Scattering and effective interactions of ultracold atoms with spin-orbit coupling

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We derive an analytical expression for the scattering amplitude of two ultracold atoms of arbitrary spin and with general spin-orbit (SO) coupling, on the basis of our recent work [Phys. Rev. A **86**, 053608 (2012)]. As an application, we demonstrate that SO coupling can induce scattering resonance in the case with finite scattering length. The same approach can be applied to calculate the two-body bound state of SO-coupled ultracold atoms. For the ultracold spin-1/2 Fermi gases in three- or two- dimensional systems with SO coupling, we also obtain the renormalization relation of effective contact interaction with momentum cutoff, as well as the applicability of Huang-Yang pseudopotential.

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I. INTRODUCTION

In the study of ultracold gases it is very important to understand the low-energy scattering properties of atoms. First, two-body and three-body collisions are the underlying physics of many important experimental phenomena, e.g., the two-body decay and three-body recombination. Second, understanding the behavior of the low-energy interatomic scattering amplitudes is indispensable in designing the effective interatomic interactions (e.g., the Huang-Yang pseudopotential [1], Bethe-Peierls boundary condition [2], and the contact interaction with momentum cutoff [3]), which are widely used in the theoretical calculations. In the low-energy cases the effective interaction and the realistic interaction potential should lead to the same two-body scattering amplitude.

In recent years, a class of synthetic gauge fields and spin-orbit (SO) coupling has been realized in ultracold Bose gases [4–8,10] and degenerate Fermi gases [11–13] with Raman laser beams [14,15]. In these systems, the atomic spin is linearly coupled with the atomic spatial momentum. There is a considerable amount of theoretical interest in understanding the SO-coupling effect in both many-body [16–44] and few-body physics [44–55].

In this paper we provide a systematic investigation on the two-body scattering amplitude of SO-coupled ultracold atoms in three-dimensional (3D) uniform space. Our research is based on the following motivations. First, in the current experiments, the amplitude of elastic interatomic collision [9] and inelastic-scattering-induced decay [9,10] of ultracold gases have been directly observed in the systems with SO coupling. The theoretical investigation for the two-body scattering amplitude is necessary to explain this kind of observations. In particular, the calculation of the inelastic scattering amplitudes is crucial for the study of stability of the SO-coupled ultracold gases in the metastable dressed state, e.g., the dark state. Second, as shown above, the criteria for the effective interaction in the ultracold gases is that the effective interaction potential and the real interaction potential should lead to the same low-energy two-body scattering amplitude. Accordingly, we should first calculate the scattering amplitude given by the real potential and then construct the correct effective interactions. This kind of work has been done for ultracold gases in quasi-one-dimensional [56] and quasi-two-dimensional [57] confinements and optical lattices [58,59], but it is still absent for the gases with SO coupling.

The calculation in this paper is based on our recent work [54] where the short-range behavior of the scattering wave functions of two SO-coupled ultracold atoms in a 3D uniform system is studied and a modified Bethe-Peierls boundary condition is derived. Based on these results, in this paper we derive an analytical expression for the scattering amplitude of two atoms with arbitrary spin and SO coupling. Our approach can also be used to calculate the low-energy bound state of two spin-1/2 atoms with SO coupling. Furthermore, we show that the SO coupling can induce the scattering resonance. Namely, for the atoms with finite scattering length, the threshold scattering amplitude diverges when the SO-coupling intensity assumes some particular value. For the SO-coupled spin-1/2 fermonic atoms, we also derive the renormalization relation of 3D and pure-two-dimensional (pure-2D) effective contact interaction with momentum cutoff, as well as study the applicability of Huang-Yang pseudopotential. We find that the form of the 3D and 2D renormalization relation is not changed by the SO coupling. Nevertheless, in the presence of SO coupling the physical parameters, i.e., the scattering length in the 3D case and bound-state binding energy in the 2D case, should be replaced by the ones which are related to the SO coupling. Furthermore, we also find that the Huang-Yang pseudopotential cannot be directly used in the presence of SO coupling.

The remainder of this paper is organized as follows: In Sec. II, we derive the exact analytical expression for the scattering amplitude of SO-coupled ultracold atoms and show the approach for the calculation of two-atom bound states. In Sec. III, we illustrate the scattering resonance induced by SO coupling. The renormalization relation of effective contact interaction and the applicability of Huang-Yang pseudopotential are investigated in Sec. IV. The main results are summarized and discussed in Sec. V, while some details of our calculations are explained in the Appendixes.

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II. SCATTERING AMPLITUDE AND BOUND STATE OF SO-COUPLED ATOMS

A. Spin-1/2 fermionic atoms

We first consider the scattering amplitude of two SO-coupled spin-1/2 fermonic atoms in 3D space. In this paper we use the term "SO coupling" to refer to the linear coupling between atomic spin and momentum, e.g., the ones realized in the current experiments with Raman laser beams. Without loss of generality, the single-atom Hamiltonian of such a system can be written as

$$H_{1b} = \frac{\vec{P}^2}{2} + \lambda \vec{M} \cdot \vec{P} + Z\,, \tag{1}$$

where $\vec{P}$ is the atomic momentum and $\vec{M}$ and Z are operators in spin space (here we have used $\hbar = 1$ and the atomic mass $m = 1$). The term $\lambda \vec{M} \cdot \vec{P}$ describes the SO coupling and Z accounts for the residual spin-dependent part. Here, the eigenvalues of $\vec{M}$ are of the order of unity, and λ indicates the intensity of the SO coupling. It is pointed out that the term $\lambda \vec{M} \cdot \vec{P}$ in Hamiltonian in Eq. (1) can be used to describe *arbitrary* type of linear spin-momentum coupling. For instance, for effective spin-1/2 systems in Refs. [11,12], one has $\lambda = 2k_r$, $\vec{M} = (\hat{\sigma}_z,0,0)$, and $Z = \delta\hat{\sigma}_z/2 + \Omega\hat{\sigma}_x/2$, where δ is the two-photon detuning, k_r is the recoil momentum, Ω is the Raman-coupling strength, and $\hat{\sigma}_{x,y,z}$ is the Pauli operator. Similarly, for the system with Rashba SO coupling in the 3D space, we have $\vec{M} = (\hat{\sigma}_x,\hat{\sigma}_y,0)$.

For the two-atom scattering problem, the Hilbert space $\mathcal{H}$ can be expressed as $\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_{s1} \otimes \mathcal{H}_{s2}$, with $\mathcal{H}_r$ for the interatomic relative motion in the spatial space, and $\mathcal{H}_{si}$ ($i = 1,2$) for the spin of the ith atom. In this paper we use $|\rangle\rangle$ to denote the state in $\mathcal{H}$, $|)$ for the state in $\mathcal{H}_r$, $|\rangle$ for the state in $\mathcal{H}_{s1} \otimes \mathcal{H}_{s2}$, and $|\rangle_i$ for the state in $\mathcal{H}_{si}$. In Secs. II, III, and IV.C we work in the representation of interatomic relative position, where the state $|\psi\rangle\rangle$ is described by the "spinor wave function" $|\psi(\vec{r})\rangle \equiv (\vec{r}|\psi\rangle\rangle$. Here $|\vec{r})$ is the eigenstate of the interatomic relative position, with corresponding eigenvalue $\vec{r} = (x,y,z)$. It is clear that $|\psi(\vec{r})\rangle$ can also be considered as a $\vec{r}$-dependent spin state.

The total Hamiltonian of the two atoms is given by $H_{1b}^{(1)} + H_{1b}^{(2)} + U(\vec{r})$, where $H_{1b}^{(i)}$ ($i = 1,2$) is for the ith atom, and $U(\vec{r})$ is the spin-dependent interaction potential between the two atoms. Because the total momentum of the two atoms is conserved, the relative motion of these two can be separated from their mass-center motion. The Hamiltonian for the relative motion is then

$$H = \vec{p}^2 + \lambda\vec{c}\cdot\vec{p} + B(\vec{K}) + U(\vec{r}) \equiv H_0 + U(\vec{r}), \tag{2}$$

where $\vec{p}$ is the relative-momentum operator of the two atoms. In the $\vec{r}$ representation we have $\vec{p} = -i\nabla$. The total momentum $\vec{K} = \vec{P}^{(1)} + \vec{P}^{(2)}$ of the two atoms is conserved during the scattering process and behaves as a constant in our calculation. The operators $\vec{c}$ and $B(\vec{K})$ read

$$\vec{c} = \vec{M}^{(1)} - \vec{M}^{(2)}, \tag{3}$$

$$B(\vec{K}) = Z^{(1)} + Z^{(2)} + \frac{\lambda}{2}\vec{K}\cdot(\vec{M}^{(1)} + \vec{M}^{(2)})\,. \tag{4}$$

