|}{\pi} \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{1/2}}. \quad (90)$$

Note that t_2 depends on the scattering length only through t_0 . The second-order gradient correction of the gap is $\Delta_2(\mathbf{R}) = t_2(\mathbf{R})\alpha(\mathbf{R})$ in the MF-BCS model. Using the same approximation for the density the second-order gradient correction of the density is

$$n_2 = \frac{1}{4\pi^2} \left(\frac{2m\alpha(\mathbf{R})}{\hbar^2} \right)^{3/2} t_2 j'_1(t_0) + g_2. \quad (91)$$

These are the first nontrivial gradient expansion terms. The simplification in the MF-BCS model has arisen from the fact that in Eq. (77) the ∂_1 derivatives (i.e., the derivatives with respect to the density) are zero.

VI. UNIVERSAL PREFACTOR OF THE VON WEIZSÄCKER-TYPE CORRECTION

The present paper supplies the derivation of some of the relations used already in our earlier paper [10]. To compare with the results of [10] one has to apply the limit $a \rightarrow \infty$ to Eqs. (88)–(91) (see also Appendix B in applying this limit). The leading order $t_0(\mathbf{R})$ profile is constant, which can be seen from Eq. (83). Let us denote by T the root of $i_1(T) = 0$, then

$$t_0(\mathbf{R}) = T \approx 1.1622, \quad j_1(T) \approx 1.4688, \quad (92)$$

where T is defined by the requirement $i_1(T) = 0$ in order that Eq. (83) remains meaningful in the limit $a \rightarrow \infty$. See also (B7)–(B9). It leads to

$$2n(\mathbf{R}) = (\mu - U_{\text{ext}})^{3/2} \frac{1}{2\pi^2} j_1(T) \left(\frac{2m}{\hbar^2} \right)^{3/2} \left(1 - \frac{\hbar^2}{2m} j_1(0) \frac{21}{48} \frac{\nabla^2 U_{\text{ext}}}{(\mu - U_{\text{ext}})^2} - \frac{\hbar^2}{2m} j_1(0) \frac{21}{192} \frac{(\nabla U_{\text{ext}})^2}{(\mu - U_{\text{ext}})^3} \right). \quad (93)$$

Note that $n = n_{\uparrow} = n_{\downarrow}$ in our notation. Similarly from Eqs. (74), (79), (89), and (90) one gets

$$\Delta(\mathbf{R}) = T(\mu - U_{\text{ext}}) - \frac{4 + 7T^2 \hbar^2}{36T} \frac{\nabla^2 U_{\text{ext}}}{2m(\mu - U_{\text{ext}})} - \frac{7T^2 - 8 \hbar^2}{144T} \frac{(\nabla U_{\text{ext}})^2}{2m(\mu - U_{\text{ext}})^2}. \quad (94)$$

Equation (93) can be rewritten as

$$\mu - U_{\text{ext}} = (j_1(T))^{-2/3} (2\pi^2)^{2/3} \frac{\hbar^2}{2m} (2n)^{2/3} + \frac{7\hbar^2}{72m} \left\{ \frac{(\nabla(\mu - U_{\text{ext}}))^2}{4(\mu - U_{\text{ext}})^2} - \frac{\nabla^2(\mu - U_{\text{ext}})}{(\mu - U_{\text{ext}})} \right\}, \quad (95)$$

where we have taken into account that the second term in the right-hand side of the equation is a correction. The first step of the iteration on the right-hand side leads after a rearrangement to the Thomas-Fermi-Weizsäcker-type equation:

$$-\kappa_W \frac{\hbar^2}{2m} \frac{\nabla^2 n^{1/2}}{n^{1/2}} + \xi \kappa_F (2n)^{2/3} + U_{\text{ext}} = \mu. \quad (96)$$

Here,

$$\kappa_W = \frac{7}{27}, \quad \xi = \left(\frac{2}{3j_1(T)} \right)^{2/3}, \quad \kappa_F = \frac{\hbar^2}{2m} (3\pi^2)^{2/3}. \quad (97)$$

