Universal Relations of an Ultracold Fermi Gas with Arbitrary Spin-Orbit Coupling

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We derive the universal relations for an ultracold two-component Fermi gas with an spin-orbit coupling (SOC) \( \sum_{\alpha,\beta=x,y,z} \lambda_{\alpha\beta} \sigma_\alpha p_\beta \), where \( p_{x,y,z} \) and \( \sigma_{x,y,z} \) are the single-atom momentum and Pauli operators for pseudo spin, respectively, and the SOC intensity \( \lambda_{\alpha\beta} \) could take arbitrary value. We consider the system with an s-wave short-range interspecies interaction, and ignore the SOC-induced modification for the value of the scattering length. Using the first-quantized approach developed by S. Tan (Phys. Rev. Lett. 107, 145302 (2011)), we obtain the short-range and high-momentum expansions for the one-body real-space correlation function and momentum distribution function, respectively. For our system these functions are 2 × 2 matrix in the pseudo-spin basis. We find that the leading-order (1/\( k^4 \)) behavior of the diagonal elements of the momentum distribution function (i.e., \( n_\uparrow\uparrow(k) \) and \( n_\downarrow\downarrow(k) \)) is not modified by the SOC. However, the SOC can significantly modify the large-\( k \) behaviors of the distribution difference \( \delta n(k) \equiv n_\uparrow\uparrow(k) - n_\downarrow\downarrow(k) \) as well as the non-diagonal elements of the momentum distribution function, i.e., \( n_\uparrow\downarrow(k) \) and \( n_\downarrow\uparrow(k) \). In the absence of the SOC, the leading order of \( \delta n(k) \), \( n_\uparrow\downarrow(k) \) and \( n_\downarrow\uparrow(k) \) are \( \mathcal{O}(1/k^6) \). When SOC appears, it can induce a term on the order of 1/\( k^7 \) for these elements. We further derive the adiabatic relation and the energy functional. Our results show the SOC can induce a new term in the energy functional, which describe the contribution from the SOC to the total energy. In addition, the form of the adiabatic relation for our system is not modified by the SOC. Our results are applicable for the systems with any type of single-atom trapping potential, which could be either diagonal or non-diagonal in the pseudo-spin basis.

I. INTRODUCTION

In the recent decade a number of new kinds of experimental methods, such as magnetic and optical Feshbach resonances, were invented to tune the inter-atomic interactions for alkali and alkaline-earth atoms [1, 2]. A vast number of efforts were devoted to investigate the strongly interacting state of matter in such systems [3, 4]. The existence of strong correlation effects and the lack of small parameters for perturbative calculations make it very difficult to obtain any rigorous results for such strongly interacting systems. In recent years, a series of exact universal relations were established which for the first time set up a bridge between the microscopic short distance correlations and the macroscopic thermodynamic characters of the system [3, 26]. These relations show that many important properties of the system (e.g., the one-body momentum distribution, one-body spatial correlation function and many-body total energy) are related together via a parameter which contains the information of the interaction effect in the high-momentum limit, and is usually called as contact. These relations has already been confirmed in several different experiments [27, 30].

Another recent important progress in the research of ultracold gases is the successful experimental realization of synthetic coupling between atomic (pseudo) spin and momentum [31, 39]. Here we call this coupling as spin-orbit coupling (SOC). In these systems the SOC can strongly affect the one-body dispersion and thus seriously change the many-body properties. Therefore, the SO-coupled ultracold gases have attracted many attentions from both theorists and experimentalists [37, 42]. Thus, it is very natural to consider the universal relations in the SO-coupled ultracold gases. Recently S. Peng et. al. studied this problem for a system with a three-dimensional isotropic SOC \( (\sigma \cdot \mathbf{p}) \)-type) [13]. Here we derive the universal relations for the ultracold gases with arbitrary type of SOC. Explicitly, we consider an ultracold gas of identical Fermi atoms with pseudo spin \( \uparrow \) and \( \downarrow \), with a general type SOC which can be expressed as \( \sum_{\alpha,\beta=x,y,z} \lambda_{\alpha\beta} \sigma_\alpha p_\beta \), where \( p_{x,y,z} \) are the components of single-atom momentum and the SOC intensity \( \lambda_{\alpha\beta} \) could be arbitrary real numbers. In our system there could also be a general single-atom trapping potential, which can be expressed as an arbitrary atomic-position-dependent 2 × 2 matrix in the pseudo-spin basis.

We further assume that there is an s-wave short-range interaction between two atoms in different pseudo-spin states, which is described by the scattering length \( a \). In principle, the SOC may modify the value of \( a \) [39, 43]. Nevertheless, previous analytical [39] and numerical studies [44] have shown that in many ultracold gases, including the current experimental systems with Raman-beam-induced one-dimensional SOC, the SOC-induced modification of scattering length is negligible when the characteristic length of the SOC (defined as the inverse of the SOC intensity) is much larger than the range of the two-body interaction (i.e., the van der Waals...
length). This is normal situation in cold atom system. Thus, the starting point of our paper is that the scattering length is not changed by the SOC. This starting point is very different from the assumption in the recent work by S. Peng et. al. [13].

A. Our main results

For the convenience of the readers, here we briefly summarize the results we obtained.

(A) We derive the short-range expansion of the single-atom spatial correlation function \( \rho_{\sigma\sigma'}(r, r + b) \) (\( \sigma, \sigma' = \uparrow, \downarrow \)) of a many-body state \( |\Psi\rangle \), which is defined as

\[
\rho_{\sigma\sigma'}(r, r + b) \equiv \langle \Psi | \hat{d}_{\sigma}^\dagger(r) \hat{d}_{\sigma'}(r + b) |\Psi\rangle
\]

in the second quantized language and can form a 2 × 2 matrix in the pseudo-spin basis. Here \( \hat{d}_{\sigma}^\dagger(r) \) and \( \hat{d}_{\sigma}(r) \) are the creation and annihilation operators of an atom with pseudo spin \( \sigma \) at position \( r \). For the case where \( b \equiv |b| \) is small, we expand \( \rho_{\sigma\sigma'}(r, r + b) \) up to the 2nd order of \( b \) (see Eq. (11)). We find that the behavior of \( \rho_{\sigma\sigma'}(r, r + b) \) is not changed by the SOC in the 0th and 1st order of \( b \). Nevertheless, in the 2nd order of \( b \) a new non-analytical term can be induced by the SOC. This term is the leading non-analytical term of the non-diagonal elements \( \rho_{\uparrow\downarrow}(r, r + b) \) and \( \rho_{\downarrow\uparrow}(r, r + b) \).

(B) We derive the high-momentum expansion of the single-atom momentum distribution function \( n_{\sigma\sigma'}(k) \) (\( \sigma, \sigma' = \uparrow, \downarrow \)) of a many-body state \( |\Psi\rangle \), which is defined as

\[
n_{\sigma\sigma'}(k) \equiv (2\pi)^3 \langle \Psi | \hat{d}_{\sigma}^\dagger(k) \hat{d}_{\sigma'}(k) |\Psi\rangle,
\]

with \( \hat{d}_{\sigma}^\dagger(k) \) and \( \hat{d}_{\sigma}(k) \) being the creation and annihilation operators of an atom with pseudo spin \( \sigma \) and in the plane-wave state \( |k\rangle \) defined by \( |k\rangle = e^{ikr}/(2\pi)^3 \) [14]. It is clear that \( n_{\sigma\sigma'}(k) \) can also form a 2 × 2 matrix in the pseudo-spin basis. In previous researches people mainly study the behavior of the diagonal elements \( n_{\uparrow\uparrow}(k) \) and \( n_{\downarrow\downarrow}(k) \). For our system the non-diagonal terms \( n_{\uparrow\downarrow}(k) \) and \( n_{\downarrow\uparrow}(k) \) are also non-zero and should be studied. In the large-\( k \) limit we expand all the four elements \( n_{\sigma\sigma'}(k) \) to the order of \( 1/k^6 \) (see Eq. (19) and (25)), and find that:

- The leading-order (1/k^2) behavior of the diagonal elements \( n_{\uparrow\uparrow}(k) \) and \( n_{\downarrow\downarrow}(k) \) are not modified by the SOC. No matter if there is an SOC or not, we always have \( \lim_{k \to \infty} n_{\uparrow\uparrow}(k) = \lim_{k \to \infty} n_{\downarrow\downarrow}(k) = C/k^4 \). Here the parameter \( C \) can be defined as the contact corresponding to the state \( |\Psi\rangle \). As in the systems without SOC, the value of \( C \) is also related to the small-\( b \) behavior of \( \rho_{\sigma\sigma'}(r, r + b) \).