In the stationary scattering theory, the incident state is regarded as the eigenstate of the Hamiltonian H_0 for the free motion of the two fermionic atoms. With the Pauli's principle being taken into account, such an incident state for two spin-1/2 fermonic atoms can be expressed as

$$\left|\Psi_t^{(0)}(\vec{r})\right\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{4\pi^{3/2}}|\alpha,\vec{k}\rangle - \frac{e^{-i\vec{k}\cdot\vec{r}}}{4\pi^{3/2}}P_{12}|\alpha,\vec{k}\rangle, \tag{5}$$

with $\vec{k}$ being the relative momentum of the two atoms and P_{12} being the permutation operator of the spin of the two atoms. Here the state $|\alpha,\vec{k}\rangle$ ($\alpha = 1,2,3,4$) of the two-atom spin is defined as the αth eigenstate of the operator $h_0(\vec{k}) \equiv \lambda\vec{c}\cdot\vec{k} + B(\vec{K})$, with eigenenergy $\mathcal{E}(\alpha,\vec{K},\vec{k})$. The symbol satisfies $\alpha \geqslant \alpha'$ when $\mathcal{E}(\alpha,\vec{K},\vec{k}) \geqslant \mathcal{E}(\alpha',\vec{K},\vec{k})$. In this paper, we denote

$$t = (\alpha,\vec{K},\vec{k}) \tag{6}$$

as the set of these three quantum numbers. It is easy to prove that $|\Psi_t(\vec{r})\rangle$ in Eq. (5) is an eigenstate of H_0 with eigenenergy

$$E_t = k^2 + \mathcal{E}(\alpha,\vec{K},\vec{k}). \tag{7}$$

In this paper, we assume that $U(\vec{r})$ is a short-range potential with effective range r_*. In the region $r \equiv |\vec{r}| \gtrsim r_*$, we have $U(\vec{r}) \simeq 0$ and furthermore the low-energy scattering state $|\Psi_t^{(+)}(\vec{r})\rangle$ with respect to the incident state $|\Psi_t^{(0)}(\vec{r})\rangle$ can be expressed as [48,57]

$$|\Psi_t^{(+)}(\vec{r})\rangle \approx |\Psi_t^{(0)}(\vec{r})\rangle + B_t G_0(E_t;\vec{r},0)\,|\mathrm{S}\rangle, \tag{8}$$

with $|\mathrm{S}\rangle = (|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2)/\sqrt{2}$ being the singlet spin state. Here B_t is a $\vec{r}$-independent constant and related with $|\Psi_t^{(+)}(\vec{r})\rangle$ through the relation

$$\int d\vec{r}\,' U(\vec{r}\,')|\Psi_t^{(+)}(\vec{r}\,')\rangle = B_t|\mathrm{S}\rangle. \tag{9}$$

For details, see Appendix A. In Eq. (8) the free Green's function $G_0(\eta;\vec{r},\vec{r}\,')$ is defined as

$$G_0(\eta;\vec{r},\vec{r}\,') = \frac{1}{\eta + i0^+ - H_0}\delta(\vec{r} - \vec{r}\,'), \tag{10}$$

and is a $(\vec{r},\vec{r}\,')$-dependent operator for the two-atom spin. In this paper we consider the low-energy case with $k \ll 1/r_*$ and further assume that the SO coupling is weak enough so that $\lambda \ll 1/r_*$. Furthermore, we have proved [54] that, in the *short-range region* $r_* \lesssim r \ll 1/k$ the function $|\Psi_t^{(+)}(\vec{r})\rangle$ behaves as

$$|\Psi_t^{(+)}(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a_{\mathrm{R}}}\right)|\mathrm{S}\rangle - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|\mathrm{S}\rangle. \tag{11}$$

Here, the scattering length a_{R} is determined by both the detail of the potential $U(\vec{r})$ and the SO coupling. In some special systems, e.g., the systems with $[U(\vec{r}),\vec{c}] = 0$ and those in the current experiments [4–10], the scattering length a_{R} is independent of the SO coupling and takes the same value as the scattering length in the systems without SO coupling [54].

We can now calculate the coefficient B_t in Eq. (8) and the interatomic scattering amplitude. As in Refs. [48,57], B_t can be obtained from Eq. (11) and the behavior of $G_0(\eta;\vec{r},\vec{r}\,')|\mathrm{S}\rangle$ in the short-range region $r_* \lesssim r \ll 1/k$. With calculations shown

in Appendix B, we find that

$$G_0(\eta;\vec{r},0) \approx -\frac{1}{4\pi}\left(\frac{1}{r}+i\eta^{1/2}\right)+F(\eta)+i\frac{\lambda}{8\pi}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right) \quad (\text{for } r_* \lesssim r \ll 1/k), \tag{12}$$

where the operator $F(\eta)$ is defined as

$$F(\eta)=\frac{1}{(2\pi)^3}\int d\vec{k}''\mathcal{F}(\eta,\vec{k}''), \tag{13}$$

where

$$\mathcal{F}(\eta,\vec{k}'')=\sum_{\alpha''}\left(\frac{|\alpha'',\vec{k}''\rangle\langle\alpha'',\vec{k}''|}{\eta+i0^+-E_{t''}}-\frac{|\alpha'',\vec{k}''\rangle\langle\alpha'',\vec{k}''|}{\eta+i0^+-k''^2}\right), \tag{14}$$

with $t''=(\alpha'',\vec{K},\vec{k}'')$ and $k''=|\vec{k}''|$. It is clear that the fact $\lim_{|\vec{k}|\to\infty}h_0(\vec{k})=\lambda\vec{c}\cdot\vec{k}$ gives $\lim_{k''\to\infty}[\mathcal{F}(\eta,\vec{k}'')+\mathcal{F}(\eta,-\vec{k}'')]\propto 1/k''^4+O(1/k''^5)$. Therefore, using $\int d\vec{k}''=\int_0^\infty k''^2dk''\int d\Omega_{\vec{k}''}$ with $\Omega_{\vec{k}''}$ being the solid angle of $\vec{k}''$, it is easy to prove that the integration in the right-hand side of Eq. (13) converges to a finite operator. Apparently, $\mathcal{F}(\eta)$ can be re-expressed as $\mathcal{F}(\eta)=(2\pi)^{-3}\int d\vec{k}''[\mathcal{F}(\eta,\vec{k}'')+\mathcal{F}(\eta,-\vec{k}'')]/2$. Such an expression maybe convenient for the numerical calculation of the integration.

By substituting Eq. (12) into Eq. (8), we get the expression for $|\Psi_t^{(+)}(\vec{r})\rangle$ in the short-range region

$$|\Psi_t^{(+)}(\vec{r})\rangle=\left|\Psi_t^{(0)}(0)\right\rangle+iB_t\frac{\lambda}{8\pi}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|\mathrm{S}\rangle+B_t\left[-\frac{1}{4\pi}\left(\frac{1}{r}+iE_t^{1/2}\right)+F(E_t)\right]|\mathrm{S}\rangle \quad (\text{for } r_*\lesssim r\ll 1/k). \tag{15}$$

By comparing Eq. (15) to Eq. (11) and using the fact that $F(\eta)|\mathrm{S}\rangle\propto|\mathrm{S}\rangle$, we obtain

$$B_t=\frac{4\pi\langle\mathrm{S}|\Psi_t^{(0)}(0)\rangle}{1/a_\mathrm{R}+iE_t^{1/2}-4\pi\langle\mathrm{S}|F(E_t)|\mathrm{S}\rangle}. \tag{16}$$

According to scattering theory [60], the scattering amplitude $f(t'\leftarrow t)$ between the incident state $|\Psi_t^{(0)}(\vec{r})\rangle$ and an energy-conserved output state $|\Psi_{t'}^{(0)}(\vec{r})\rangle$ with $t'=(\alpha',\vec{K},\vec{k}')$ is defined as

$$f(t'\leftarrow t)=-2\pi^2\int d\vec{r}\left\langle\Psi_{t'}^{(0)}(\vec{r})|U(\vec{r})|\Psi_t^{(+)}(\vec{r})\right\rangle. \tag{17}$$

It is pointed out that, since $U(\vec{r})\simeq 0$ in the region $r\gtrsim r_*$, the integration in the right-hand side of the above equation is only done in the region $r\lesssim r_*$. Under the low-energy condition $k\ll 1/r_*$, in this region we have $\langle\Psi_{t'}^{(0)}(\vec{r})|\approx\langle\Psi_{t'}^{(0)}(0)|$, and then $f(t'\leftarrow t)$ can be re-expressed as

$$f(t'\leftarrow t)=-2\pi^2\left\langle\Psi_{t'}^{(0)}(0)\right|\int d\vec{r}\,U(\vec{r})|\Psi_t^{(+)}(\vec{r})\rangle=-2\pi^2\left\langle\Psi_{t'}^{(0)}(0)|\mathrm{S}\right\rangle B_t, \tag{18}$$

where we have used Eq. (9). Thus, using Eq. (16), we finally have

$$f(t'\leftarrow t)=-(2\pi)^3\left\langle\Psi_{t'}^{(0)}(0)\right|\frac{1}{1/a_\mathrm{R}+iE_t^{1/2}-4\pi F(E_t)}\times\left|\Psi_t^{(0)}(0)\right\rangle, \tag{19}$$

with $E_t^{1/2}\equiv i\sqrt{|E_t|}$ for $E_t<0$. This is the exact analytical expression for the low-energy scattering amplitude of two spin-1/2 fermonic atoms with SO coupling.