Note that ξ is the usual universal constant introduced for the homogeneous system by the definition $\mu = \xi \epsilon_F$ (ϵ_F being the Fermi energy $\hbar^2 k_F^2 / (2m)$, where $k_F = (6\pi^2 n)^{1/3}$). The previous value is valid in the MF-BCS model [2,10]. Numerically, $\xi = 0.59$ in this model, while the Monte Carlo simulations have provided $\xi = 0.37 - 0.44$ [2,24]. Note that for a normal system at unitarity $\xi = 0.55$ [25–27], the corresponding MF-BCS value is $\xi = 1$ (i.e., free gas value), since $\xi_N = \alpha + \beta$, where α is the ratio of the mass and the effective mass (being unity in the MF-BCS model) and β is zero (see Ref. [27] and references therein). The first term on the left-hand side of Eq. (96) is of the form of the von Weizsäcker correction to the Thomas-Fermi theory (see for the early history of the problem Ref. [28]). By now it is well established that $\kappa_W = 1$ (originally derived by von Weizsäcker) is the correct value in case of a rapidly varying density with a small amplitude, while in the case of a smooth external potential $\kappa_W = 1/9$. This value of κ_W was first derived by Kirzhnits [29] and by Kompaneets and Pavlovskii [30] (see for reviews of the density gradient expansions [11,31,32]).

It is worth mentioning that $\kappa_W = 1/9$ was found [33] the optimal value when the energy of a free gas in a harmonic oscillator potential was compared with the quantum mechanical result via second-order perturbation theory. This suggests that such an external potential occurring in trapped gases is well suited for a gradient expansion of the density.

There has been a renewed interest in recent years concerning the von Weizsäcker correction in the case of the trapped unitary Fermi gas [34–43]. The value of $\kappa_W = 1$ has been chosen in [34,35], while $\kappa_W = 1/4$ has been obtained in [36,37,39,40] by assuming the validity of a kind of Ginzburg-Landau theory at zero temperature. Furthermore,

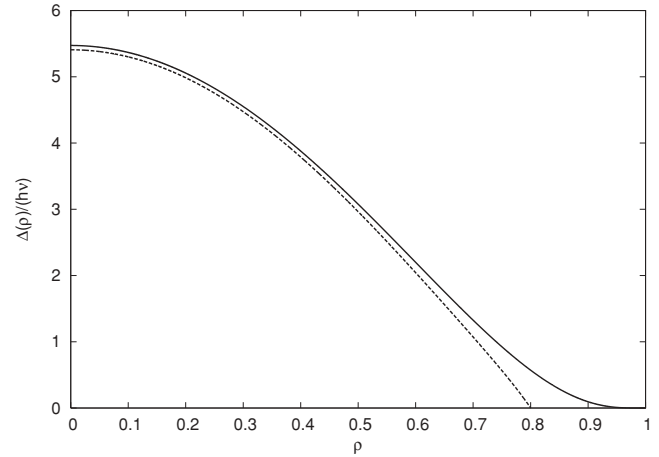


FIG. 3. Solutions of the gap equation without (solid line) and with (dashed line) the second-order gradient corrections as a function of the dimensionless radius $\rho = R/R_{\text{TF}}$, and measured in units of $\hbar\omega_0 = \hbar v$ (see text). Parameters are $a/d = 1/(3\pi)$, $R_{\text{TF}}/d = 8$.

an expansion in powers of $d = 4 - \epsilon$ spatial dimensions has led to $\kappa_W = 0.176$ [42] by extrapolating the result to three dimensions. A comparison between the choices $\kappa = 1/9$ and $\kappa = 1/4$ has been carried out in [43] by studying fermion systems at unitarity with particle numbers up to 50. It has been found that the choice $\kappa_W = 1/4$ provides better results for the energy except at few particle numbers. This finding backs our result for $\kappa_W = 7/27$, which is quite close to this value.

VII. ISOTROPIC HARMONIC TRAPPING

As an application of Eqs. (88)–(91) let us apply our results to the special case of isotropic harmonic trapping potential,

$$U(\mathbf{R}) = \frac{1}{2} m \omega_0^2 R^2. \quad (98)$$

In local density approximation the Thomas-Fermi radius R_{TF} is introduced by the relation,

$$\mu = \frac{1}{2} m \omega_0^2 R_{\text{TF}}^2, \quad (99)$$

which ensures $n_0(R_{\text{TF}}) = 0$. It is advantageous to use the dimensionless combination,

$$\varrho = R/R_{\text{TF}}, \quad (100)$$

for the radial distance. A natural characteristic length of the harmonic oscillator problem is the oscillator length $d = \sqrt{\hbar/(m\omega_0)}$. The LDA gap equation (83) for harmonic confinement,