- The SOC can modify the behavior of \( n_{\uparrow\downarrow}(k) \) and \( n_{\downarrow\uparrow}(k) \) in the sub-leading order (1/k^3) by inducing a new term which is proportional to the contact \( C \). However, the behavior of the total momentum distribution \( n(k) \equiv n_{\uparrow\uparrow}(k) + n_{\uparrow\downarrow}(k) \) is still not modified by the SOC on this order.

- In the absence of the SOC, the difference \( \delta n(k) \equiv n_{\uparrow\uparrow}(k) - n_{\downarrow\downarrow}(k) \) of the diagonal elements, as well as the non-diagonal elements \( n_{\uparrow\downarrow}(k) \) and \( n_{\downarrow\uparrow}(k) \), are of the order of \( O(1/k^6) \) in the large-\( k \) limit. However, in the presence of SOC, a new term can be induced in the order \( 1/k^3 \) for these elements. This term is proportional to \( C \). Therefore, the SOC can significantly modify the leading-order behavior of \( \delta n(k) \), \( n_{\uparrow\downarrow}(k) \) and \( n_{\downarrow\uparrow}(k) \).

(C) We find that the adiabatic relation is not modified by the SOC. Explicitly, when \( |\Psi\rangle \) is an eigen-state of the many-body Hamiltonian \( H \), i.e., \( H |\Psi\rangle = E |\Psi\rangle \), then we still have \( \frac{\partial E}{\partial (\gamma_{-1/2})} = \frac{k^2}{4\pi m} C \), with \( m \) being the single-atom mass.

(D) We derive the energy functional for our system (see Eq. (37)), in which the average energy \( E = \langle \Psi | H |\Psi\rangle \) of an arbitrary many-body state \( |\Psi\rangle \) is expressed in terms of the single-atom momentum and position distribution functions (i.e., \( \rho_{\sigma\sigma'}(r, r) \) and \( n_{\sigma\sigma'}(k) \)), as well as the contact \( C \). We find that the SOC induce a new term for the energy functional, which is the average value of the SOC term in the Hamiltonian of all the atoms.

Our above results show that in the large-momentum limit the leading-order behavior of the universal relations are usually not modified by the SOC. This is can be explained as follows. The SOC is a linear function of the one-atom momentum \( p \), while the kinetic energy \( p^2/(2m) \) is a quadratic function of \( p \). Thus, in the large-momentum limit the SOC is much smaller than \( p^2/(2m) \), and thus cannot modify the leading-order behavior of the system.

The remainder of this paper is organized as follows. In Sec. II we describe our model and notations. In Sec. III we derive the short-range expansion of the single-atom spatial correlation function \( \rho_{\sigma\sigma'}(r, r + b) \). Using this result, in Sec. IV we derive the large-momentum expansion of the single-atom momentum distribution function \( n_{\sigma\sigma'}(k) \). The adiabatic relation and energy functional are derived in In Sec. V, and a summary and discussion are given in Sec. VI. In the appendix we present some details of our calculation.

II. SYSTEM AND WAVE FUNCTION

As shown above, we consider the system with \( N \) identical ultracold SO-coupled pseudo-spin-1/2 Fermi atoms. The single-atom Hamiltonian is given by

\[
H_{1b} = \frac{p^2}{2m} + \sum_{\alpha, \beta=x, y, z} \lambda_{\alpha\beta} \sigma_{\alpha} p_{\beta} + U(r),
\]

with \( p \) and \( r \) being the atomic momentum and position, respectively, and \( \sigma_{\alpha} \) (\( \alpha = x, y, z \)) being the Pauli operators of the atomic spin. Here \( U(r) \) is the single-atom...
trapping potential, which could be either diagonal or non-diagonal in the pseudo-spin basis.

The Hilbert space \( \mathcal{H} \) of our system is given by \( \mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_s \), where \( \mathcal{H}_r \) and \( \mathcal{H}_s \) are the Hilbert spaces for the \( N \)-atom spatial motion and \( N \)-atom spin, respectively. Here we use \(| \rangle \rangle \) to denote the total quantum state in \( \mathcal{H} \), and use \(| r \rangle \rangle s \) to denote the states in \( \mathcal{H}_r \) and \( \mathcal{H}_s \), respectively. In this paper we work in the “coordinate representation” where the \( N \)-body state \(| \Psi \rangle \rangle \) is described by a spinor wave function \(| \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle \), which is defined as

\[
| \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle = \langle r | \cdots | r | \Psi \rangle ,
\]

with \(| r \rangle \rangle \) being the eigen-state of the position of the atoms. Notice that \(| \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle \) is a \((\mathbf{r}_1, \ldots, \mathbf{r}_N)\)-dependent vector in the space \( \mathcal{H}_s \).

We further assume that there is an \( s \)-wave short-range two-body interaction between atoms in different pseudo-spin state. In the presence of SOC this interaction can be described by various zero-range models, e.g., the renormalized delta interaction [33] and the modified Bethe-Peierls boundary condition (MPBC) [39]. In this work we use the MPBC approach. In this approach, the wave function \(| \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle \) are defined in the region with \( \mathbf{r}_i \neq \mathbf{r}_j \) for \( \forall i, j \in (1, \ldots, N) \), and the total Hamiltonian \( H \) of the \( N \) atoms is just the summation of the free-Hamiltonians of each atom, i.e.,

\[
H = \sum_{i=1}^{N} H_{1b}^{(i)},
\]

with \( H_{1b}^{(i)} \) being the one-body Hamiltonian of the \( i \)-th atom. In addition, when two atoms (for instance, atoms 1 and 2) are close, in our notation the \( N \)-body wave function should satisfy

\[
\lim_{|\mathbf{r}_{12}| \to 0} | \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle = \left\{ \left( \frac{1}{|\mathbf{r}_{12}|} - \frac{1}{a} \right) | S \rangle \rangle_{12} \right\} \otimes | \Psi_{r_1} + \cdots + \Psi_{r_N} \rangle \rangle,
\]

Here \( \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 \), \( a \) is the scattering length, \(| S \rangle \rangle_{12} = (| \uparrow \rangle | \downarrow \rangle - | \downarrow \rangle | \uparrow \rangle ) / \sqrt{2} \) is the singlet spin state of the atoms 1 and 2, and \( G = (G_x, G_y, G_z) \) is a vector-type spin operator with the component \( G_\beta = \sum_{a=x,y,z} \lambda_{\alpha \beta} | \sigma_\alpha \rangle \rangle - \langle \sigma_\alpha | / 2 (\beta = x, y, z) \), where \( | \sigma_\alpha \rangle \rangle \) is the Pauli operator of the \( i \)-th atom. The term with operator \( G \) describes the SOC-induced modification for the short-range behavior of the wave function. In Eq. (3) \(| A(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle \rangle_{3, \ldots, N} \) is a spin state of the atoms \( 3, \ldots, N \), which depends on the positions of these atoms as well as the center-of-mass position of the atoms 1 and 2. As shown below, the important parameters in the universal relations, e.g., the contact \( C \), can be expressed in terms of \(| A \rangle \rangle_{3, \ldots, N} \).