B. Atoms with arbitrary spin

This approach can be straightforwardly generalized to the general case of two fermonic or bosonic atoms with any kind of SO coupling and arbitrary spin. In these cases, the single-atom motion and the relative motion of the two atoms are still given by Eqs. (1) and (2), respectively. The incident state can be expressed as

$$\left|\Psi_t^{(0)}(\vec{r})\right\rangle=\frac{e^{i\vec{k}\cdot\vec{r}}}{4\pi^{3/2}}|\alpha,\vec{k}\rangle\pm\frac{e^{-i\vec{k}\cdot\vec{r}}}{4\pi^{3/2}}P_{12}|\alpha,\vec{k}\rangle, \tag{20}$$

where $\pm$ are for the systems of bosonic and fermonic atoms, respectively.

The scattering wave function with respect to incident state $|\Psi_t^{(0)}(\vec{r})\rangle$ can still be denoted as $|\Psi_t^{(+)}(\vec{r})\rangle$. In the region with $r\gtrsim r_*$ we have (Appendix A)

$$|\Psi_t^{(+)}(\vec{r})\rangle\approx|\Psi_t^{(0)}(\vec{r})\rangle+G_0(E_t;\vec{r},0)|\phi\rangle \tag{21}$$

with the $\vec{r}$-independent spin state $|\phi\rangle$ satisfying

$$|\phi\rangle=\int d\vec{r}\,'U(\vec{r}\,')|\Psi_t^{(+)}(\vec{r})\rangle. \tag{22}$$

This is very similar to Eq. (8), but the spin state $|\phi\rangle$ is not unique. Instead, $|\phi\rangle$ can be different for different incident state $|\Psi_t^{(0)}(\vec{r})\rangle$. Furthermore, as shown in Ref. [54], in the short-range region $r_*\lesssim r\ll 1/k$ the scattering wave function $|\Psi_t^{(+)}(\vec{r})\rangle$ behaves as

$$|\Psi_t^{(+)}(\vec{r})\rangle=\left(\frac{1}{r}-A_\mathrm{R}\right)|\chi\rangle-i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|\chi\rangle. \tag{23}$$

Here $|\chi\rangle$ is another $\vec{r}$-independent spin state, and A_R is a $\vec{r}$-independent operator in the spin space, which is also determined by the detail of the interaction potential $U(\vec{r})$ and the SO coupling. For the cases of spin-1/2 fermonic atoms, we have $A_\mathrm{R}=1/a_\mathrm{R}$, and Eq. (23) reduces to Eq. (11). As in the above section, in the current experiments [4–10] for bosonic atoms with one-dimensionl (1D) SO coupling, A_R is independent of the SO coupling. For instance, for the ultracold gases with spin-1 ^{87}Rb atoms, we have

$$A_\mathrm{R}=\frac{1}{a_0}\mathcal{P}_{F=0}+\frac{1}{a_2}\mathcal{P}_{F=2}, \tag{24}$$

where a_0 (a_2) is the scattering length with respect to the total atomic spin $F=0$ ($F=2$) and $\mathcal{P}_{F=0,2}$ are the associated projection operators.

Using Eq. (12), we can obtain the expression of $|\Psi_t^{(+)}(\vec{r})\rangle$ in the short-range region. By comparing such an expression with Eq. (23), we have

$$|\phi\rangle=-4\pi|\chi\rangle=\frac{4\pi}{A_\mathrm{R}+iE_t^{1/2}-4\pi F(E_t)}\left|\Psi_t^{(0)}(0)\right\rangle \tag{25}$$

and the exact analytical expression

$$f(t'\leftarrow t)=-(2\pi)^3\left\langle\Psi_{t'}^{(0)}(0)\right|\frac{1}{A_\mathrm{R}+iE_t^{1/2}-4\pi F(E_t)}\times\left|\Psi_t^{(0)}(0)\right\rangle \tag{26}$$

for the scattering amplitude of SO-coupled ultracold atoms with arbitrary spin. In Ref. [10] we have used this result to quantitatively explain the collisional decay observed in our experiments with SO-coupled ^{87}Rb atoms.

It is pointed out that in the presence of SO coupling, the state $|\Psi_t^{(0)}(0)\rangle$ depends on the quantum number $t = (\alpha, \vec{K}, \vec{k})$, and thus changes with the direction of the atomic relative momentum $\vec{k}$. Therefore, the scattering amplitude $f(t' \leftarrow t)$ in Eq. (26) is anisotropic with respect to the directions of the incident momentum $\vec{k}$ and output momentum $\vec{k}'$. This anisotropicity is also observed in the experiment by Spielman *et al.* [9].

In the end of this section we consider a simple case where $A_{\rm R} = 1/a$ with a being a constant c number and $|a|$ being much smaller than the eigenvalues of the operator $iE_t^{1/2} - 4\pi F(E_t)$. In this case Eq. (26) can be simplified as $f(t' \leftarrow t) \approx -a(2\pi)^3 \langle \Psi_{t'}^{(0)}(0)|\Psi_t^{(0)}(0)\rangle$. This approximate result can also be obtained with Fermi's golden rule. On the other hand, if the eigenvalues of $A_{\rm R}$ are comparable to or smaller than the ones of the operator $iE_t^{1/2} - 4\pi F(E_t)$, the contribution from that operator becomes significant and the Fermi's golden rule is no longer applicable.

C. Two-atom bound state

In the above subsections we derived the analytical expression of the scattering amplitude of two ultracold atoms with SO coupling. The Green's function approach used in our calculations can also be applied to derive the low-energy bound state of two SO-coupled atoms. We denote the energy of the bound state as E_b, and then the binding energy can be defined as $E_{\rm binding} \equiv -(E_b - E_{\rm th})$, where $E_{\rm th}$ is the energy of scattering threshold or the lowest eigenenergy of H_0. As shown in Appendix B, when $E_{\rm binding} \ll r_*^{-2}$, the wave function $|\Psi_b(\vec{r})\rangle$ of low-energy bound state is given by

$$|\Psi_b(\vec{r})\rangle \approx N_b G_0(E_b; \vec{r}, 0)\,|\phi_b\rangle, \tag{27}$$

in the region $r \gtrsim r_*$. Here N_b is the normalization factor and $|\phi_b\rangle$ is a $\vec{r}$-independent spin state. Furthermore, in the short-range region $r_* \lesssim r \ll E_{\rm binding}^{-1/2}$, $|\Psi_b(\vec{r})\rangle$ has the same behavior as the low-energy scattering state $|\Psi_t^{(+)}(\vec{r})\rangle$ and thus can be expressed as $|\Psi_b(\vec{r})\rangle = (1/r - A_{\rm R})|\chi_b\rangle - i(\lambda/2)\vec{c}\cdot(\vec{r}/r)|\chi_b\rangle$, with $|\chi_b\rangle$ being a $\vec{r}$-indepedent state in the spin space. As in the above section, with this fact and the short-range behavior of $G_0(\eta; \vec{r}, 0)$ given by Eq. (12), we find that $|\chi_b\rangle$, $|\phi_b\rangle$ and E_b can be obtained by

$$\left[-iE_b^{1/2} + 4\pi F(E_b)\right]|\chi_b\rangle = A_{\rm R}|\chi_b\rangle, \tag{28}$$

$$|\chi_b\rangle = -\frac{1}{4\pi} N_b |\phi_b\rangle, \tag{29}$$

with $E_b^{1/2} \equiv i\sqrt{|E_b|}$ for $E_b < 0$. In particular, for two spin-1/2 fermonic atoms, we have $A_{\rm R} = 1/a_{\rm R}$ and $|\phi_b\rangle = |{\rm S}\rangle$. Then Eq. (28) becomes

$$-iE_b^{1/2} + 4\pi \langle {\rm S}|F(E_b)|{\rm S}\rangle = \frac{1}{a_{\rm R}}. \tag{30}$$

With this equation one can obtain the bound-state energy E_b.

III. SO-COUPLING-INDUCED RESONANCE

In above discussions, we derive the general analytical expression (26) for the scattering amplitude of ultracold atoms with SO coupling. As an application, in this section we show that SO coupling can induce scattering resonance of two ultracold atoms. For simplicity, here we only consider the scattering of two spin-1/2 fermoinc atoms.

In such a system, the incident state $|\Psi_t^{(0)}(\vec{r})\rangle$ takes the form in Eq. (5), and one has $|\Psi_t^{(0)}(0)\rangle \propto |{\rm S}\rangle$. Thus, the interatomic scattering amplitude $f(t' \leftarrow t)$ in Eq. (19) can be rewritten as

$$f(t' \leftarrow t) = -(2\pi)^3 \frac{\langle \Psi_{t'}^{(0)}(0)|{\rm S}\rangle\langle {\rm S}|\Psi_t^{(0)}(0)\rangle}{1/a_{\rm R} + d(\lambda, E_t)}, \tag{31}$$

with the function $d(\lambda, E_t)$ defined as

$$d(\lambda, E_t) = iE_t^{1/2} - 4\pi \langle {\rm S}|F(E_t)|{\rm S}\rangle. \tag{32}$$

We first consider the case of threshold scattering with $E_t = E_{\rm th}$. In this case, we have $|\Psi_{t'}^{(0)}(\vec{r})\rangle = |\Psi_t^{(0)}(\vec{r})\rangle$ and $d(\lambda, E_{\rm th})$ usually takes a real value. Therefore, when the condition

$$\frac{1}{a_{\rm R}} + d(\lambda, E_{\rm th}) = 0 \tag{33}$$

is satisfied, the threshold scattering amplitude diverges and a scattering resonance occurs. Since the scattering length $a_{\rm R}$ can be finite, such a resonance is induced by the SO coupling. By comparing Eq. (33) to Eq. (30), we further find that a bound state with zero binding energy appears at the resonance point. In experiments, one can observe the SO-coupling-induced resonance by tuning the scattering length or the SO-coupling intensity [61].