$$1 = \frac{2}{\pi} \frac{|a|R_{\text{TF}}}{d^2} (1 - \varrho^2)^{1/2} i_1(t_0), \quad (101)$$

provides us a profile $t_0(\varrho)$, which depends on the single dimensionless parameter $|a|R_{\text{TF}}/d^2$. Up to second-order gradient corrections the gap can be expressed as

$$\frac{\Delta(\varrho)}{\hbar\omega_0} \cong \frac{1}{2} \left(\frac{R_{\text{TF}}}{d} \right)^2 (1 - \varrho^2) \left(t_0(\varrho) + \frac{d^4}{R_{\text{TF}}^4} \delta \tilde{t}(\varrho) \right), \quad (102)$$

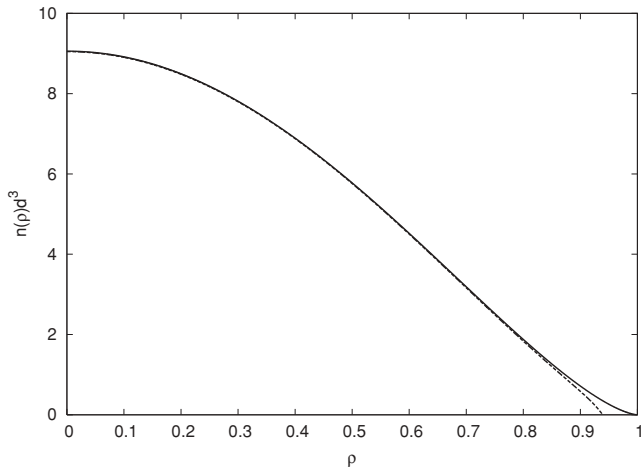


FIG. 4. Density profiles without (solid line) and with (dashed line) the second-order gradient corrections as a function of the dimensionless radius $\rho = R/R_{\text{TF}}$, and measured in units of $1/d^3$. Parameters are $a/d = 1/(3\pi)$, $R_{\text{TF}}/d = 8$.

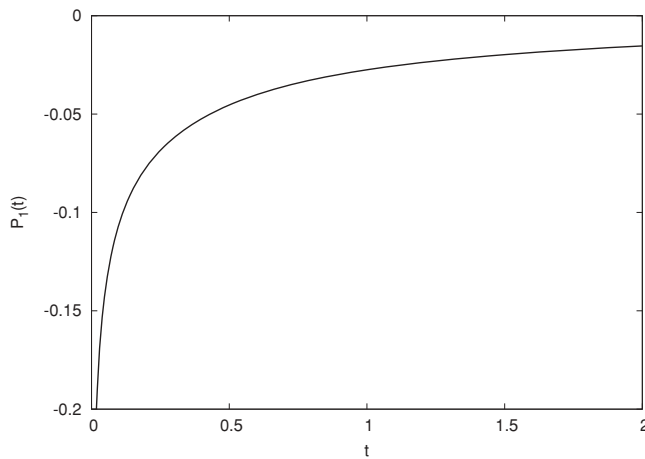


FIG. 5. The $P_1(t)$ function [see Eq. (B3)].

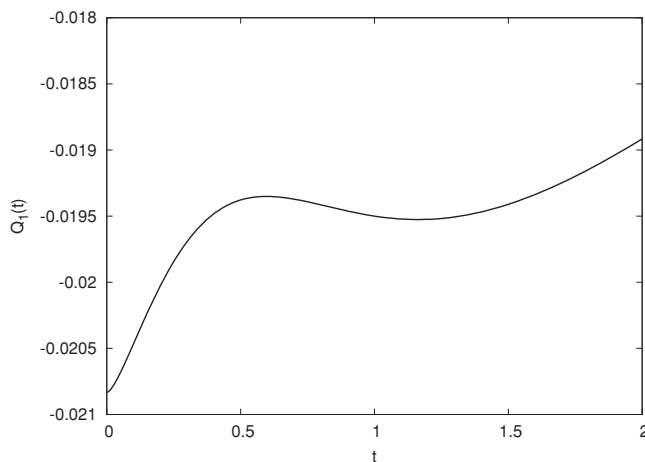


FIG. 6. The $Q_1(t)$ function [see Eq. (B4)].

