Modified Bethe-Peierls boundary condition for ultracold atoms with spin-orbit coupling

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We show that the Bethe-Peierls (BP) boundary condition should be modified for ultracold atoms with spin-orbit (SO) coupling. Moreover, we derive a general form of the modified BP boundary condition, which is applicable to a system with an arbitrary kind of SO coupling. In the modified BP condition, an anisotropic term appears and the interatomic scattering length is normally SO-coupling dependent. For the special system in the current experiments, however, it can be proved that the scattering length is SO-coupling independent, and it takes the same value as in the case without SO coupling. Our result is helpful for the study of both few-body and many-body physics in SO-coupled ultracold gases.

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I. INTRODUCTION

In the study of ultracold atomic gases [1–9], the Bethe-Peierls (BP) boundary condition [10] is widely used as a replacement for the realistic interaction between two atoms. With this approach, one only needs to solve the Schrödinger equation with the Hamiltonian for atomic free motion, and thus the calculation is significantly simplified. As a result, the BP boundary condition is very useful in the research of few-body and many-body physics in ultracold gases, especially those with large interatomic scattering lengths. Many achievements have been obtained. For instance, for two-component Fermi gases, Petrov and co-workers obtained the atom-dimer [4] and the dimer-dimer [5] scattering lengths, and Werner and Castin [6] rederived the well-known Tan's relations [11–13] using the BP boundary condition.

In recent years, a class of synthetic gauge fields and spin-orbit (SO) coupling has been realized in ultracold Bose gases [14–20] and degenerate Fermi gases [21,22]. A considerable amount of theoretical interest has been stimulated to understand the SO-coupling effect in both few-body [23–27] and many-body physics [28–48], including for gases with large interatomic scattering lengths [35–44]. It becomes now an urgent task to carefully examine the BP boundary condition in SO-coupled ultracold gases.

In this paper we show that, in SO-coupled systems, the BP boundary condition should be modified and moreover we derive a general form of the modified BP boundary condition that is applicable to a system with any kind of SO coupling and arbitrary atomic spin. The relevance to the current experiments is discussed.

II. MODIFIED BP BOUNDARY CONDITION FOR SPIN-1/2 FERMIONIC ATOMS

In this section we shall consider a system of two spin-1/2 fermonic atoms with a short-ranged and spin-dependent interaction potential $U(\vec{r})$, where $\vec{r} = (x,y,z)$ is the relative position of the two atoms. The interaction $U(\vec{r})$ has an effective range r_* such that $U(\vec{r}) \simeq 0$ for $r \equiv |\vec{r}| \gtrsim r_*$. Furthermore, we shall focus on the case of low-energy scattering for which the difference ε between the energy of atomic relative motion and the scattering threshold is much smaller than $1/r_*^2$.

Let $|\uparrow\rangle$ and $|\downarrow\rangle$ represent the spin eigenstates of a single atom; the quantum state of the relative atomic motion can be described by a spinor wave function

$$|\psi(\vec{r})\rangle = \psi_S(\vec{r})|\mathrm{S}\rangle + \sum_{j=1}^{3} \psi_{T_j}(\vec{r})|\mathrm{T}_j\rangle, \tag{1}$$

where $|\mathrm{S}\rangle = (|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2)/\sqrt{2}$ is the singlet spin state and $|\mathrm{T}_j\rangle$ $(j = 1,2,3)$ are the three triplet states. In dilute ultracold gases, the interatomic distance is much larger than the effective range r_*, and the physical property of the system is determined by the behavior of the wave function $|\psi(\vec{r})\rangle$ in the region $r \gtrsim r_*$.

Our task is to investigate the behavior of the wave function $|\psi(\vec{r})\rangle$ in the presence of SO coupling, and then establish the correct BP boundary condition.