In Fig. 1 we plot the amplitude $f(t \leftarrow t)$ of the threshold scattering of two spin-1/2 fermoinc atoms with 1D SO coupling, i.e., $\vec{M} = (\hat{\sigma}_z, 0, 0)$ and $Z = \kappa\hat{\sigma}_x$, as in current experiments. In our calculation we assume the total momentum $\vec{K}$ of the two atoms is along the x direction, i.e., $\vec{K} = (K_0, 0, 0)$. The scattering amplitudes with respect to different values of K_0 are illustrated versus $1/a_{\rm R}$ and the SO coupling intensity λ. The appearance of resonance is clearly shown.

Next, when the scattering energy E_t is larger than the scattering threshold, the function $d(\lambda, E_t)$ takes a complex value. Thus, the scattering amplitude $f(t' \leftarrow t)$ cannot be divergent. Nevertheless, as a function of $1/a_{\rm R}$, the absolute value of the scattering amplitude still achieves a local maximum value when the condition ${\rm Re}[1/a_{\rm R} + d(\lambda, E_t)] = 0$ or $1/a_{\rm R} = -{\rm Re}[d(\lambda, E_t)]$ is satisfied. To illustrate this effect, we also calculate the scattering amplitude $f(t' \leftarrow t)$ for two spin-1/2 fermoinc atoms with $\vec{M} = (\hat{\sigma}_z, 0, 0)$ and $Z = \kappa\hat{\sigma}_x$. In Fig. 2 we plot $|f(t' \leftarrow t)|$ versus $1/a_{\rm R}$ for the cases with $\vec{K} = 0$, $t = (2, 0, 0)$ and $t' = t_{0,1,2,3}$ where $t_0 = t$, $t_1 = (4, 0, \sqrt{\lambda^4 - \kappa^2}/\lambda)$, $t_2 = (4, 0, \sqrt{\lambda^4 - \kappa^2}/\lambda - 0.5\kappa^{1/2})$, and $t_3 = (4, 0, \sqrt{\lambda^4 - \kappa^2}/\lambda - 0.8\kappa^{1/2})$. The peak behavior of the scattering amplitude is clearly illustrated.

We mention again that the resonance discussed here is essentially induced by the SO-coupling term in the Hamiltonian H_0 defined in Eq. (2). From Eq. (2) one can easily find that such a term can be omitted when $k \gg \lambda$, and therefore the SO-coupling-induced resonance is significant only when the atomic relative momentum k is small enough, i.e., $k \lesssim \lambda$.

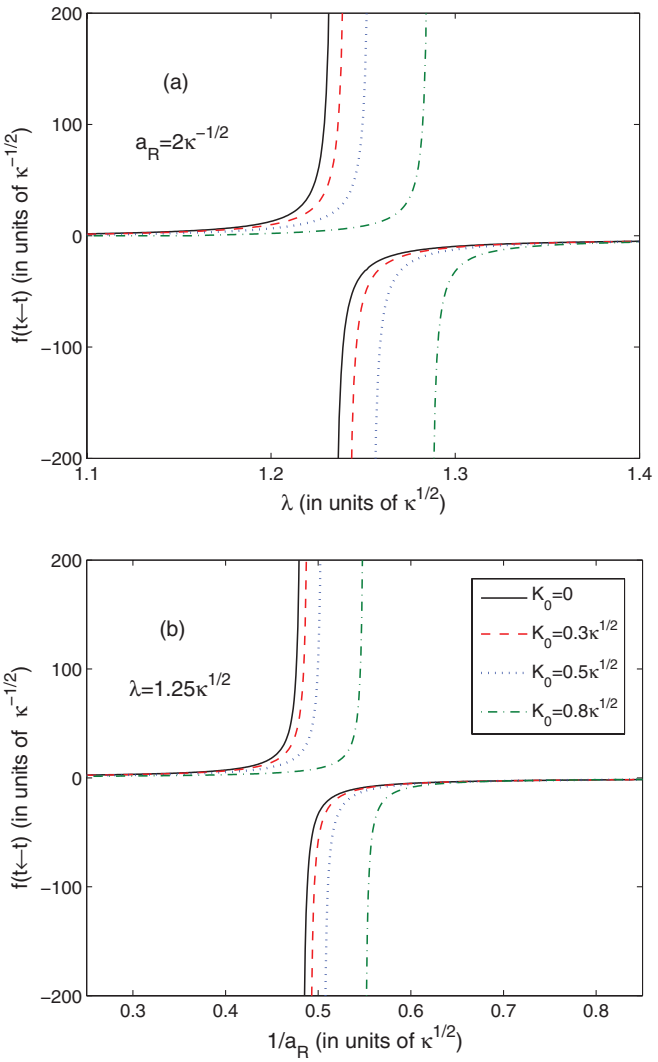

FIG. 1. (Color online) The threshold scattering scattering amplitude $f(t \leftarrow t)$ of two spin-1/2 fermoinc atoms with 1D SO coupling. We plot the $f(t \leftarrow t)$ as a function of SO-coupling intensity λ with the scattering length $a_R = 2\kappa^{-1/2}$ (a) and a function a_R with $\lambda = 1.25\kappa^{1/2}$ (b). Here we have used the natural unit with $\hbar = m = 1$ and set the total momentum of the two atoms to be $\vec{K} = (K_0,0,0)$, with $K_0 = 0$ (black solid line), $0.3\kappa^{1/2}$ (red [gray] dashed line), $0.5\kappa^{1/2}$ (green [gray] dotted line), and $0.8\kappa^{1/2}$ (blue [gray] dashed-dotted line).

Finally, we emphasize that the calculations in this section can be directly generalized to the systems of atoms with arbitrary spin and SO coupling, and the SO-coupling-induced resonance can also appear.

IV. EFFECTIVE INTERACTIONS

In the many-body theory of ultracold gases, the interatomic interaction is usually modeled by some simple effective potentials. The most widely used effective interactions include the Huang-Yang pseudopotential [1], the Bethe-Peierls boundary condition [2], and the contact interaction with a momentum cutoff [3].

For a given system, the interatomic scattering amplitude given by the effective inter-atomic interaction should be the same as the one from the realistic interaction potential $U(\vec{r})$.

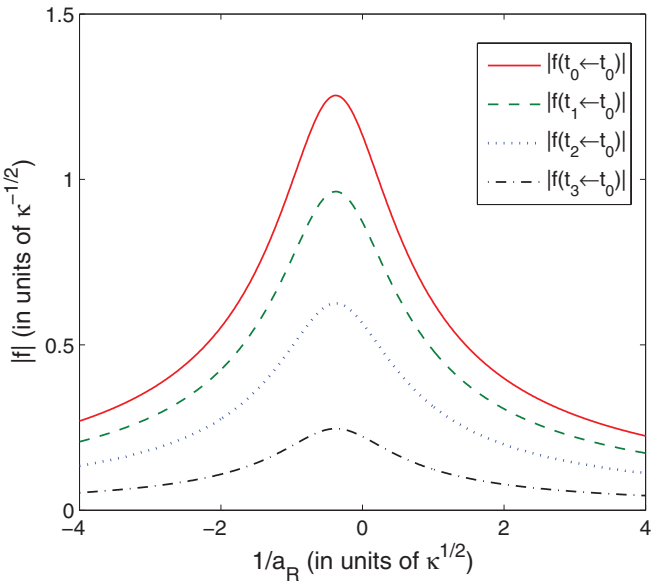

FIG. 2. (Color online) The absolute value of scattering amplitude of two spin-1/2 fermonic atoms with 1D SO coupling. Here we plot $|f(t' \longleftarrow t)|$ for the cases with $\vec{K} = 0$, $\lambda = 1.25\kappa^{1/2}$, and $E_t > E_{\rm th}$. We take $t = (2,0,0)$ and $t' = t_0$ (blue [gray] solid line), t_1 (green [gray] dashed line), t_2 (red [gray] dotted line), and t_3 (black dashed-dotted line), with $t_{0,1,2,3}$ defined in Sec. III.

In our previous works [48,54], we have shown that to satisfy such a condition, the Bethe-Peierls boundary condition for 3D ultracold gases, as well as the renormalization relation for the contact interaction of quasi-2D gases, should be modified in the presence of SO coupling. In this section, we consider the contact interaction with a momentum cutoff in a 3D and pure-2D uniform system of the SO-coupled spin-1/2 Fermi gas, as well as the Huang-Yang pseudo potential.