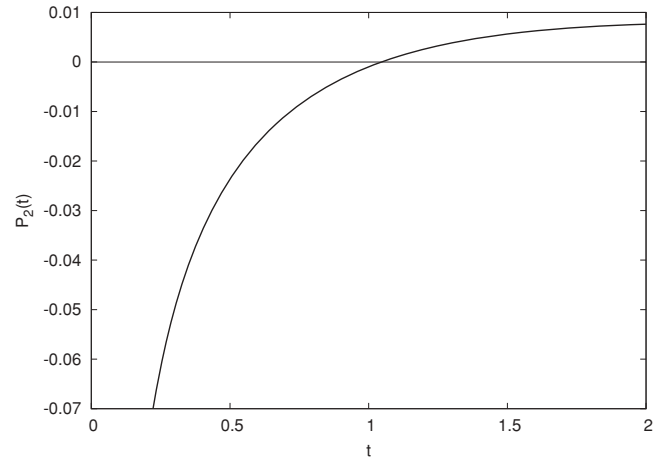


FIG. 7. The $P_2(t)$ function [see Eq. (B5)].

where $\delta\tilde{t}$ can be read off from (90) as

$$\delta t = \frac{1}{t_0 i_1'(t_0)} \left(\frac{16\varrho^2 P_2(t_0)}{(1-\varrho^2)^3} + \frac{24 Q_2(t_0)}{(1-\varrho^2)^2} \right). \quad (103)$$

Equation (91) together with the leading LDA for the density can be expressed as

$$d^3 n(\varrho) \cong \frac{(1-\varrho^2)^{3/2}}{4\pi^2} \frac{R_{\text{TF}}^3}{d^3} \left[j_1(t_0) + \frac{d^4}{R_{\text{TF}}^4} \delta\tilde{n}(\varrho, t_0) \right], \quad (104)$$

where

$$\delta\tilde{n}(\varrho, t_0) = \frac{16\varrho^2}{(1-\varrho^2)^3} \left(P_1(t_0) + \frac{j_1'(t_0)}{t_0 i_1'(t_0)} P_2(t_0) \right) + \frac{24}{(1-\varrho^2)^2} \left(Q_1(t_0) + \frac{j_1'(t_0)}{t_0 i_1'(t_0)} Q_2(t_0) \right). \quad (105)$$

It is clearly seen that the small parameter of the problem is d/R_{TF} . The magnitude of the correction as compared to the leading term is proportional to $(d/R_{\text{TF}})^4$ both for the density and the gap.

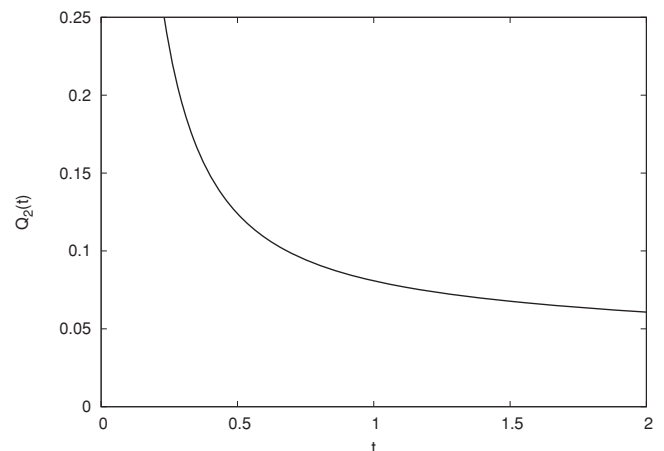


FIG. 8. The $Q_2(t)$ function [see Eq. (B6)].

At the Feshbach point ($a \rightarrow \infty$) our results can further simplify

$$\delta\tilde{\tau} = -\frac{7T^2 - 8}{36T} \frac{\varrho^2}{(1 - \varrho^2)^3} - \frac{7T^2 + 4}{6T} \frac{1}{(1 - \varrho^2)^2}, \quad (106)$$

$$\delta\tilde{n} = -7j_1(T) \left(\frac{1}{24} \frac{\varrho^2}{(1 - \varrho^2)^3} + \frac{1}{4} \frac{1}{(1 - \varrho^2)^2} \right). \quad (107)$$

$\delta\tilde{\tau}$ and $\delta\tilde{n}$ are universal at unitarity (at the Feshbach resonance) for a spherical parabolic trap: They do not contain any parameter of the two-particle interaction.