### III. SINGLE-ATOM SPATIAL CORRELATION FUNCTION

In this section we derive the expansion of the single-atom spatial correlation function \( \rho_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b}) \) \((\sigma, \sigma' = \uparrow, \downarrow)\) in the short-range limit \( b \equiv | \mathbf{b} | \to 0 \). Our calculation is done via the approach in Ref. [12].

In the coordinate representation, \( \rho_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b}) \) \((\sigma, \sigma' = \uparrow, \downarrow)\) corresponding to a state \(| \Psi \rangle \rangle \), which is defined in Eq. (1), can be expressed as

\[
\rho_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b})
= N \times \text{Tr}_{2, \ldots, N} \int D_2 \left| \langle 1 | (\sigma' | \Psi_{\mathbf{r}+\mathbf{b}} \rangle \rangle_{s} | \Psi_{\mathbf{r}} | \sigma \rangle_1 \right|
\]

where \( D_2 = \prod_{i=2}^{N} d\mathbf{r}_i \),

\[
| \Psi_{\mathbf{r}} \rangle \rangle_{s} = | \Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N) \rangle \rangle_{s},
\]

\(| \sigma \rangle_{1} (\sigma = \uparrow, \downarrow)\) is the pseudospin states of atom 1, and \( \text{Tr}_{2, \ldots, N} \) is the trace for the spin states of atoms 2, ..., \( N \). To derive the small-\( b \) behavior of \( \rho_{\sigma, \sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b}) \), we divide the integration \( \int D_2 \) in Eq. (7) as

\[
\int D_2 = \int_{\mathcal{R}_e} D_2 + \int_{\mathcal{R}_c} D_2.
\]

Here \( \varepsilon \) is a small positive distance which satisfies \( \varepsilon > b \), \( \mathcal{R}_e \) is the region with \( | \mathbf{r} - \mathbf{r}_1 | > \varepsilon \) for \( \forall i = 2, \ldots, N \), i.e., the region where the distances between atom 1 and all the other atoms are larger than \( \varepsilon \), and \( \mathcal{R}_c \) is the complementary of \( \mathcal{R}_e \). Since \( \varepsilon > b \), in \( \mathcal{R}_c \) we also have \( | \mathbf{r} + \mathbf{b} - \mathbf{r}_1 | > 0 \) for \( \forall i = 2, \ldots, N \). According to (4), this fact implies that in the region \( \mathcal{R}_e \) the wave function \(| \Psi_{\mathbf{r}+\mathbf{b}} \rangle \rangle_{s} \), as a function of \( \mathbf{f} \), is analytical when \( | \mathbf{f} | \leq | \mathbf{b} | \). Thus, in \( \mathcal{R}_c \) we can expand \(| \Psi_{\mathbf{r}+\mathbf{b}} \rangle \rangle_{s} \) as a Taylor series of \( \mathbf{b} \):

\[
| \Psi_{\mathbf{r}+\mathbf{b}} \rangle \rangle_{s} = | \Psi_{\mathbf{r}} \rangle \rangle_{s} + \mathbf{b} \cdot \nabla_{\mathbf{r}} | \Psi_{\mathbf{r}} \rangle \rangle_{s} + \frac{1}{2} \sum_{\alpha, \beta = x, y, z} b_\alpha b_\beta \frac{\partial^2}{\partial r_\alpha \partial r_\beta} | \Psi_{\mathbf{r}} \rangle \rangle_{s} + \ldots(10)
\]
where \( b_{x,y,z} \) and \( r_{x,y,z} \) are the components of \( b \) and \( r \), respectively. On the other hand, in \( \tilde{R}_r \), the wave function \(|\Psi_{r+b}\rangle\) may diverges at some point \( f_b \) which satisfies \(|f_b| > |b| \). Namely, \(|b| \) may larger than the divergence radius of the function \(|\Psi_{r+b}\rangle\). Thus, in \( \tilde{R}_r \) we cannot do the expansion \(|10\rangle\) for \(|\Psi_{r+b}\rangle\). Therefore, in Eq. (11) we can use the expression \(|10\rangle\) to calculate the integration \( \int_{\tilde{R}_r} D_2 \), and use Eq. (8) with \( r_1 = r + b \) or \( r_1 = r \) to calculate \( \int_{\tilde{R}_r} D_2 \). For the small-\( b \)-case, with direct calculation we finally expand \( \rho_{\sigma,\sigma'}(r, r+b) \) as a series of \( b \) (Appendix A.1):

\[
\rho_{\sigma,\sigma'}(r, r+b) = \\
\rho_{\sigma,\sigma'}(r, r) + b \cdot u_{\sigma,\sigma'}(r) - \frac{b^2}{8\pi} C(r) \delta_{\sigma,\sigma'} + \\
\frac{b^2}{24\pi a} C(r) \delta_{\sigma,\sigma'} + \frac{1}{2} \sum_{\alpha,\beta = x,y,z} \nu_{\alpha\beta}(r) b_{\alpha} b_{\beta} + \\
-\frac{\pi}{2} b b \cdot [3 w(r) + w^*(r)] \delta_{\sigma,\sigma'} + s_{\sigma,\sigma'}(r, b) + O(b^3),
\]

where \( \delta_{\sigma,\sigma'} \) is the Kronecker symbol.

The quantities in each order of the r.h.s of Eq. (11) are defined and explained as follows.

0th order term: \( \rho_{\sigma,\sigma'}(r, r) \) is (up to a global factor) the density matrix element of the atom at position \( r \). If the SOC were absent and the trapping potential \( U(r) \) is diagonal in the pseudo-spin basis, we have \( \rho_{\uparrow\uparrow}(r, r) = \rho_{\downarrow\downarrow}(r, r) = 0 \).

1st-order terms: The factors \( u_{\sigma,\sigma'}(r) \) and \( C(r) \) are defined as

\[
\lim_{\eta \to 0^+} \int_{\tilde{R}_r} D_2 [1\langle \sigma' | (\nabla_r |\Psi_r\rangle_s \rangle \langle \Psi_r | \sigma \rangle_1],
\]

and

\[
C(r) = 8\pi^2 N(N-1) \int D_3 [3\ldots,N |A_r|A_r|3\ldots,N],
\]

respectively, with \( D_3 = \Pi_{i=3}^N dr_i \) and

\[
|A_r|3\ldots,N \equiv |A(r, r_3, \ldots, r_N)|3\ldots,N.
\]

Below we will show that the contact \( C \) for our systems can be defined as the integration of the factor \( C(r) \) with \( r \). Thus, \( C(r) \) can be considered the “contact density” of our system.

2nd order terms: The factors \( \nu_{\alpha\beta}(r) \), \( w(r) \) and \( s_{\sigma,\sigma'}(r, b) \) are given by

\[
\lim_{\eta \to 0^+} \int_{\tilde{R}_r} D_2 [1\langle \sigma' | (\frac{\partial^2}{\partial r_{\alpha} \partial r_{\beta}} |\Psi_r\rangle_s \rangle \langle \Psi_r | \sigma \rangle_1],
\]

and

\[
w(r) = \frac{1}{2} N(N-1) \int D_3 [3\ldots,N |A_r|A_r|3\ldots,N],
\]

respectively, with \( r_{x,y,z} \) being the components of \( r \) and

\[
B_{\sigma,\sigma'}^{(\alpha)} = \langle \sigma' | \sigma^{(1)}_\alpha | \sigma \rangle_1.
\]

In the absence of the SOC, the term \( s_{\sigma,\sigma'}(r, b) \) of Eq. (11) would disappear from the expansion of \( \rho_{\sigma,\sigma'}(r, r+b) \), while all the other terms still remain. Thus, the SOC does not affect the behavior of \( \rho_{\sigma,\sigma'}(r, r+b) \) in the 0th and 1st order of \( b \), and modify the behavior in the 2nd order by inducing the last term in the r.h.s. of Eq. (11), which is a non-analytical term and proportional to the contact density \( C(r) \) and the SOC intensity \( \lambda_{\alpha\beta} \). Especially, for the non-diagonal elements \( \rho_{\uparrow\downarrow}(r, r+b) \) and \( \rho_{\downarrow\uparrow}(r, r+b) \) this SOC-induced term is the lowest-order non-analytical term.