A. Contact interaction in 3D system

In this and the next subsection we give up the $\vec{r}$ representation and use the Dirac symbol $|\rangle\rangle$ defined in Sec. II A to describe the state in the total Hilbert space H. In a 3D system, the contact interaction $\hat{U}_{\rm eff}$ with a momentum cutoff can be expressed as an operator in H:

$$\hat{U}_{\rm eff} = \frac{U_0}{(2\pi)^3}\int_{|\vec{k}|,|\vec{k}'|<k_c} |\vec{k}\rangle(\vec{k}'| \otimes |{\rm S}\rangle\langle{\rm S}| d\vec{k}d\vec{k}'. \qquad (34)$$

Here k_c is a cutoff momentum and $|\vec{k}) \equiv (2\pi)^{-3/2}\int d\vec{r} e^{i\vec{k}\cdot\vec{r}}|\vec{r})$ is a state in the space H_r. It is pointed out that in many references about the many-body theory of ultracold gases, the systems are first assumed to have finite volume $\mathcal{V}$, and the final result is obtained in the limit $\mathcal{V}\to\infty$. In these cases the second-quantized form $\hat{U}_{\rm eff}$ is given by $\hat{U}_{\rm eff} = U_0/\mathcal{V}\sum'_{\vec{k},\vec{k}',\vec{K}} a^\dagger_{\vec{K}/2+\vec{k},\uparrow} a^\dagger_{\vec{K}/2-\vec{k},\downarrow} a_{\vec{K}/2-\vec{k}',\downarrow} a_{\vec{K}/2+\vec{k}',\uparrow}$, where $a^\dagger_{\vec{p},\sigma}$ and $a_{\vec{p},\sigma}$ are the creation and annihilation operators for an atom with momentum $\vec{p}$ and spin σ. The summation $\sum'_{\vec{k},\vec{k}',\vec{K}}$ is under the condition $\max(|\vec{k}|,|\vec{k}'|) < k_c$ with k_c being the cutoff momentum.

The renormalization relation for this contact potential, i.e., the relationship between U_0 and k_c, can be obtained from

the condition that $\hat{U}_{\rm eff}$ and the realistic interatomic interaction should lead to the same low-energy scattering amplitude. For the cases without SO coupling, the standard calculation gives the well-known result

$$\frac{1}{4\pi a_s} = \frac{1}{U_0} + \frac{1}{(2\pi)^3}\int_{k''<k_c} d\vec{k}''\frac{1}{k''^2}, \tag{35}$$

with a_s being the s-wave scattering length.

In the presence of SO coupling, the correct renormalization relation can be obtained by the same procedure. The effective scattering amplitude $f_{\rm eff}(t'\leftarrow t)$ given by $\hat{U}_{\rm eff}$ can be obtained from the Lippmman-Schwinger equation for the two-body T operator $\hat{T}_{\rm eff}(\eta)$ with respect to $\hat{U}_{\rm eff}$:

$$\hat{T}_{\rm eff}(\eta) = \hat{U}_{\rm eff} + \hat{U}_{\rm eff}\hat{G}_0(\eta)\hat{T}_{\rm eff}(\eta), \tag{36}$$

where the Green's operator $\hat{G}_0(\eta)$ is defined as

$$\hat{G}_0(\eta) = \frac{1}{\eta + i0^+ - H_0} \tag{37}$$

$$= \sum_\alpha \int d\vec{k}\frac{|\vec{k})(\vec{k}|\otimes|\alpha,\vec{k}\rangle\langle\alpha,\vec{k}|}{\eta + i0^+ - E_t}, \tag{38}$$

where we have $t = (\alpha,\vec{K},\vec{k})$ as before.

Using the Lippmann-Schwinger equation, we can obtain the equation for the T-matrix element:

$$\begin{aligned} &T_{\rm eff}(\eta,t',t) \\ &= \frac{U_0}{(2\pi)^3}\langle\alpha',\vec{k}'|{\rm S}\rangle\langle{\rm S}|\alpha,\vec{k}\rangle + \frac{U_0}{(2\pi)^3}\langle\alpha',\vec{k}'|{\rm S}\rangle \\ &\quad\times\left(\sum_{\alpha''}\int_{|\vec{k}''|<k_c} d\vec{k}''\frac{\langle{\rm S}|\alpha'',\vec{k}''\rangle}{\eta + i0^+ - E_{t''}}T_{\rm eff}(\eta,t'',t)\right), \end{aligned} \tag{39}$$

where we have $t' = (\alpha',\vec{K}',\vec{k}')$ and $T_{\rm eff}(\eta,t',t) = (\vec{k}'|\langle\alpha',\vec{k}'|\hat{T}_{\rm eff}(\eta)|\alpha,\vec{k}\rangle|\vec{k})$. The notations t'' and $T_{\rm eff}(\eta,t'',t)$ are defined similarly. From Eq. (39), we find that $T_{\rm eff}(\eta,t',t)$ can be expressed as

$$T_{\rm eff}(\eta,t',t) = \frac{U_0}{(2\pi)^3}\langle\alpha',\vec{k}'|{\rm S}\rangle u(\eta,\alpha,\vec{k}), \tag{40}$$

where $u(\eta,\alpha,\vec{k})$ is independent of α' and $\vec{k}'$. By substituting Eq. (40) into Eq. (39), we get the result

$$u(\eta,\alpha,\vec{k}) = \frac{\langle{\rm S}|\alpha,\vec{k}\rangle}{1 - \frac{U_0}{(2\pi)^3}\left(\sum_{\alpha''}\int_{k''<k_c} d\vec{k}''\frac{|\langle{\rm S}|\alpha'',\vec{k}''\rangle|^2}{\eta+i0^+-E_{t''}}\right)}. \tag{41}$$

By substituting Eq. (41) into Eq. (40), we can obtain the expression of the T-matrix element $T_{\rm eff}(\eta,t',t)$.

The scattering amplitude $f_{\rm eff}(t'\leftarrow t)$ for two spin-1/2 fermionic atoms is defined as

$$f_{\rm eff}(t'\leftarrow t) = -2\pi^2\left\langle\left\langle\Psi_{t'}^{(0)}\middle|\hat{T}_{\rm eff}(E_t)\middle|\Psi_t^{(0)}\right\rangle\right\rangle, \tag{42}$$

where the incident state is $|\Psi_t^{(0)}\rangle\rangle = 2^{-1/2}[|\alpha,\vec{k}\rangle|\vec{k}) - (P_{12}|\alpha,\vec{k}\rangle)|-\vec{k})]$, with P_{12} being the permutation operator for the spin of the two atoms. Therefore, it is apparent that we have

$$f_{\rm eff}(t'\leftarrow t) = -2\pi^2[T_{\rm eff}(E_t,t',t) - T'_{\rm eff}(E_t,t',t)] \tag{43}$$

with $T'_{\rm eff}(E_t,t',t) = (\vec{k}'|\langle\alpha',\vec{k}'|\hat{T}_{\rm eff}(\eta)[{\rm P}_{12}|\alpha,\vec{k}\rangle]|-\vec{k})$. By substituting our result of $T_{\rm eff}(E_t,t',t)$ into Eq. (43), we have

$$f_{\rm eff}(t'\leftarrow t) = -\frac{\frac{U_0}{2\pi}\langle\alpha',\vec{k}'|{\rm S}\rangle\langle{\rm S}|\alpha,\vec{k}\rangle}{1 - \frac{U_0}{(2\pi)^3}\left(\sum_{\alpha''}\int_{k''<k_c} d\vec{k}''\frac{|\langle{\rm S}|\alpha'',\vec{k}''\rangle|^2}{\eta+i0^+-E_{t''}}\right)}. \tag{44}$$

By requiring that the zero-energy effective scattering amplitude $f_{\rm eff}(t'\leftarrow t)$ be equal to the realistic scattering amplitude, i.e.,

$$f_{\rm eff}(t'\leftarrow t) = f(t'\leftarrow t) \tag{45}$$

with $E_t = 0$ and $f(t'\leftarrow t)$ given by Eq. (19), we obtain the following renormalization relation for systems with SO coupling in the limit $k_c\to\infty$:

$$\frac{1}{4\pi a_{\rm R}} = \frac{1}{U_0} + \frac{1}{(2\pi)^3}\int_{k''<k_c} d\vec{k}''\frac{1}{|\vec{k}''|^2}. \tag{46}$$

Here we have used Eq. (B3). By comparing Eq. (35) with Eq. (46), we find that for the 3D contanct potential with momentum cutoff, the form of the renormalization relation is not changed by the SO coupling. In the presence of SO coupling one only needs to replace the scattering length a_s with $a_{\rm R}$.

We mention that Eq. (28) for the bound-state energy E_b can also be obtained from the contact potential $\hat{U}_{\rm eff}$ with renormalization relation (46).

B. Contact potential in pure-2D system

Our above discussion can be directly generalized to pure-2D ultracold gases of spin-1/2 fermonic atoms with SO coupling. We assume the atoms are moving in the x-y plane. Thus, the single-atom Hamiltonian is also given by Eq. (1), with $\vec{P} = (P_x,P_y)$ being the single-atom momentum in the x-y plane. The Hamiltonian for the relative motion is then

$$H^{(2D)} = \vec{p}^2 + \lambda\vec{c}\cdot\vec{p} + B(\vec{K}) + U_{2D}(\vec{\rho}) \equiv H_0^{(2D)} + U_{2D}(\vec{\rho}), \tag{47}$$

where $\vec{K}$ is the two-atom total momentum, $\vec{\rho} = (x,y)$ is the two-atom relative position in the x-y plane, and U_{2D} is the two-atom interaction potential in the 2D space, with effective range ρ_*. Here the operators $\vec{c}$ and $B(\vec{K})$ in the two-atom spin space are defined as in Sec. II, and SO-coupling intensity λ is also assumed to be small enough so that the condition $\lambda \ll 1/\rho_*$ is satisfied.