VIII. SUMMARY AND CONCLUSIONS

We have calculated the gradient corrections on the BCS side of the Feshbach resonance to the generalized Thomas-Fermi model, which represents the LDA in the presence of pairing. Though the correction terms have a prefactor, which is small for typical trap potentials already at moderately large particle numbers, the corrections get large due to the singularities at the LDA border of the cloud. At unitarity a von Weizsäcker-type correction appears whose universal prefactor has been derived as $\kappa_W = 7/27$. This value is quite close to $1/4$ proposed in Refs. [36,39–41] and is also not far from the ϵ -expansion result [42] as extrapolated to three dimensions.

It is remarkable that by inverting the functional $n[U_{\text{ext}}]$ to order \hbar^2 , as it has been done in Sec. VI, the singularities at $\mu = U_{\text{ext}}$ disappear and the density can be continued to infinity. This situation is similar to what happens in the case of the free gas, and perhaps, the most physical justification, which starts the calculation at finite temperature and the zero temperature limit is taken at the end [31,44,45]. One has to keep in mind, however, that it does not mean that even the asymptotic decay of the density follows the true one in general.

Away from unitarity, however, the situation is much more complicated and needs further study. Instead, then, one can use the treatment applied in Sec. VII (i.e., to regard the gradient terms as corrections and keep away from the surface region, which becomes, however, larger and larger when tending to the BCS limit).

In Fig. 3 we have depicted the gap profile $\Delta(\varrho)/\hbar\omega_0$ both in LDA and with gradient corrections. At a certain radius ϱ_2 the gap with gradient corrections becomes zero.

In Fig. 4 we show the dimensionless density profile at the same parameters as for Fig. 3. The deviation from the LDA profile is much less pronounced at those particular parameters in the region where the gradient expansion is applicable. Note that in the figures both curves are calculated at the same μ values, so they belong to slightly different particle numbers.

The distance ϱ_1 from the origin, where $\Delta(\varrho_1)/\hbar\omega_0 = 1$, decreases when the magnitude of the scattering length becomes shorter, which means that the most suitable situation exists at the Feshbach resonance. In the weak coupling (BCS) limit Δ is smaller than $\hbar\omega_0$ already at the point $\mathbf{r} = 0$. For $\varrho > \varrho_1$ the $\Delta(\varrho)/\hbar\omega_0$ function steeply goes to zero (see Fig. 3) beyond which point even its formal continuation becomes meaningless reflecting the fact that such an expansion is not adequate when the gap function $\Delta(\mathbf{r})$ gets smaller than the level spacing of the trap. One has to emphasize that this behavior has been shown when the first nonzero correction is treated perturbatively.

More generally, the solution levels off for increasing ϱ and one can define the radius ϱ_2 in such a way $\Delta(\varrho)/\hbar\omega_0 < \delta$ for $\varrho > \varrho_2$ with δ as a suitable chosen small parameter. Actually, in the region $\varrho > \varrho_2$ one has to apply another method instead of the one developed in this paper to get more accurate results, but the difference might be small. This problem goes beyond the scope of the present paper and is planned as a forthcoming work.

Note added: After submission of the paper we have learned that the density matrix in case of the inhomogeneous superfluid Fermi systems was derived in Ref. [46] to $o(\hbar^2)$ using the Wigner-Kirkwood \hbar -expansion method by regarding the pair potential as an external one, which is an intermediate step in our work (see also [8]). We are grateful to Professor Schuck for informing us of the papers [21,46].

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APPENDIX A: MOMENTUM INTEGRALS

In the zeroth order two types of momentum integrals occur:

$$K_1 = \int \frac{d^3 p}{(2\pi\hbar)^3} \left(\frac{1}{E} - \frac{2m}{p^2} \right) = \frac{A(\alpha)}{\alpha} i_1(t)|_{t=\Delta/\alpha}, \quad (A1)$$

$$L_1 = \int \frac{d^3 p}{(2\pi\hbar)^3} \left(1 - \frac{v}{E} \right) = A(\alpha) j_1(t)|_{t=\Delta/\alpha}, \quad (A2)$$

where $A(\alpha)$ has been introduced in (73) with α the local chemical potential (64). The dimensionless integrals $i_1(t)$ and $j_1(t)$ are defined as

$$i_1(t) = \int_0^\infty dx \left(\frac{x^2}{\sqrt{(x^2 - 1)^2 + t^2}} - 1 \right). \quad (A3)$$

$$j_1(t) = \int_0^\infty x^2 dx \left(1 - \frac{x^2 - 1}{\sqrt{(x^2 - 1)^2 + t^2}} \right). \quad (A4)$$