A. Without SO coupling

For completeness, we start with the case without SO coupling, for which the relative motion of the two atoms is governed by the Hamiltonian

$$H = \vec{p}^{\,2} + B + U(\vec{r}), \tag{2}$$

where $\vec{p} = -i\nabla$ is the relative momentum and the natural units $\hbar = m = 1$ (where m is the single-atom mass) are used. Operator B acts in the spin space and accounts for the possible $\vec{r}$-independent contribution, e.g., from the Zeeman effect. We assume the differences of the eigenenergies of B are much smaller than $1/r_*^2$.

We first consider the property of $|\psi(\vec{r})\rangle$ in the short-range region $r_* \lesssim r \ll 1/\sqrt{\varepsilon}$. According to low-energy scattering theory (Appendix A), when $|\psi(\vec{r})\rangle$ is a low-energy eigenfunction of H, one has

$$|\psi(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a}\right)|\mathrm{S}\rangle \quad \text{for} \quad r_* \lesssim r \ll 1/\sqrt{\varepsilon}, \tag{3}$$

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with the scattering length a being determined by the detail of $U(\vec{r})$. Note that Eq. (3) does not depend on the eigenvalue of H for $|\psi(\vec{r})\rangle$ and is thus applicable to all low-energy wave functions.

With Eq. (3), one can obtain the behavior of a low-energy wave function $|\psi(\vec{r})\rangle$ in the whole region $r \gtrsim r_*$. Let $|\phi(\vec{r})\rangle$ be the solution of the Schrödinger equation with Hamiltonian $\vec{p}^{\,2} + B$; together with the BP boundary condition

$$\lim_{r\to 0} |\phi(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a}\right)|\mathrm{S}\rangle + O(r), \tag{4}$$

the realistic wave function $|\psi(\vec{r})\rangle$ and the pseudo one $|\phi(\vec{r})\rangle$ will have the same behavior for $r \gtrsim r_*$. Therefore, in the study of few-body and many-body physics in systems with interaction $U(\vec{r})$, one can replace the realistic potential $U(\vec{r})$ by the BP condition (4). Theoretical calculations can be greatly simplified.

B. With one-dimensional SO coupling

We now consider a simple case with one-dimensional SO coupling. Without loss of generality, the single-atom Hamiltonian of the system can be written as

$$H_{1\mathrm{b}} = \frac{\vec{P}^2}{2} + \lambda\hat{\sigma}_z P_x + Z, \tag{5}$$

where $\vec{P}$ is the atomic momentum, $\hat{\sigma}$ is the Pauli operator, λ indicates the intensity of the SO coupling, and Z accounts for the residual spin-dependent part. In this paper we shall consider the case of weak SO coupling, $\lambda \ll 1/r_*$, as in the current experiments. We assume the differences between the eigenvalues of Z are much smaller than $1/r_*^2$.

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

$$H = \vec{p}^{\,2} + \lambda\big(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)}\big)p_x + B(\vec{K}) + U(\vec{r}) \equiv H_0 + U(\vec{r}), \tag{6}$$

where $B(\vec{K}) = Z^{(1)} + Z^{(2)} + \lambda(\hat{\sigma}_z^{(1)} + \hat{\sigma}_z^{(2)})K_x/2$ and the vector $\vec{K} = (K_x, K_y, K_z)$ is just the total momentum of the two atoms.

For the aim of establishing a correct BP boundary condition, one should also examine the behavior of the eigenfunction $|\psi(\vec{r})\rangle$ of H in Eq. (6) in the short-range region, now defined as $r_* \lesssim r \ll r_s$ with $r_s = \min(1/\sqrt{\varepsilon}, 1/\lambda)$. Comparing Eq. (6) to Eq. (2), one finds that due to the SO coupling, the Hamiltonian H is modified by a term $\lambda(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)})p_x$. This term exists in the whole range of the interatomic distance r, including the short-range region and the region $r \lesssim r_*$. Therefore, the short-range behavior of $|\psi(\vec{r})\rangle$ can no longer be described by Eq. (3), and the BP boundary condition in Eq. (4) cannot be directly applied.