As in Sec. II A, the incident state in the scattering, or the eigenstate of the Hamiltonian $H_0^{(2D)}$, can be described by the spinor wave function

$$\left|\Psi_t^{(0)}(\vec{r})\right\rangle = \frac{e^{i\vec{k}\cdot\vec{\rho}}}{2^{3/2}\pi}|\alpha,\vec{k}\rangle - \frac{e^{-i\vec{k}\cdot\vec{\rho}}}{2^{3/2}\pi}P_{12}|\alpha,\vec{k}\rangle \tag{48}$$

in the $\vec{r}$ representation. Here the state $|\alpha,\vec{k}\rangle$ for the two-atom spin is defined as in Sec. II A, and we have $t = (\alpha,\vec{K},\vec{k})$ as before. In Ref. [48], we have calculated the 2D scattering amplitude $f^{(2D)}(t'\leftarrow t)$ between $|\Psi_t^{(0)}(\vec{r})\rangle$ and $|\Psi_{t'}^{(0)}(\vec{r})\rangle$ for the cases with Rashba SO coupling. The method applied there can be directly used for the cases with arbitrary type of SO

coupling. The straightforward calculation yields

$$f^{(2D)}(t' \longleftarrow t) = -\frac{4\pi^3 \langle \Psi_{t'}^{(0)}(0)|S\rangle\langle S|\Psi_t^{(0)}(0)\rangle}{\frac{i\pi}{2} - \ln E_t^{1/2} - C - \ln\frac{d_R}{2} - 2\pi\mathcal{F}^{(2D)}(E_t)}, \quad (49)$$

where $C = 0.5772\ldots$ is the Euler Γ number and E_t is the eigenvalue of $H_0^{(2D)}$, with respect to the eigenstate $|\Psi_t^{(0)}(\vec{r})\rangle$. In Eq. (49) the function $\mathcal{F}^{(2D)}(\eta)$ is defined as

$$\mathcal{F}^{(2D)}(\eta) = \frac{1}{(2\pi)^2}\sum_{\alpha''}\int d\vec{k}''|\langle S|\alpha'',\vec{k}''\rangle|^2 \times\left(\frac{1}{\eta + i0^+ - E_{t''}} - \frac{1}{\eta + i0^+ - |\vec{k}''|^2}\right), \quad (50)$$

with $t'' = (\alpha'', \vec{K}, \vec{k}'')$. The parameter d_R in Eq. (49) can be determined by the following condition (see Appendix B of Ref. [48] where d_R is denoted by d): In the region with $\rho_* < |\vec{\rho}| \ll 1/k$, the solution $|\psi_R(\vec{\rho})\rangle$ of equation

$$[\mathcal{T}(\vec{\rho})H^{(2D)}\mathcal{T}^\dagger(\vec{\rho})]|\psi_T(\vec{\rho})\rangle = E_t|\psi_T(\vec{\rho})\rangle \quad (51)$$

satisfies $|\psi_T(\vec{\rho})\rangle \propto (\ln|\vec{\rho}| - \ln d_R)|S\rangle$. Here the rotation $\mathcal{T}(\vec{\rho})$ is defined as $\mathcal{T}(\vec{\rho}) = \exp(i\lambda c_x x/2)\exp(i\lambda c_y y/2)$.

Now we consider the 2D contact potential which takes the form

$$\hat{U}_{\rm eff}^{(2D)} = \frac{U_0}{(2\pi)^2}\int_{|\vec{k}|,|\vec{k}'|<k_c}|\vec{k}\rangle(\vec{k}'|\otimes|S\rangle\langle S|d\vec{k}d\vec{k}', \quad (52)$$

where k_c is a cutoff momentum. Similar to the 3D case, in the references where the area $\mathcal{S}$ of the system is first assumed to be finite, the second-quantized form $\hat{U}_{\rm eff}^{(2D)}$ is given by $\hat{U}_{\rm eff}^{(2D)} = U_0^{(2D)}\mathcal{S}^{-1}\sum_{\vec{k},\vec{k}',\vec{K}}{}' a^\dagger_{\vec{K}/2+\vec{k},\uparrow}a^\dagger_{\vec{K}/2-\vec{k},\downarrow}a_{\vec{K}/2-\vec{k}',\downarrow}a_{\vec{K}/2+\vec{k}',\uparrow}$ where $a^\dagger_{\vec{p},\sigma}$, $a_{\vec{p},\sigma}$, and $\sum'_{\vec{k},\vec{k}',\vec{K}}$ have similar definitions as in Sec. IV B. The renormalization relation for this contact potential can be obtained from the condition that $\hat{U}_{\rm eff}^{(2D)}$ and the realistic interatomic interaction should lead to the same low-energy scattering amplitude. In the absence of SO coupling, the standard calculation gives [62]

$$\frac{1}{U_0^{(2D)}} = -\frac{1}{(2\pi)^2}\int_{k''<k_c}d\vec{k}''\frac{1}{\varepsilon + k''^2}, \quad (53)$$

where the physical parameter $\varepsilon > 0$ is the binding energy of the 2D two-atom bound state for the cases without SO coupling.

In the presence of SO coupling, the effective scattering amplitude $f_{\rm eff}(t' \leftarrow t)$ given by $\hat{U}_{\rm eff}$ can be obtained with the method used in Sec. IV. A. The straightforward calculation gives

$$f_{\rm eff}^{(2D)}(t' \longleftarrow t) = -\frac{4\pi^3 \langle \Psi_{t'}^{(0)}(0)|S\rangle\langle S|\Psi_t^{(0)}(0)\rangle}{\frac{i\pi}{2} - \ln E_t^{1/2} + \frac{2\pi}{U_0^{(2D)}} + \ln k_c - 2\pi\mathcal{F}^{(2D)}(E_t)}. \quad (54)$$

By requiring that $f_{\rm eff}^{(2D)}(t' \leftarrow t) = f^{(2D)}(t' \leftarrow t)$ with $f^{(2D)}(t' \leftarrow t)$ given by Eq. (49), we obtain the following renormalization relation for systems with SO coupling in the limit $k_c \to \infty$:

$$\frac{1}{U_0^{(2D)}} = -\frac{1}{(2\pi)^2}\int_{k''<k_c}d\vec{k}''\frac{1}{\varepsilon_R + k''^2}, \quad (55)$$

with $\varepsilon_R = 4\exp(-2C)/d_R^2$. By comparing Eq. (53) with Eq. (55), we find that for the 2D contact potential with momentum cutoff, the form of the renormalization relation is not changed by the SO coupling. In the presence of SO coupling one only needs to replace ε with ε_R.

C. Huang-Yang pseudopotential

In the end of this section consider the Huang-Yang pseudopotential [1] for the SO-coupled spin-1/2 Fermi gas in a 3D system. In the $\vec{r}$ representation, the Huang-Yang pseudopotential [1] is given by

$$U_{HY} = 4\pi a\delta(\vec{r})\frac{\partial}{\partial r}(r\cdot), \quad (56)$$

with being a the scattering length. Since U_{HY} is a zero-range potential, the scattering state with respect to U_{HY}, i.e., the solution of the equation

$$[H_0 + U_{HY}]|\psi_t^{(+)}(\vec{r})\rangle = E_t|\psi_t^{(+)}(\vec{r})\rangle \quad (57)$$

with outgoing boundary condition, should take the form

$$|\psi_t^{(+)}(\vec{r})\rangle = |\Psi_t^{(0)}(\vec{r})\rangle + B_t G_0(E_t;\vec{r},0)|S\rangle \quad (58)$$

in the region with $r \equiv |\vec{r}| > 0$, and thus satisfy the Bethe-Peierls boundary condition. In the absence of SO coupling, the Bethe-Peierls boundary condition is

$$\lim_{r\to 0}|\psi_t^{(+)}(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a}\right)|S\rangle. \quad (59)$$

According to this condition, the function $r|\psi_t^{(+)}(\vec{r})\rangle$ is continuous in the point $r = 0$. Therefore, the partial derivative $\partial/\partial r$ in U_{HY} is well defined for the function $r|\psi_t^{(+)}(\vec{r})\rangle$. Namely, the operation of the Huang-Yang pseudopotential U_{HY} on the wave function $|\psi_t^{(+)}(\vec{r})\rangle$ is well defined.

Nevertheless, in the presence of the SO coupling, as shown in Ref. [54], the Bethe-Peierls boundary condition is modified to

$$\lim_{r\to 0}|\psi_t^{(+)}(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a}\right)|S\rangle - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|S\rangle. \quad (60)$$

Due to the anisotropic term $-i\lambda\vec{c}\cdot\vec{r}/(2r)|S\rangle$, the function $r|\psi_t^{(+)}(\vec{r})\rangle$ is *not*continuous in the point $r = 0$. As a result, the partial derivative $\partial/\partial r$ in U_{HY} is not well defined for the function $r|\psi_t^{(+)}(\vec{r})\rangle$, and thus the operation of U_{HY} on the wave function $|\psi_t^{(+)}(\vec{r})\rangle$ is no longer well defined. Therefore, in the presence of SO coupling, the Huang-Yang pseudopotential is not consistent with the modified Bethe-Peierls boundary condition and thus cannot be directly used in the theoretical calculations.