$i_1(t)$ and $j_1(t)$ can be expressed in terms of complete elliptic integrals $K(k)$ and $E(k)$ (see Ref. [47]):

$$K(k) = \int_0^{\pi/2} d\varphi \frac{1}{\sqrt{1 - k^2 \sin^2 \varphi}}, \quad (A5)$$

$$E(k) = \int_0^{\pi/2} d\varphi \sqrt{1 - k^2 \sin^2 \varphi}, \quad (A6)$$

as

$$i_1(t) = \sqrt[4]{1 + t^2} [K(k) - 2E(k)], \quad (A7)$$

$$j_1(t) = \frac{1}{3} \sqrt[4]{1 + t^2} \left[\frac{t^2 K(k)}{1 + \sqrt{(1 + t^2)}} + 2E(k) \right], \quad (A8)$$

where the modulus k is connected to t by

$$k = \sqrt{\frac{1}{2} \left(1 + \frac{1}{\sqrt{1 + t^2}} \right)}. \quad (A9)$$

In the special case $t = 0$: $k = 1$, $i_1(0) = \infty$, $j_1(0) = 2/3$. In higher orders one needs the generalizations of the

integrals (A1) and (A2). For $n = 3, 5, \dots$ let us consider the momentum integrals:

$$K_n = \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{E^n} = \frac{A(\alpha)}{\alpha^n} i_n(t)|_{t=\Delta/\alpha}, \quad n > 1, \quad (\text{A10})$$

$$L_n = \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{v}{E^n} = \frac{A(\alpha)}{\alpha^{n-1}} j_n(t)|_{t=\Delta/\alpha}, \quad n > 1. \quad (\text{A11})$$

Here the new dimensionless integrals $i_n(t)$, $j_n(t)$ are defined for odd n as

$$i_n(t) = \int_0^\infty x^2 dx \left(\frac{1}{\sqrt{(x^2 - 1)^2 + t^2}} \right)^n, \quad n > 1, \quad (\text{A12})$$

$$j_n(t) = \int_0^\infty x^2 dx \frac{x^2 - 1}{(\sqrt{(x^2 - 1)^2 + t^2})^n}, \quad n > 1. \quad (\text{A13})$$

(For similar integrals written in a different way see Ref. [48].) They can be obtained analytically from $i_1(t)$ and $j_1(t)$ using the rules,

$$i_{2n+1}(t) = (-1)^n \frac{1}{1 \cdot 3 \cdots (2n-1)} \left(\frac{1}{t} \frac{\partial}{\partial t} \right)^n i_1(t), \quad (\text{A14})$$

$$j_{2n+1}(t) = (-1)^{n-1} \frac{1}{1 \cdot 3 \cdots (2n-1)} \left(\frac{1}{t} \frac{\partial}{\partial t} \right)^n j_1(t), \quad (\text{A15})$$

which can be easily seen from definitions (A12) and (A13), respectively. Useful properties performing the gradient expansions are

$$j'_1(t) = t i_3(t), \quad (\text{A16})$$

$$i'_n(t) = -n t i_{n+2}(t), \quad (\text{A17})$$

$$j'_n(t) = -n t j_{n+2}(t), \quad n > 1. \quad (\text{A18})$$

In calculating explicitly $i_n(t)$ and $j_n(t)$ for odd n using the well-known formula for the derivatives of complete elliptic functions [47] it turns out that they are linear combinations of $i_1(t)$ and $j_1(t)$:

$$i_n(t) = A_n(t) i_1(t) + B_n(t) j_1(t), \quad (\text{A19})$$

$$j_n(t) = C_n(t) i_1(t) + D_n(t) j_1(t), \quad (\text{A20})$$

where the coefficients $A_n(t)$, $B_n(t)$, $C_n(t)$, and $D_n(t)$ are rational functions of t .