To overcome this difficulty, we introduce a unitary transformation (rotation) $\mathcal{R}(\vec{r})$ as

$$\mathcal{R}(\vec{r}) = e^{i\lambda(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)})x/2}, \tag{7}$$

with x the relative position in the x direction, and we define the rotated wave function $|\psi(\vec{r})\rangle_{\mathrm{R}}$ as

$$|\psi(\vec{r})\rangle_{\mathrm{R}} = \mathcal{R}(\vec{r})|\psi(\vec{r})\rangle. \tag{8}$$

An immediate observation is that since $|\psi(\vec{r})\rangle$ is an eigenfunction of Hamiltonian H, the rotated wave function $|\psi(\vec{r})\rangle_{\mathrm{R}}$ is an eigenfunction of the rotated Hamiltonian

$$H_{\mathrm{R}} = \mathcal{R}(\vec{r})H\mathcal{R}^{\dagger}(\vec{r}). \tag{9}$$

Straightforward calculations yield

$$H_{\mathrm{R}} = \vec{p}^{\,2} + W(\vec{r}) + U_{\mathrm{R}}(\vec{r}) \tag{10}$$

with

$$U_{\mathrm{R}}(\vec{r}) = \mathcal{R}(\vec{r})U(\vec{r})\mathcal{R}^{\dagger}(\vec{r}), \tag{11}$$

$$W(\vec{r}) = \mathcal{R}(\vec{r})B(\vec{K})\mathcal{R}^{\dagger}(\vec{r}) - \frac{\lambda^2}{4}\big(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)}\big)^2. \tag{12}$$

Equation (10) shows that the SO coupling *disappears* in the rotated Hamiltonian H_{R}. Furthermore, in the region $r \ll 1/\lambda$, we have $W(\vec{r}) \simeq W(0)$, and then

$$H_{\mathrm{R}} \approx H_{\mathrm{SR}} \equiv \vec{p}^{\,2} + W(0) + U_{\mathrm{R}}(\vec{r}). \tag{13}$$

Thus, the eigenfunctions of H_{R} and H_{SR} have the same behavior in the short-range region $r_* < r \ll r_s$. Further, Eq. (13) has the same behavior as Eq. (2). Therefore, the eigenfunction $|\psi(\vec{r})\rangle_{\mathrm{R}}$ behaves as

$$|\psi(\vec{r})\rangle_{\mathrm{R}} \propto \left(\frac{1}{r} - \frac{1}{a_{\mathrm{R}}}\right)|\mathrm{S}\rangle \quad \text{for} \quad r_* \lesssim r \ll r_s, \tag{14}$$

analogous to Eq. (3). It should be pointed out that a_{R} is the scattering length with respect to the rotated interaction potential $U_{\mathrm{R}}(\vec{r})$. On the basis of Eq. (14), the behavior of the wave function $|\psi(\vec{r})\rangle$ in the unrotated frame can be obtained by the inverse unitary transformation $\mathcal{R}^{\dagger}(\vec{r})$. The result is

$$|\psi(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a_{\mathrm{R}}}\right)|\mathrm{S}\rangle - i\frac{\lambda}{2}(\hat{\sigma}_{z1} - \hat{\sigma}_{z2})\left(\frac{x}{r}\right)|\mathrm{S}\rangle, \quad \text{for} \quad r_* \lesssim r \ll r_s. \tag{15}$$

As in the above ssection, Eq. (15) does not depend on whether or not $|\psi(\vec{r})\rangle$ is an eigenfunction of H, and thus it is generally applicable. Finally, we emphasize that the last term in Eq. (15) is of the order of unity and cannot be neglected.