Furthermore, the appearance of the term \( s_{\sigma,\sigma'}(r, b) \) in Eq. (11) can be mathematically interpreted as follows. As shown above, to calculate \( \rho_{\sigma,\sigma'}(r, r+b) \) via Eq. (7) we require to do the integration \( \int_{\tilde{R}_r} D_2 \) in the region \( \tilde{R}_r \). Furthermore, in that region the states \(|\Psi_r\rangle_s \) and \(|\Psi_{r+b}\rangle_s \) in the to-be-integrated function \( i\langle \sigma' |\Psi_{r+b}\rangle_s \langle \Psi_r | \sigma \rangle_1 \) should be expanded via the MPBC shown in Eq. (8). The direct calculation shows that \( s_{\sigma,\sigma'}(r, b) \) is lead by the contribution from the SOC-induced term of the MPBC (i.e., the term proportional to \( G \) in Eq. (3)) to the integration \( \int_{\tilde{R}_r} D_2 \).

IV. MOMENTUM DISTRIBUTION FUNCTION

Using our above results on the short-range expansion of \( \rho_{\sigma,\sigma'}(r, r+b) \), we can now study the high-momentum behavior of the single-atom momentum distribution function \( n_{\sigma,\sigma'}(k) \) defined in (2). This factor is related to \( \rho_{\sigma,\sigma'}(r, r+b) \) via

\[
n_{\sigma,\sigma'}(k) = \int dr d\mathbf{b} e^{-i\mathbf{k} \cdot \mathbf{b}} \rho_{\sigma,\sigma'}(r, r+b).
\]

Substituting Eq. (11) into Eq. (18), we can obtain the expression of \( n_{\sigma,\sigma'}(k) \) in the large-\( k \) limit (Appendix A.2). In the following we investigate the SOC-induced effect for the diagonal and non-diagonal elements of the momentum distribution function.
A. Diagonal elements

In the large-$k$ limit the diagonal elements $n_{\uparrow \uparrow}(k)$ and $n_{\downarrow \downarrow}(k)$ are given by

$$n_{\sigma \sigma}(k) = \frac{C}{k^4} - \frac{i}{k^6} \mathbf{k} \cdot (3\mathbf{w} + \mathbf{w}^*) - \eta_\sigma \frac{4C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta + O \left( \frac{1}{k^6} \right), \quad (19)$$

for $\sigma = \uparrow, \downarrow$, with $\eta_\uparrow = +1$, $\eta_\downarrow = -1$. Here $k_{x,y,z}$ are the components of $\mathbf{k}$ and $\mathbf{w} = \int \mathbf{w}(r) \, dr$. In Eq. (19) the factor $C$ is defined as

$$C = \int d\mathbf{r} C(\mathbf{r}). \quad (20)$$

It is the contact of our system.

Eq. (19) shows that the leading-order behaviors of $n_{\uparrow \uparrow}(k)$ and $n_{\downarrow \downarrow}(k)$ are not changed by the SOC. Explicitly, no matter if there is an SOC we always have

$$\lim_{k \to \infty} n_{\uparrow \uparrow}(k) = \lim_{k \to \infty} n_{\downarrow \downarrow}(k) = \frac{C}{k^4}. \quad (21)$$

Nevertheless, in the sub-leading-order $(1/k^5)$ the SOC modify the behaviors of $n_{\uparrow \uparrow}(k)$ and $n_{\downarrow \downarrow}(k)$ by introducing a new term $-\frac{4C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta$, which is proportional to the SOC intensity $\lambda_{\alpha \beta}$ and the contact $C$.

Furthermore, when we calculate $n_{\sigma \sigma}(k)$ by substituting Eq. (11) into Eq. (18), we can find that the term $-\eta_\sigma \frac{4C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta$ of Eq. (19) is actually induced by the term $s_{\sigma \sigma}(r, b)$ of Eq. (11) (Appendix A). In addition, as shown in the end of Sec. III, $s_{\sigma \sigma}(r, b)$ is lead by the SOC-induced term (i.e., the term proportional to $G$) of the MBPC Eq. (6), which describes the behavior of the wave function in the short-range limit. Therefore, the SOC-induced term $-\eta_\sigma \frac{4C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta$ in Eq. (19) can be interpreted as a result of the SOC-induced modification of the short-range behavior of the wave function.

With the above results we can further get the behavior of the total momentum distribution $n(k)$, which is given by

$$n(k) = n_{\uparrow \uparrow}(k) + n_{\downarrow \downarrow}(k). \quad (22)$$

Substituting Eq. (19) into Eq. (22) we obtain that in the large-$k$ limit

$$n(k) = \frac{2C}{k^4} - \frac{32\pi^2}{k^6} \mathbf{k} \cdot (3\mathbf{w} + \mathbf{w}^*) + O \left( \frac{1}{k^6} \right). \quad (23)$$

In the absence of the the SOC, both of the two terms in the r.h.s. of Eq. (23) still exists. Thus, the behavior of $n(k)$ is not modified by the SOC up to the order of $1/k^5$.

We can further define the momentum-distribution difference of atoms with spin $\uparrow$ and $\downarrow$ as

$$\delta n(k) = n_{\uparrow \uparrow}(k) - n_{\downarrow \downarrow}(k). \quad (24)$$

Thus, Eq. (19) yields that

$$\delta n(k) = -\frac{8C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta + O \left( \frac{1}{k^6} \right). \quad (25)$$

This result shows that, if there were no SOC (i.e., $\lambda_{\alpha \beta} = 0$), then $\delta n(k)$ is at most on the order of $O(1/k^6)$, no matter if the trapping potential $U(r)$ is diagonal or non-diagonal in the pseudo-spin basis. However, in the presence of the SOC, a term $-\frac{8C}{k^6} \sum_{\beta = x,y,z} \lambda_{z\beta} k_\beta$ can be induced in the order of $1/k^5$. Namely, the SOC can significantly modify the behavior of $\delta n(k)$ by changing the leading order from at most $1/k^6$ to $1/k^5$. This result also implies that the SOC-induced modification of the single-atom momentum distribution may be experimentally detected via the measurement of the large-$k$ behavior of $\delta n(k)$.

B. Non-diagonal elements

The situation is quite different for the non-diagonal elements $n_{\uparrow \downarrow}(k)$ and $n_{\downarrow \uparrow}(k)$. Substituting Eq. (11) into Eq. (18), we find that in the large-$k$ limit we have

$$n_{\uparrow \downarrow}(k) = -\frac{4C}{k^6} \sum_{\beta = x,y,z} (\lambda_{x\beta} + i\lambda_{y\beta}) k_\beta + O \left( \frac{1}{k^6} \right), \quad (26)$$

and $n_{\downarrow \uparrow}(k) = n_{\uparrow \downarrow}(k)^*$. Therefore, similar as $\delta n(k)$, the large-$k$ behaviors of $n_{\uparrow \downarrow}(k)$ and $n_{\downarrow \uparrow}(k)$ are also significantly modified by the SOC and the leading order of these terms is changed from at most $1/k^6$ to $1/k^5$.