V. DISCUSSION

In this paper we derive the analytical expression of the scattering amplitude of two ultracold atoms with SO coupling. Our approach can also be used to calculate the wave function and

the energy of two-body bound state. Moreover, we show that the SO coupling can induce interatomic scattering resonance. The influence of such a resonance in the many-body physics of the SO-coupled ultracold gases remains to be explored. With the expression of scattering amplitude, we further prove that the renormalization relations of the 3D and 2D contact potentials with momentum cutoff are not changed by the SO coupling. Nevertheless, in the presence of SO coupling the physical parameters in the renormalization relation should be replaced by the ones which are related to the SO coupling. Our result provides a solid basis for some previous theoretical works (e.g., Refs. [25,33,46]) where the renormalizations relation with these forms are used for the SO-coupled gases without proof. We also show that in the presence of the SO coupling, the Huang-Yang pseudopotential is no longer consistent with the modified Bethe-Peierls boundary condition and thus cannot be directly used in the theoretical calculations.

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APPENDIX A: BEHAVIOR OF SCATTERING WAVE FUNCTION

In this Appendix we give the explicit definition of the effective range r_* for the potential $U(\vec{r})$ and prove Eqs. (8), (9), (21), (22), and (27) for the behavior of the scattering state $|\Psi_t^{(+)}(\vec{r})\rangle$ and bound state $|\Psi_b(\vec{r})\rangle$ in the region $r \gtrsim r_*$. Although this problem has been discussed by us in Refs. [54] and [48], the treatment there is not fully rigorous. Here we provide a more explicit analysis.

We first consider the case of spin-1/2 atoms. According to the scattering theory, $|\Psi_t^{(+)}(\vec{r})\rangle$ is determined by the Lippmman-Schwinger equation

$$|\Psi_t^{(+)}(\vec{r})\rangle = |\Psi_t^{(0)}(\vec{r})\rangle + \int d\vec{r}\,' G_0(E_t,\vec{r},\vec{r}\,')U(\vec{r}\,')|\Psi_t^{(+)}(\vec{r}\,')\rangle, \tag{A1}$$

with the Green's function G_0 defined in Eq. (10). Here we assume the potential $U(\vec{r})$ is negligible when the interatomic distance is larger than a characteristic length r_0, i.e., $U(\vec{r}) \simeq 0$ in the region $r \gtrsim r_0$. Thus, the integration in Eq. (A1) is only effective in the region $r' \lesssim r_0$.

If the momentum k is low enough so that $k \ll 1/r_0$, when $r \to \infty$ and $r' \lesssim r_0$, the function $G_0(E,\vec{r},\vec{r}\,')$ varies very slowly with respect to $\vec{r}\,'$ and we have $G_0(E,\vec{r},\vec{r}\,') \approx G_0(E,\vec{r},0)$. Therefore, in the limit $r \to \infty$, the solution of Eq. (A1) takes the form

$$|\Psi_t^{(+)}(\vec{r})\rangle \approx \left|\Psi_t^{(0)}(\vec{r})\right\rangle + G_0(E_t,\vec{r},0)|\phi\rangle, \tag{A2}$$

where the spin state $|\phi\rangle$ is related to $|\Psi_t^{(+)}(\vec{r})\rangle$ via the equation

$$|\phi\rangle = \int d\vec{r}\,' U(\vec{r}\,')|\Psi_t^{(+)}(\vec{r}\,')\rangle. \tag{A3}$$

Furthermore, due to the fact that $P_{12}|\Psi_t^{(+)}(-\vec{r})\rangle = -|\Psi_t^{(+)}(\vec{r})\rangle$ and $P_{12}U(-\vec{r})P_{12} = U(\vec{r})$ with P_{12} being the permutation operator of the spin of the two atoms, one finds that $P_{12}[U(-\vec{r})|\Psi_t^{(+)}(-\vec{r})\rangle] = -U(\vec{r})|\Psi_t^{(+)}(\vec{r})\rangle$. This result yields

$$|\phi\rangle = \int d\vec{r}\,' U(\vec{r}\,')|\Psi_t^{(+)}(\vec{r}\,')\rangle = B_t|\mathrm{S}\rangle\,, \tag{A4}$$

with B_t a constant number. Therefore, when the interatomic distance r is *large enough*, we have

$$|\Psi_t^{(+)}(\vec{r})\rangle \approx \left|\Psi_t^{(0)}(\vec{r})\right\rangle + B_t G_0(E_t,\vec{r},0)|\mathrm{S}\rangle. \tag{A5}$$

A direct result is that there exists a characteristic length r_* and Eq. (A5) is applicable in the region $r \gtrsim r_*$. It is apparent that we have $r_* \gtrsim r_0$. In this paper we define such a characteristic length as the effective range of the potential $U(\vec{r})$. Therefore, Eqs. (A5) and (A3) or Eqs. (8) and (9) are naturally satisfied when $r \gtrsim r_*$.

When $U(\vec{r})$ is spherical, in the low-energy case one only needs to take into account the s-wave scattering. The straightforward calculation shows that, as a result of the s-wave approximation, we have $r_* = r_0$. When $U(\vec{r})$ is anisotropic, the effective range r_* is larger than r_0. In our current paper and Ref. [54], we assume the kinetic energy of atomic relative motion is low enough so that the effective ranges of $U(\vec{r})$ and the "rotated potential"

$$U_{\mathrm{R}}(\vec{r}) \equiv e^{i\lambda c_z x/2}e^{i\lambda c_y y/2}e^{i\lambda c_x z/2}U(\vec{r})e^{-i\lambda c_x x/2}e^{-i\lambda c_y y/2}e^{-i\lambda c_z z/2} \tag{A6}$$

are much smaller than $1/k$. This condition can be satisfied in the dilute gases, in particular, in the systems where the condition $r_0 \ll 1/k$ is satisfied and the anistropicity of $U(\vec{r})$ and $U_{\mathrm{R}}(\vec{r})$ is small enough so that the relevant effective ranges of U and U_{R} are in the same order of magnitude with r_0.

Our above analysis can be directly generalized to the general cases of atoms with arbitrary spin. In that case the scattering state $|\Psi_t^{(+)}(\vec{r})\rangle$ takes the form in Eq. (A2) in the whole region with $r \gtrsim r_*$, and the $\vec{r}$-independent state $|\phi\rangle$ is also related to $|\Psi_t^{(+)}(\vec{r})\rangle$ via Eq. (A3). Nevertheless, now $|\phi\rangle$ is not unique. It can be different for different incident states $|\Psi_t^{(0)}(\vec{r})\rangle$. Then we can obtain the result in Eqs. (21) and (22).

Now we consider the low-energy bound state of two SO-coupled atoms. It is clear that the wave function $|\Psi_b(\vec{r})\rangle$ of the bound state is given by the equation

$$|\Psi_b(\vec{r})\rangle = N_b \int d\vec{r}\,' G_0(E_b,\vec{r},\vec{r}\,')U(\vec{r}\,')|\Psi_b(\vec{r}\,')\rangle \tag{A7}$$

with E_b being the energy of the bound state and N_b being the normalization factor. As above, when $|E_{\mathrm{binding}}| \ll 1/r_0^2$ we have

$$|\Psi_b(\vec{r})\rangle \approx N_b G_0(E_b,\vec{r},0)|\phi_b\rangle \tag{A8}$$

in the region $r > r_*$. That is the result in Eq. (27). In this paper we assume the condition $|E_{\mathrm{binding}}| \ll 1/r_*^2$ is satisfied.

APPENDIX B: THE SHORT-RANGE BEHAVIORS OF FREE GREEN'S FUNCTION

In this Appendix we prove Eq. (12) for the short-range behaviors of $G_0(E_t,\vec{r},0)$ with the following three steps:

First, with the fact

$$\delta(\vec{r}-\vec{r}\,') = \int d\vec{k}'' \frac{e^{i\vec{k}''\cdot(\vec{r}-\vec{r}\,')}}{(2\pi)^3}\left(\sum_{\alpha''}|\alpha'',\vec{k}''\rangle\langle\alpha'',\vec{k}''|\right), \quad \text{(B1)}$$

it is easy to show that

$$G_0(\eta,\vec{r},0) = \sum_{\alpha}\int d\vec{k}'' \frac{e^{i\vec{k}''\cdot\vec{r}}}{(2\pi)^3}\frac{|\alpha'',\vec{k}''\rangle\langle\alpha,\vec{k}''|}{\eta+i0^+-E_{t''}}. \quad \text{(B2)}$$

with $t''=(\alpha'',\vec{K},\vec{k}'')$. Equation (B2) and the completeness relationship $\sum_{\alpha''}|\alpha'',\vec{k}''\rangle\langle\alpha'',\vec{k}''|=1$ leads to the result

$$G_0(\eta,\vec{r},0) = \int d\vec{k}'' \frac{e^{i\vec{k}''\cdot\vec{r}}}{(2\pi)^3}\frac{1}{\eta+i0^+-k''^2} + \int d\vec{k}'' \frac{e^{i\vec{k}''\cdot\vec{r}}}{(2\pi)^3}\mathcal{F}(\eta,\vec{k}''), \quad \text{(B3)}$$