Let $|\phi(\vec{r})\rangle$ be the wave function given by the Schrödinger equation with Hamiltonian H_0 in Eq. (6) together with the *modified* BP boundary condition

$$\lim_{r\to 0} |\phi(\vec{r})\rangle \propto \left(\frac{1}{r} - \frac{1}{a_{\mathrm{R}}}\right)|\mathrm{S}\rangle - i\frac{\lambda}{2}\big(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)}\big)\left(\frac{x}{r}\right)|\mathrm{S}\rangle + O(r). \tag{16}$$

It is clear that in the whole region $r \gtrsim r_*$, $|\phi(\vec{r})\rangle$ has the same behavior with the solution of the Schrödinger equation with Hamiltonian H in Eq. (6). Therefore, theoretical calculation can be done by replacing $U(\vec{r})$ with condition (16).

So far we have obtained the modified BP boundary condition (16) for the system with one-dimensional SO coupling. Comparing Eq. (16) to Eq. (4), we find that the SO coupling has two effects on the BP condition. First, the modified BP condition includes an anisotropic term

$-i\lambda(\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)})x/(2r)|\mathrm{S}\rangle$. Second, the scattering length a_R is determined by the detail of the rotated interaction potential $U_\mathrm{R}(\vec{r})$ defined in Eq. (11).

In general, to obtain the value of a_R we need to explicitly solve the Schrödinger equation with potential $U_\mathrm{R}(\vec{r})$ for a given SO coupling. As shown below, however, in the special case of the current experiments [21,22], the SO coupling *does not* change the scattering length. Namely, a_R equals to the scattering length a_0 for the case without SO coupling.

In Refs. [21,22], the spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ are two hyperfine states of the ^{6}Li or ^{40}K atom, and the single-atom Hamiltonian in the Schrödinger picture is given by

$$H_\mathrm{1bS} = \frac{\vec{P}^2}{2} + \frac{\Omega}{2}(\hat{\sigma}_+ e^{2ik_r X} + \hat{\sigma}_- e^{-2ik_r X}) + \frac{\delta}{2}\hat{\sigma}_z, \quad (17)$$

with X the single-atom coordinate in the x direction, $\hat{\sigma}_+ = |\uparrow\rangle\langle\downarrow|$, and $\hat{\sigma}_- = \hat{\sigma}_+^\dagger$. Here Ω and δ are the Rabi frequency and the two-photon detuning, respectively. Then, in the Schrödinger picture the two-atom Hamiltonian is $H_\mathrm{2bS} = H_\mathrm{1bS}^{(1)} + H_\mathrm{1bS}^{(2)} + U_0(\vec{r})$, where the bare interatomic interaction potential $U_0(\vec{r})$ has scattering length a_0.

The SO coupling term emerges after the spin rotation along the z axis or the unitary transformation $\mathcal{T}(X) = \exp[-ik_r X\hat{\sigma}_z]$ is applied. In the transformed picture, the single-atom Hamiltonian is given by $H_\mathrm{1b} = \mathcal{T}(X)H_\mathrm{1bS}\mathcal{T}^\dagger(X)$. It can be shown that H_1b takes the form in Eq. (5) with $\lambda = 2k_r$ and $Z = \Omega\hat{\sigma}_x/2 + \delta\hat{\sigma}_z/2$.

The two-atom Hamiltonian in the transformed picture can be written as $H_\mathrm{1b}^{(1)} + H_\mathrm{1b}^{(2)} + U(\vec{r})$, and the transformed interaction potential $U(\vec{r})$ is given by

$$\begin{aligned} U(\vec{r}) &= \mathcal{T}(X_1)\mathcal{T}(X_2)U_0(r)\mathcal{T}^\dagger(X_2)\mathcal{T}^\dagger(X_2) \\ &= e^{-ik_r[\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)}]x} U_0(\vec{r}) e^{ik_r[\hat{\sigma}_z^{(1)} - \hat{\sigma}_z^{(2)}]x}, \end{aligned} \quad (18)$$

where the relative coordinate x satisfies $x = X_1 - X_2$ and we have used the fact that $[U_0(\vec{r}), \hat{\sigma}_z^{(1)} + \hat{\sigma}_z^{(2)}] = 0$, arising from the conservation of the total z component of hyperfine spin during the collision process. We emphasize that, in the transformed picture where the SO-coupling term $\hat{\sigma}_z P_x$ appears, the interatomic interaction is not the bare potential $U_0(\vec{r})$, but the transformed one $U(\vec{r})$.