V. MANY-BODY ENERGY

In this section we use our above results to study the relations between the many-body energy and the contact, and derive the adiabatic relation and energy functional for our SO-coupled system.

A. Adiabatic relation

We consider the case that $|\Psi\rangle$ is an eigen-state (e.g., the ground state) of the Hamiltonian $H$, which satisfies the eigen-equation $H|\Psi\rangle = E|\Psi\rangle$ as well as the MBPC (40) with scattering length a. Thus, the eigen-energy $E$ depends on the value of $a$. Now we derive the adiabatic relation which connects $\partial E/\partial \langle -1/a \rangle$ and the contact $C$ for our SO-coupled system, with the approach shown in Ref. [17]. To this end we consider two systems $\alpha$ and $\beta$ with scattering lengths $a_\alpha$ and $a_\beta$, respectively, and assume $|\Psi^{(n)}\rangle$ ($n = \alpha, \beta$) is the normalized eigen-state of $H$ for system $n$, with corresponding eigen-energy $E_n$. We further assume these two eigen-energies have the same rank for each system. For instance, $|\Psi^{(\alpha)}\rangle$ and $|\Psi^{(\beta)}\rangle$ are
the ground states of the systems $\alpha$ and $\beta$, respectively, and $E_{\alpha, \beta}$ are the ground-state energies. Therefore, we have

$$\lim_{a_\alpha \to a_\beta} E_\alpha = E_\beta; \quad \lim_{a_\alpha \to a_\beta} \langle \Psi^{(\alpha)} \Psi^{(\beta)} \rangle = 1. \tag{27}$$

On the other hand, with the direct generalization of the approach used in Ref. \[17\], we can prove that (Appendix B) taking the limit $A_\beta - A_\alpha \to (\Psi^{(\alpha)})^\dagger \Psi^{(\beta)}$

$$= \frac{2\pi \hbar^2}{m} N(N-1) \int dr \int D_3 \left[ \sum_{\alpha, \beta} |A_\alpha(r)|^2 |A_\beta(r)|^2 \right]. \tag{28}$$

Here $|A_\alpha(n)\rangle_{3,\ldots,N}$ ($n = \alpha, \beta$) is the state of $A(r_1, r_2, \ldots, r_N)$ system $n$, and thus satisfies $\lim_{a_\alpha \to a_\beta} |A_\alpha(n)\rangle_{3,\ldots,N} = |A_\beta(n)\rangle_{3,\ldots,N}$. Substituting taking the limit $a_\alpha \to a_\beta$ for Eq. (28) and using Eqs. \[27\] \[12\] \[20\], we obtain the adiabatic relation

$$\frac{\partial E}{\partial (-1/a)} = \frac{\hbar^2}{4\pi m}, \tag{29}$$

which has the same form as in the systems without SOC.

### B. Energy functional

If $|\Psi\rangle$ is an arbitrary many-body state, the average energy can be defined as $\mathcal{E} = \langle \Psi | H | \Psi \rangle$ and can be expressed as a functional of the single-atom momentum and position distribution function. Now we derive the expression of this energy functional, with the help of our previous result in Eq. \[11\]. Here we use the similar approach as Ref. \[16\]. We first define a function $J(\beta)$ as

$$J(\beta) = \frac{1}{(2\pi)^3} \sum_{\sigma = \uparrow, \downarrow} \int dk n_{\sigma, \sigma}(k) e^{-\beta \frac{k^2}{2m}}. \tag{30}$$

Substituting Eq. \[13\] into this definition, we find that $J(\beta)$ can be re-expressed as

$$J(\beta) = \sum_{\sigma = \uparrow, \downarrow} \int dr \rho_\sigma(r) U_\beta(b) \rho_\sigma(r, r + b), \tag{31}$$

where $U_\beta(b) = (2\pi \hbar^2/m) \frac{\beta e^{-\beta \frac{b^2}{2m}}}{b}$. Using Eq. \[11\], we further obtain

$$J(\beta) = N - \frac{Ch\beta}{\sqrt{2m\pi^2}} + \frac{C\beta^2}{4\pi^2} + \beta K + O(\beta^{3/2}), \tag{32}$$

with $N = \int dr [\rho_{\uparrow}(r, r) + \rho_{\downarrow}(r, r)]$ being the total atom number and $K = \int dr_\alpha(r)$. On the other hand, the definition $\mathcal{E} = \langle \Psi | H | \Psi \rangle$ of the average energy yields

$$\mathcal{E} = \int dr U(r) - K + \sum_{\sigma, \sigma' = \uparrow, \downarrow} \int dk \left[ \lambda_{\sigma\beta} B_{\sigma\sigma'}^{(\alpha)} k_\beta n_{\sigma', \sigma}(k) \right] \tag{33}$$

where $B_{\sigma\sigma'}^{(x,y,z)}$ are the matrix-elements of the Pauli operator, as defined in Eq. \[17\], and $U_\beta(r) = \sum_{\sigma, \sigma' = \uparrow, \downarrow} U_{\sigma\sigma'}(r) d_{\sigma\sigma'}(r)$, with $U_{\sigma\sigma'}(r)$ being the matrix-element of the trapping potential in the one-body pseudospin basis and

$$d_{\sigma\sigma'}(r, r) = \rho_{\sigma\sigma'}(r, r). \tag{34}$$

Substituting Eq. \[33\] into Eq. \[34\] and using Eq. \[30\] as well as the relation

$$\frac{\hbar}{2\pi^2 \sqrt{2m\beta}} = \frac{1}{(2\pi)^3} \int dk \left( \frac{\hbar^2}{mk^2} e^{-\beta \frac{k^2}{2m}} \right), \tag{35}$$

we find that

$$\frac{1}{(2\pi)^3} \sum_{\sigma = \uparrow, \downarrow} \int dk e^{-\beta \frac{k^2}{2m}} \left[ n_{\sigma\sigma}(k) - \frac{C}{k^4} \right] = N + \frac{C\beta \hbar^2}{4\pi^2 m} - \beta \left[ \mathcal{E} - \int dr U(r) \right]$$

$$+ \beta \sum_{\alpha, \beta = x, y, z, \sigma, \sigma' = \uparrow, \downarrow} \int dk \left[ \lambda_{\alpha\beta} B_{\sigma\sigma'}^{(\alpha)} k_\beta n_{\sigma', \sigma}(k) \right] + O(\beta^{3/2}). \tag{36}$$

Doing the operation $\Delta_{\sigma\sigma'}(\ldots)|_{\beta=0}$ for both of the two sides of Eq. \[36\], we finally obtain the expression of the energy functional:

$$\mathcal{E} \mathcal{E} = \frac{\hbar^2}{4\pi^2 m} + \frac{1}{(2\pi)^3} \sum_{\sigma = \uparrow, \downarrow} \int dk \left( \frac{\hbar^2}{2m} \right) \left[ n_{\sigma\sigma}(k) - \frac{C}{k^4} \right]$$

$$+ \sum_{\sigma, \sigma' = \uparrow, \downarrow} \int dr \left[ U_{\sigma\sigma'}(r) d_{\sigma\sigma'}(r) \right]$$

$$+ \frac{1}{(2\pi)^3} \sum_{\alpha, \beta = x, y, z, \sigma, \sigma' = \uparrow, \downarrow} \int dk \left[ \lambda_{\alpha\beta} B_{\sigma\sigma'}^{(\alpha)} k_\beta n_{\sigma', \sigma}(k) \right]. \tag{37}$$

This result shows that the SOC modify the energy functional by introducing the last term of Eq. \[37\], which is just the average value of the SOC term in the total Hamiltonian $H$ on state $|\Psi\rangle$. Thus, this energy functional is the direct generalization of the one for the systems without SOC.