with the operator $\mathcal{F}(\eta,\vec{k}'')$ defined in Eq. (14). Similarly as in Sec. II, the fact that $\lim_{|\vec{k}|\to\infty}h_0(\vec{k})=\lambda\vec{c}\cdot\vec{k}$ gives $\lim_{k''\to\infty}[\mathcal{F}(\eta,\vec{k}'')e^{i\vec{k}''\cdot\vec{r}}+\mathcal{F}(\eta,-\vec{k}'')e^{-i\vec{k}''\cdot\vec{r}}]\propto\cos(\vec{k}''\cdot\vec{r})[1/k''^4+\mathcal{O}(1/k''^5)]+\sin(\vec{k}''\cdot\vec{r})[1/k''^3+\mathcal{O}(1/k''^4)]$. Therefore, using $\int d\vec{k}''=\int_0^\infty k''^2dk''\int d\Omega_{\vec{k}''}$ with $\Omega_{\vec{k}''}$ the solid angle of $\vec{k}''$ it is easy to prove that the integration in the right-hand side of Eq. (B3) does not diverge. On the other hand, we also have

$$\int d\vec{k}'' \frac{e^{i\vec{k}''\cdot\vec{r}}}{(2\pi)^3}\frac{1}{\eta+i0^+-k''^2} = -\frac{e^{i\sqrt{\eta}r}}{4\pi r} \quad \text{(B4)}$$

with $\arg\eta\in(-\pi,\pi]$. Due to these facts, we have

$$\lim_{r\to0}G_0(\eta,\vec{r},0) = -\frac{1}{4\pi r}+\mathcal{O}(r^0). \quad \text{(B5)}$$

Second, as in Ref. [54], we introduce a unitary transformation $\mathcal{R}(\vec{r})$ as

$$\mathcal{R}(\vec{r}) = e^{i\lambda c_z x/2}e^{i\lambda c_y y/2}e^{i\lambda c_x z/2}, \quad \text{(B6)}$$

with $\vec{c}\equiv(c_x,c_y,c_z)$. The rotated free Hamiltonian $H_{0\mathrm{R}}=\mathcal{R}(\vec{r})H_0\mathcal{R}^\dagger(\vec{r})$ can be calculated as

$$H_{0\mathrm{R}} = \vec{p}^{\,2}-2\lambda\vec{d}(\lambda\vec{r})\cdot\vec{p}+W(\vec{r}) \quad \text{(B7)}$$

with operators $\vec{d}\equiv(d_x,d_y,d_z)$ and W given by

$$d_x(\lambda\vec{r}) = 0; \quad \text{(B8)}$$

$$d_y(\lambda\vec{r}) = e^{i\lambda c_z z/2}\frac{c_y}{2}e^{-i\lambda c_z z/2}-\mathcal{R}(\vec{r})\frac{c_y}{2}\mathcal{R}^\dagger(\vec{r}); \quad \text{(B9)}$$

$$d_z(\lambda\vec{r}) = \frac{c_z}{2}-\mathcal{R}(\vec{r})\frac{c_z}{2}\mathcal{R}^\dagger(\vec{r}), \quad \text{(B10)}$$

and

$$W(\vec{r}) = i\lambda[\nabla\cdot\vec{d}(\lambda\vec{r})]+\mathcal{R}(\vec{r})B(\vec{K})\mathcal{R}^\dagger(\vec{r}) + \lambda^2\left[|\vec{d}(\lambda\vec{r})|^2-\mathcal{R}(\vec{r})\frac{|\vec{c}|^2}{4}\mathcal{R}^\dagger(\vec{r})\right]. \quad \text{(B11)}$$

Now we define the rotated Green's function $G_{0\mathrm{R}}(\eta,\vec{r},0)$ as the Green's function with respect to $H_{0\mathrm{R}}$, i.e.,

$$G_{0\mathrm{R}}(\eta,\vec{r},0) = \frac{1}{\eta+i0^+-H_{0\mathrm{R}}}\delta(\vec{r}). \quad \text{(B12)}$$

According to Eqs. (B8)–(B10), we have $\vec{d}(\lambda\vec{r})=\mathcal{O}(\lambda r)$. Namely, the SO-coupling term in H_{R} vanishes in the limit $r\to0$. Due to this fact, in such a limit $G_{0\mathrm{R}}(\eta,\vec{r},0)$ has the same behavior with the Green's function $G_W(\eta,\vec{r},0)$, which is defined as

$$G_W(\eta,\vec{r},0) = \frac{1}{\eta+i0^+-[\vec{p}^{\,2}+W(0)]}\delta(\vec{r}) = -\sum_n|W_n\rangle\langle W_n|\frac{e^{i\sqrt{\eta-W_n}r}}{4\pi r}, \quad \text{(B13)}$$

with W_n and $|W_n\rangle$ being the nth eigenvalue and eigenstate of the operator $W(0)$, respectively. Since $\lim_{r\to0}G_W(\eta,\vec{r},0)$ is the sum of $-1/(4\pi r)$ and a $\vec{r}$-independent operator, we have

$$\lim_{r\to0}G_{0\mathrm{R}}(\eta,\vec{r},0) = -\frac{1}{4\pi r}+G_0'(\eta), \quad \text{(B14)}$$

with $G_0'(\eta)$ being a $\vec{r}$-independent operator in the space of two-atom spin.

As in Ref. [54], the result in Eq. (B14) can be proved as follows. According to the definition of $G_{0\mathrm{R}}$, it is obvious that

$$G_0(\eta,\vec{r},0) = \mathcal{R}(\vec{r})G_{0\mathrm{R}}(\eta,\vec{r},0). \quad \text{(B15)}$$

Due to this relation and Eq. (B5), $G_{0\mathrm{R}}(\eta,\vec{r},0)$ can be expressed as the sum of $-1/(4\pi r)$ and another term which converges in the limit $r\to0$. Then we have

$$G_{0\mathrm{R}}(\eta,\vec{r},0) = -\frac{1}{4\pi r}+\sum_{n=0}^{\infty}r^nG_n'(\eta) + \sum_{l=1}^{\infty}\sum_{m_l=-l}^{l}\sum_{n=0}^{\infty}r^nY_{l,m_l}(\theta,\phi)J_{l,m_l,n}(\eta), \quad \text{(B16)}$$

with (r,θ,ϕ) the spherical coordinate. Here $Y_{l,m_l}(\theta,\phi)$ are the spherical harmonic functions, $G_n'(\eta)$ and $J_{l,m_l,n}(\eta)$ are $\vec{r}$-independent operators in the space of two-atom spin.

In the region $r>0$, the Green's function $G_{0\mathrm{R}}(\eta,\vec{r},0)$ satisfies

$$[\vec{p}^{\,2}-2\lambda\vec{d}(\lambda\vec{r})\cdot\vec{p}+W(\vec{r})]G_{0\mathrm{R}}(\eta,\vec{r},0) = \eta G_{0\mathrm{R}}(\eta,\vec{r},0). \quad \text{(B17)}$$

By substituting Eq. (B16) into Eq. (B17) and comparing the coefficients of the term r^{-2} in both sides, we find that because $d(\lambda\vec{r})=\mathcal{O}(\lambda r)$, one has $J_{l,m_l,0}(\eta)=0$. Therefore, in the limit $r\to0$, $G_{0\mathrm{R}}(\eta,\vec{r},0)$ behaves as in Eq. (B14).

Third, using Eq. (B15) and Eq. (B14), we finally have

$$\lim_{r\to0}G_0(\eta,\vec{r},0) = -\frac{1}{4\pi r}+i\frac{\lambda}{8\pi}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)+G_0'(\eta). \quad \text{(B18)}$$

Now we derive the $\vec{r}$-independent operator $G_0'(\eta)$ in the space of two-atom spin. Therefore, we have

$$G_0'(\eta) = \lim_{r\to0}\frac{1}{2}\left[G_0(\eta,\vec{r},0)+G_0(\eta,-\vec{r},0)+\frac{1}{2\pi r}\right]. \quad \text{(B19)}$$

Using the Eqs. (B3) and (B4) and the fact

$$\lim_{r\to0}\left[\int d\vec{k}\,f(\vec{k})e^{i\vec{k}\cdot\vec{r}}+\int d\vec{k}\,f(\vec{k})e^{-i\vec{k}\cdot\vec{r}}\right] = \lim_{r\to0}\int d\vec{k}\,f(\vec{k})(e^{i\vec{k}\cdot\vec{r}}+e^{-i\vec{k}\cdot\vec{r}}) = 2\int d\vec{k}\,f(\vec{k}), \quad \text{(B20)}$$

we find that

$$G_0'(\eta) = -\frac{i\eta^{1/2}}{4\pi} + F(\eta). \tag{B21}$$

with the operator $F(\eta)$ defined in Eq. (13).

In the short-range region, the behavior of $G_0(\eta;\vec{r},0)$ is given by $\lim_{r\to 0} G_0(\eta,\vec{r},0)$. Thus, by substituting Eq. (B21) into Eq. (B18), we obtain

$$G_0(\eta;\vec{r},0) \approx -\frac{1}{4\pi}\left(\frac{1}{r} + i\eta^{1/2}\right) + F(\eta) + i\frac{\lambda}{8\pi}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right) \quad (\text{for } r_* \lesssim r \ll 1/k). \tag{B22}$$

That is the result in Eq. (12).

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