APPENDIX B: SECOND-ORDER COEFFICIENTS

Here we enumerate some dimensionless functions used in the main text. Functions occurring in Eq. (75) are

$$48H_1(t) = 8t^2 i_5(t) - 10t^4 i_7(t) - t^2 j_5(t) - 10t^4 j_7(t),$$

$$8H_2(t) = 5t^3 j_7(t) - 2t j_5(t),$$

$$48H_3(t) = 2i_3(t) - 17t^2 i_5(t) + 15t^4 i_7(t) + 2j_5(t), \quad (\text{B1})$$

$$48H_4(t) = 2t i_3(t) + 5t^3 i_5(t) - 10t^5 i_7(t) - 4t j_5(t) + 10t^3 j_7(t),$$

$$16H_5(t) = 4t^2 i_5(t) - 5t^4 i_7(t),$$

and those used in (76) are

$$48M_1(t) = 10t^3 j_7(t) - 4t j_5(t) + 2t i_3(t) + 5t^3 i_5(t) - 10t^5 i_7(t),$$

$$8M_2(t) = i_3(t) - 5t^2 i_5(t) + 5t^4 i_7(t),$$

$$48M_3(t) = 11t j_5(t) - 15t^3 j_7(t) + 2t i_5(t), \quad (\text{B2})$$

$$48M_4(t) = -3j_3(t) - t^2 j_5(t) + 10t^4 j_7(t) - 10t^2 i_5(t) + 10t^4 i_7(t),$$

$$16M_5(t) = 5t^3 j_7(t) - 2t j_5(t).$$

Straightforward, but lengthy, calculation leads to the analytic forms of the coefficient functions $P_1(t)$, $Q_1(t)$ occurring first in Eq. (88):

$$P_1(t) = -\frac{[8 + 3t^2]i_1(t)}{384(1+t^2)} - \frac{5j_1(t)}{128(1+t^2)} - \frac{t^4[1+t^2]i_1^4(t)}{192(3j_1(t) - t^2 i_1(t))^3} - \frac{t^2 i_1^3(t)[t^2 + 3]}{192(3j_1(t) - t^2 i_1(t))^2} - \frac{i_1^2(t)[4 + 3t^2]}{384(3j_1(t) - t^2 i_1(t))}, \quad (\text{B3})$$

$$Q_1(t) = \frac{t^2 i_1(t)}{96(1+t^2)} - \frac{j_1(t)}{32(1+t^2)} + \frac{t^2 i_1^2(t)}{96(3j_1(t) - t^2 i_1(t))}. \quad (\text{B4})$$

Similar calculation gives the expressions, for $P_2(t)$, $Q_2(t)$ [used in Eq. (89)]:

$$P_2(t) = -\frac{j_1(t)}{48t} + \frac{5t[i_1(t) + 3j_1(t)]}{384(1+t^2)} - \frac{t i_1(t)[5i_1(t) + 7j_1(t)]}{384(t^2 i_1(t) - 3j_1(t))} + \frac{t i_1(t)[-8i_1^2(t) + i_1(t)j_1(t) + 21j_1^2(t)]}{384(t^2 i_1(t) - 3j_1(t))^2} + \frac{[i_1(t) + 3j_1(t)] t i_1(t) j_1(t) [10i_1(t) + 21j_1(t)]}{192(t^2 i_1(t) - 3j_1(t))^3}, \quad (\text{B5})$$

$$Q_2(t) = \frac{i_1(t) + 3j_1(t)}{72t} + \frac{t[i_1(t) + 3j_1(t)]}{96(1+t^2)} - \frac{t i_1(t)[10i_1(t) + 21j_1(t)]}{288(t^2 i_1(t) - 3j_1(t))}. \quad (\text{B6})$$

The functions $P_1(t)$, $Q_1(t)$, $P_2(t)$ and $Q_2(t)$ are shown in Figs. 5, 6, 7, and 8 respectively. At the Feshbach resonance $i_1(T) = 0$ should be taken. In this case,

$$P_1(T) = -\frac{5j_1(T)}{128(1+T^2)}, \quad Q_1(T) = -\frac{j_1(T)}{32(1+T^2)}, \quad (\text{B7})$$

$$P_2(T) = -\frac{j_1(T)}{48T} + \frac{5Tj_1(T)}{128(1+T^2)}, \quad (\text{B8})$$

$$Q_2(T) = \frac{j_1(T)}{24T} + \frac{Tj_1(T)}{32(1+T^2)}. \quad (\text{B9})$$

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