### VI. SUMMARY

In this paper we derive the universal relations for ultracold two-component Fermi gases with arbitrary type
SOC. We obtain the short-range and high-momentum expansions of the single-atom spatial correlation function $\rho_{\sigma\sigma'}(\mathbf{r} + \mathbf{b}) \ (\sigma, \sigma' = \uparrow, \downarrow)$ and momentum distribution function $n_{\sigma\sigma'}(\mathbf{k})$. We find that the SOC significantly modify the leading-order behaviors of $n_{\uparrow\uparrow}(\mathbf{k})$, $n_{\downarrow\downarrow}(\mathbf{k})$ and the distribution difference $n_{\uparrow\downarrow}(\mathbf{k}) - n_{\downarrow\uparrow}(\mathbf{k})$, and modify the sub-leading-order behaviors of each diagonal element $n_{\uparrow\uparrow}(\mathbf{r}, \mathbf{r} + \mathbf{b})$ and $n_{\downarrow\downarrow}(\mathbf{k})$ as well as all the four elements of $\rho_{\sigma\sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b})$. All of these modifications are proportional to the contact $C$, and are induced by the SOC-induced term in the MBPC \(\mathcal{G}\), i.e., the term proportional to the operator $G$. We further derive the adiabatic relation and energy functional for our system. Our calculations can be generalized to the two-dimensional systems.

Our results are helpful for the further theoretical and experimental studies of ultracold gases with SOC or the ultracold gases where the single-atom trapping potential $U(\mathbf{r})$ is non-diagonal in the pseudo-spin basis. We should also be careful that, the expressions of the SOC intensity $\lambda_{\alpha\beta} \ (\alpha, \beta = x, y, z)$ and the potential $U(\mathbf{r})$ are “frame-dependent”. For instance, for the experimental systems with one-dimensional SOC induced by the Raman laser beams, in the lab frame we have $U(\mathbf{r}) = \frac{\hbar}{2} \Omega(\mathbf{r}) |\uparrow\downarrow| + \text{h.c.}$, while in the rotated frame we have $U(\mathbf{r}) = \frac{\hbar}{2} \Omega(\mathbf{r}) |\uparrow\downarrow| + \text{h.c.}$ and $\lambda_{\alpha\beta} = (\hbar k_l/2) \delta_{\alpha z} \delta_{\beta x}$. Here $\Omega$ and $k_l$ being the effective Rabi frequency and wave vector of the Raman beams, respectively. Therefore, when working in a certain frame we should correctly use the corresponding expressions of $\lambda_{\alpha\beta}$ and the potential $U(\mathbf{r})$.

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Note added.-Recently, we became aware of a parallel paper by P. Zhang and N. Sun \cite{46}, where the large-$k$ expansion of the single-atom momentum distribution and the adiabatic relation are derived for the systems with one-dimensional and three-dimensional isotropic SOC and $U(\mathbf{r}) = 0$ via the effective-field theory approach. Our results are consistent.

Appendix A: Integrations

In this appendix we given some remarks on the calculation of the integration $\int D_2 = \int_{\mathcal{R}_2} D_2 + \int_{\mathcal{R}_x} D_2$ for Eq. (11) and the integration $\int db$ in Eq. (15). For the integration $\int D_2$, we have the following remarks:

1. To do the small-$b$ expansion, here we only need to consider the cases where both $b$ and $\varepsilon$ are very small. On the other hand, in principle, in the region $\mathcal{R}_x$ it is possible that more than one atoms are in the region with center $\mathbf{r}$ and radius $\varepsilon$. For instance, both atom 2 and atom 3 are in this region. Since in the wave function $|\Psi(\mathbf{r})\rangle$, the vector $\mathbf{r}$ is the position of atom 1, in this example the three atoms 1, 2 and 3 are very close to each other. Due to the Pauli principle, this possibility is very small and here we ignore this possibility. Namely, we assume in $\mathcal{R}_x$ only one atom is in the region with center $\mathbf{r}$ and radius $\varepsilon$.

2. In addition, since the final result of the integration $\int D_2 = \int_{\mathcal{R}_x} D_2 + \int_{\mathcal{R}_x} D_2$ is independent of the value of $\varepsilon$, here we calculate $\int_{\mathcal{R}_x} D_2$ and $\int_{\mathcal{R}_x} D_2$ to the 0th power of $\varepsilon$ and then sum the results.

3. Furthermore, also due to the identity of Fermionic atoms, the to-be-integrated function $\text{Tr}_{2,3} \langle \sigma(\mathbf{r} + \mathbf{b})|\sigma(\mathbf{r}_1)|\sigma(\mathbf{r}_2)|\Psi(\mathbf{r})\rangle$ is invariant under the exchange of $\mathbf{r}_i$ and $\mathbf{r}_j$ for $\forall i, j \in \{2, ..., N\}$. Thus, in our calculation we have

$$\int_{\mathcal{R}_x} D_2 = (N-1) \int_{\mathcal{R}_x^{(2)}} D_2,$$

(A1)

with $\mathcal{R}_x^{(2)}$ being the region with $|\mathbf{r}_2 - \mathbf{r}_1| < \varepsilon$.

For the integration $\int db$ in Eq. (15) we have the following remarks:

1. When we do this integration we first replace $\int db e^{-ik\mathbf{b}} \rho_{\sigma\sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b})$ with

$$\lim_{\zeta \to 0^+} \int db e^{-ik\mathbf{b}} e^{-\zeta b} \rho_{\sigma\sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b}),$$

and then replace $\rho_{\sigma\sigma'}(\mathbf{r}, \mathbf{r} + \mathbf{b})$ with the expansion (11).

2. In the large-$k$ limit, the contributions from the analytical terms of Eq. (11) to the Fourier transformation $\int db e^{-ik\mathbf{b}}$ would exponentially decay with $k$. Since now we want to extract the power terms which behave as $1/k^n$ with $n$ an integer, we only need to consider the contributions from the non-analytical terms of Eq. (11), i.e., the terms proportional to $b$, $b^2$, $b\mathbf{b}$ and $b\mathbf{b}_\beta$. For instance, the direct calculation gives

$$\lim_{\zeta \to 0^+} \int db e^{-ik\mathbf{b}} e^{-\zeta b} = -\frac{8\pi}{k^4} b\mathbf{b}_\beta = \frac{C(\mathbf{r})}{k^4} \delta_{\sigma\sigma'}. \quad \text{(A2)}$$

Thus, we have

$$\lim_{\zeta \to 0^+} \int db e^{-ik\mathbf{b}} e^{-\zeta b} \left[ \frac{b}{8\pi} C(\mathbf{r}) \delta_{\sigma\sigma'} \right] = \frac{C(\mathbf{r})}{k^4} \delta_{\sigma\sigma'}. \quad \text{(A3)}$$

Similarly, we also have

$$\lim_{\zeta \to 0^+} \int db e^{-ik\mathbf{b}} e^{-\zeta b} \delta_{\sigma\sigma}(\mathbf{r}, \mathbf{b}) = -\eta_\sigma \frac{4C(\mathbf{r})}{k^6} \sum_{\beta=x,y,z} \lambda_{\sigma\beta} k_\beta, \quad \text{(A4)}$$
for $\sigma = \uparrow, \downarrow$, where $s_{\sigma,\sigma}(r, b)$ is defined in Eq. (11) and $\eta_i = +1$ and $\eta_j = -1$. This result implies that the term $\eta_0 \psi(k)$ in Eq. (19) is lead by the term $s_{\sigma,\sigma}(r, b)$ of Eq. (11). The contribution from other non-analytical terms can be derived with similar calculations.

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Appendix B: Proof of Eq. (28)

In this appendix we prove Eq. (28) with the method in Ref. [17]. Our following calculation is a generalization of the calculation in Appendix B of Ref. [17] to our case with SOC. As shown in Sec. V.A of our main text, we assume $|\Psi(\alpha)\rangle$ and $|\Psi(\beta)\rangle$ are eigen-states of the many-body Hamiltonian $H$ of systems with scattering lengths $a_\alpha$ and $a_\beta$, and $E_{\alpha,\beta}$ are the corresponding eigen-energies. As in the main text, here we define the corresponding wave functions $|\psi^{(i)}\rangle_s \equiv s(r_1, ..., r_N)|\Psi^{(i)}\rangle$ ($i = \alpha, \beta$).

When $a_\alpha \neq a_\beta$, since $|\Psi(\alpha)\rangle$ and $|\Psi(\beta)\rangle$ satisfy the MBPC for different scattering lengths, in principle they are in different Hilbert spaces and thus the inner product between them is not well-defined. Nevertheless, here for our system, even if $a_\alpha \neq a_\beta$, we can still do the integration

$$I_{\alpha,\beta} \equiv \int D_1 \left( s_s^{(\alpha)}|\psi^{(\beta)}\rangle_s \right) = \int D_1 \left( |\Psi^{(\alpha)}\rangle|\psi^{(\beta)}\rangle_s \right),$$

where $D_1 = \Pi_{j=1}^N dr_j$, and the integration is defined in the region where $r_{ij} \equiv |r_i - r_j| \neq 0$ ($i, j = 1, ..., N$), as in the main text. Thus, we can define the symbol $\langle \Psi(\alpha)|\Psi(\beta)\rangle_s$ as $\langle \Psi(\alpha)|\Psi(\beta)\rangle_s \equiv I_{\alpha,\beta}$ for both the cases with $a_\alpha = a_\beta$ and the cases with $a_\alpha \neq a_\beta$. It is clear that when $a_\alpha = a_\beta$ this definition returns to the usual definition of inner product.

Under this definition, we have

$$(E_\beta - E_\alpha)\langle \Psi(\alpha)|\Psi(\beta)\rangle = \langle \Psi(\alpha)|H|\Psi(\beta)\rangle - \langle H|\Psi(\alpha)|\Psi(\beta)\rangle = N \left( \langle \Psi(\alpha)|H^{(1)}_{1b}|\Psi(\beta)\rangle - \langle H^{(1)}_{1b}|\Psi(\alpha)|\Psi(\beta)\rangle \right).$$

Here in the last step we have used Eq. (5). Using the expression (3) of the one-body Hamiltonian, we find that in our coordinate representation we have

$$\langle \Psi(\alpha)|H^{(1)}_{1b}|\Psi(\beta)\rangle - \langle H^{(1)}_{1b}|\Psi(\alpha)|\Psi(\beta)\rangle = -\frac{\hbar^2}{2m} \int D_1 \left[ s_s^{(\alpha)}\left( \nabla_{r_1}^2 |\psi^{(\beta)}\rangle_s - s_s^{(\beta)}|\psi^{(\beta)}\rangle_s \right) - i \sum_{\eta,\xi=x,y,z} \lambda_{\alpha,\beta} \int D_1 \left[ s_s^{(\alpha)}|\sigma^{(1)}_{\eta} \left( \frac{\partial}{\partial \xi_1} |\psi^{(\beta)}\rangle_s + \frac{\partial}{\partial \xi_1} |\psi^{(\beta)}\rangle_s \right) \right] \right]$$

where $\xi_1, \xi_2, \xi_3$ are the three components of $r_1$, while $s_s^{(\alpha)}|\psi^{(\beta)}\rangle_s$ and $s_s^{(\beta)}|\psi^{(\beta)}\rangle_s$ are the Dirac bra corresponding to $\nabla_{r_1}^2 |\psi^{(\beta)}\rangle_s$ and $\nabla_{r_1}^2 |\psi^{(\beta)}\rangle_s$, respectively. Notice that the integration is done in the region where $r_{ij} \equiv |r_i - r_j| \neq 0$ ($i, j = 1, ..., N$). Using the divergence theorem, we have

$$\langle \Psi(\alpha)|H^{(1)}_{1b}|\Psi(\beta)\rangle - \langle H^{(1)}_{1b}|\Psi(\alpha)|\Psi(\beta)\rangle = -\int D_2 \lim_{\epsilon \to 0} \int \{ v_{ij} \neq 1, r_{ij} > \epsilon \} dr_1 (\nabla_{r_1} \cdot I),$$

$$= \left. \int D_2 \lim_{\epsilon \to 0} \sum_{j \neq 1} \oint_{S(\epsilon, r_j)} I \cdot dS, \right|_{j=1}$$

where $D_2 = \Pi_{j=2}^N dr_j$ as we have defined before, and the surface integral $\oint_{S(\epsilon, r_j)} (j = 2, ..., N)$ is done for $r_j$ in the sphere $S(\epsilon, r_j)$ which is centered at $r_j$ and has radius $\epsilon$. Here the vector area $dS$ points out of this sphere. In Eq. (B3) the vector function $I$ is given by

$$I = \frac{\hbar^2}{2m} \left[ s_s^{(\alpha)}\left( \nabla_{r_1} |\psi^{(\beta)}\rangle_s - s_s^{(\beta)}|\psi^{(\beta)}\rangle_s \right) - i \sum_{\eta,\xi=x,y,z} \lambda_{\alpha,\beta} \int D_1 \left[ s_s^{(\alpha)}|\sigma^{(1)}_{\eta} \left( \frac{\partial}{\partial \xi_1} |\psi^{(\beta)}\rangle_s + \frac{\partial}{\partial \xi_1} |\psi^{(\beta)}\rangle_s \right) \right] \right],$$

with the spin operator $g$ being defined as $g = \sum_{j=1}^\alpha \omega_{\alpha,\beta} e_\alpha \sigma^{(1)}_{\beta} e_\beta$, while $e_{x,y,z}$ being the unit vector along the three coordinate axises. In addition, due to the identity of Fermi atoms, the function $I$ is invariant under the exchange of $r_l$ and $r_j$ ($j, l \neq 1$). Therefore, the integration $\oint_{S(\epsilon, r_j)} I \cdot dS$ is same for different $j$, and thus Eq. (B3) becomes

$$\langle \Psi(\alpha)|H^{(1)}_{1b}|\Psi(\beta)\rangle - \langle H^{(1)}_{1b}|\Psi(\alpha)|\Psi(\beta)\rangle = (N - 1) \int D_2 \lim_{\epsilon \to 0} \oint_{S(\epsilon, r_2)} I \cdot dS.$$
In addition, in the supphase $S_c(r_2)$, we can express the wave functions $|\psi^{(n)}\rangle_s$ ($n = \alpha, \beta$) via the MBPC \cite{1}. Now we define a vector $\mathbf{u}$ as $\mathbf{u} \equiv (r_1 - r_2)/r_{12}$. Thus, in supphase $S_c(r_2)$ we have $\frac{r_1 + r_2}{2} = r_2 + \epsilon \mathbf{u}/2$ and

$$|\psi^{(n)}\rangle_s = \left[ \frac{1}{\epsilon} - \frac{1}{a_n} - i\mathbf{u} \cdot \mathbf{G} + \frac{\mathbf{u}}{2} \cdot \nabla_r \right] |S\rangle_{12} \otimes |A^{(n)}_{\alpha, \beta}\rangle_{3, \ldots, N} \right|_{r=r_2} + \mathcal{O}(\epsilon); \quad (B6)$$

$$\nabla_{r_1}|\psi^{(n)}\rangle_s = \left[ \frac{\mathbf{u}}{\epsilon^2} - \frac{1}{2\epsilon} \mathbf{u} (\mathbf{u} \cdot \nabla_r) + \frac{1}{2\epsilon} \nabla_r \right] |S\rangle_{12} \otimes |A^{(n)}_{\alpha, \beta}\rangle_{3, \ldots, N} \right|_{r=r_2} + \mathcal{O}(1), \quad (B7)$$

(for $n = \alpha, \beta$),

where $|A^{(n)}_{\alpha, \beta}\rangle_{3, \ldots, N}$ is the state $|A(\mathbf{r}; r_3, \cdots, r_N)\rangle_{3, \ldots, N}$ defined in Eq. \ref{eq:A} for the system with scattering length $a_n$. Substituting Eqs. \ref{eq:B6} and \ref{eq:B7} into Eq. \ref{eq:B4} and then into Eq. \ref{eq:B5}, we obtain

$$\langle \Psi^{(\alpha)} | H^{(1)}_{1b} | \Psi^{(\beta)} \rangle - \langle H^{(1)}_{1b} | \Psi^{(\alpha)} | \Psi^{(\beta)} \rangle = \frac{(N-1)(2\pi)\hbar^2}{m} \left( \frac{1}{a_\alpha} - \frac{1}{a_\beta} \right) \int dr \int D_3 \left[ |A^{(\alpha)}_{\alpha, \beta}\rangle |A^{(\beta)}_{\alpha, \beta}\rangle \right]_{3, \ldots, N}. \quad (B8)$$

Further substituting this result into Eq. \ref{eq:B1}, we obtain Eq. \ref{eq:B2} in Sec. V.

\begin{thebibliography}{99}
\footnotesize
\bibitem{1} T. Köhler, K. Góral, and P. S. Julienne, Rev. Mod. Phys. 78, 1311 (2006).
\bibitem{2} C. Chin, R. Grimm, P. S. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
\bibitem{3} S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008).
\bibitem{4} I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
\bibitem{5} S. Tan, Ann. Phys. 323, 2952 (2008).
\bibitem{6} S. Tan, Ann. Phys. 323, 2971 (2008).
\bibitem{7} S. Tan, Ann. Phys. 323, 2987 (2008).
\bibitem{8} E. Braaten and L. Platter, Phys. Rev. Lett. 100, 205301 (2008).
\bibitem{9} E. Braaten, D. Kang, and L. Platter, Phys. Rev. Lett. 104, 223004 (2010).
\bibitem{10} E. Braaten, D. Kang, and L. Platter, Phys. Rev. A 78, 053606 (2008).
\bibitem{11} S. Zhang and A. J. Leggett, Phys. Rev. A 79, 023601 (2009).
\bibitem{12} Z. Yu, G. M. Bruun, and G. Baym, Phys. Rev. A 80, 023615 (2009).
\bibitem{13} M. Barth and W. Zwerger, Ann. Phys., 326, 2544 (2011).
\bibitem{14} M. Valiente, N. T. Zinner, and K. Molmer, Phys. Rev. A 86, 043616 (2012).
\bibitem{15} R. Combescot, F. Alzetto, and X. Leyronas, Phys. Rev. A 79, 053640 (2009).
\bibitem{16} S. Tan, Phys. Rev. Lett. 107, 145302 (2011).
\bibitem{17} F. Werner and Y. Castin, Phys. Rev. A, 80, 023615 (2009).
\bibitem{18} Z. Yu, J. H. Thywissen and S. Zhang, Phys. Rev. Lett. 115, 135304 (2015); Phys. Rev. Lett. 117, 019901 (2016).
\bibitem{19} S. M. Yoshida and M. Ueda, Phys. Rev. Lett. 115, 135303 (2015).
\bibitem{20} L. Zhang, S. Zhang and Z. Yu, Phys. Rev. A 94, 033616 (2016).
\bibitem{21} L. Zhang, S. Zhang and Z. Yu, Phys. Rev. A 95, 033609 (2017).
\bibitem{22} M. He, S. Zhang, H. Chan and Qi Zhou, Phys. Rev. Lett. 116, 045301 (2016).
\bibitem{23} S. Zhang, M. He and Qi Zhou, Phys. Rev. A 95, 062702 (2017).
\bibitem{24} M. He and Qi Zhou, arXiv:1708.00135.
\bibitem{25} J. T. Stewart, J. P. Gaebler, T. E. Drake, and D. S. Jin, Phys. Rev. Lett. 104, 235301 (2010).
\bibitem{26} Y. Sagit, T. E. Drake, R. Paudel, and D. S. Jin, Phys. Rev. Lett. 109, 220402, (2012).
\bibitem{27} S. Hoinka, M. G. Lingham, K. Fenech, H. Hu, C. J. Vale, J. E. Drut, and S. Gandolfi, Phys. Rev. Lett. 110, 055305 (2013).
\bibitem{28} C. Luciuk, S. Trotzky, S. Smale, Z. Yu, S. Zhang, J. H. Thywissen, Nature Physics 12, 599 (2016).
\bibitem{29} Y. Lin, K. Jiménez-García and I. B. Spielman, Nature 471, 83 (2011).
\bibitem{30} V. Galitski and I. B. Spielman, Nature 494, 498C54 (2013).
\bibitem{31} P. Wang, Z.-Q. Yu, Z. Fu, J. Miao, L. Huang, S. Chai, H. Zhai, and J. Zhang, Phys. Rev. Lett. 109, 095301 (2012).
\bibitem{32} L. W. Cheuk, A. T. Sommer, Z. Hadzibabic, T. Yefsah, W. S. Bakr, and M. W. Zwierlein Phys. Rev. Lett. 109, 095302 (2012).
\bibitem{33} L. Huang, Z. Meng, P. Wang, P. Peng, S.-L. Zhang, L. Chen, D. Li, Q. Zhou and J. Zhang, Nature Physics 12, 540 (2016).
\bibitem{34} Z. Wu, L. Zhang, W. Sun, X.-T. Xu, B.-Z. Wang, S.-C. Ji, Y. Deng, S. Chen, X.-J. Liu and J.-W. Pan, Science 354 (6308), 83-88.
\bibitem{35} X. Cui, Phys. Rev. A 85, 022705 (2012).
\bibitem{36} L. Zhang, Y. J. Deng and P. Zhang, Phys. Rev. A 87, 053626 (2012).
\bibitem{37} L. Zhang, S. Zhang, S. Zhang and Z. Yu, Phys. Rev. A 86, 053608 (2012).
\bibitem{38} H. Zhai, Rep. Prog. Phys. 78, 026001 (2015).
\bibitem{39} Z. H. Yu, Phys. Rev. A 85, 042711 (2012).
\bibitem{40} Y. X. Wu and Z. H. Yu, Phys. Rev. A 87, 032703 (2013).
\bibitem{41} S. Peng, C. Zhang, S. Tan and K. Jiang, arXiv:1801.07448.
\end{thebibliography}
The momentum distribution function $n_{\sigma\sigma'}(\mathbf{k})$ we defined here is normalized as $\int d\mathbf{k} [n_{\uparrow\uparrow}(\mathbf{k}) + n_{\downarrow\downarrow}(\mathbf{k})]/(2\pi)^3 = N$, with $N$ being the total atom number. This definition is consistent with the momentum distribution functions used in previous references, e.g., Ref. [16] and Ref. [17]. Explicitly, the diagonal elements $n_{\sigma\sigma}(\mathbf{k})$ ($\sigma = \uparrow, \downarrow$) in our paper has the same meaning with $\rho_{k\sigma}$ in Ref. [16] and $n_{\sigma}(\mathbf{k})$ in Ref. [17] (see Eq. (22) of Ref. [17]).

The mathematical definition of $\langle \Psi(\alpha) | \Psi(\beta) \rangle$ for the case with $a_\alpha \neq a_\beta$ is given in Appendix [13].

P. Zhang and N. Sun, arXiv:1801.07001