The scattering length a_R in the modified BP boundary condition (16) is determined by $U_R(\vec{r})$ in Eq. ((11)). Substituting Eq. (18) into Eq. (11), we find that the rotated potential $U_R(\vec{r})$ reduces to the bare potential, i.e., $U_R(\vec{r}) = U_0(r)$. Therefore, the scattering length remains unchanged with SO coupling, i.e., $a_\mathrm{R} = a_0$.

C. With arbitrary type of SO coupling

We shall now extend the above treatment to the spin-1/2 fermonic system with arbitrary type of SO coupling. In this case, the single-atom Hamiltonian can be generally written as

$$H_\mathrm{1b} = \frac{\vec{P}^2}{2} + \lambda\vec{M}\cdot\vec{P} + Z, \quad (19)$$

where $\vec{M}$ and Z as operators in the spin space and the maximum eigenvalue of $\vec{M}$ is of the order of unity. After being separated from the mass-center motion, the relative motion of the two atoms is described by the Hamiltonian

$$H = \vec{p}^{\,2} + \lambda\vec{c}\cdot\vec{p} + B(\vec{K}) \equiv H_0 + U(\vec{r}), \quad (20)$$

with $\vec{c} = \vec{M}^{(1)} - \vec{M}^{(2)}$ and $B(\vec{K}) = Z^{(1)} + Z^{(2)} + \lambda(\vec{M}^{(1)} + \vec{M}^{(2)})\cdot\vec{K}/2$.

As in the above section, to investigate the short-range behavior of the eigenfunction $|\psi(\vec{r})\rangle$ of H, we introduce a unitary transformation $\mathcal{R}(\vec{r})$ as

$$\mathcal{R}(\vec{r}) = e^{i\lambda c_x x/2} e^{i\lambda c_y y/2} e^{i\lambda c_z z/2}, \quad (21)$$

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

$$H_\mathrm{R} = \vec{p}^{\,2} - 2\lambda\vec{d}(\lambda\vec{r})\cdot\vec{p} + W(\vec{r}) + U_\mathrm{R}(\vec{r}) \quad (22)$$

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

$$d_x(\lambda\vec{r}) = 0, \quad (23)$$

$$d_y(\lambda\vec{r}) = e^{i\lambda c_z z/2}\frac{c_y}{2}e^{-i\lambda c_z z/2} - \mathcal{R}(\vec{r})\frac{c_y}{2}\mathcal{R}^\dagger(\vec{r}), \quad (24)$$

$$d_z(\lambda\vec{r}) = \frac{c_z}{2} - \mathcal{R}(\vec{r})\frac{c_z}{2}\mathcal{R}^\dagger(\vec{r}), \quad (25)$$

and

$$W(\vec{r}) = i\lambda[\nabla\cdot\vec{d}(\lambda\vec{r})] + \mathcal{R}(\vec{r})B(\vec{K})\mathcal{R}^\dagger(\vec{r}) \quad (26)$$

$$+ \lambda^2\left[|\vec{d}(\lambda\vec{r})|^2 - \mathcal{R}(\vec{r})\frac{|\vec{c}|^2}{4}\mathcal{R}^\dagger(\vec{r})\right]. \quad (27)$$

Here we have $U_\mathrm{R}(\vec{r}) = \mathcal{R}(\vec{r})U(\vec{r})\mathcal{R}^\dagger(\vec{r})$ as before.

Unlike Eq. (10) in the above section, the SO coupling still exists in the rotated Hamiltonian H_R in Eq. (22). Nevertheless, according to Eqs. (23)–(25), we have $\vec{d}(\lambda\vec{r}) = O(\lambda r)$. Namely, its zeroth-order contribution in H_R vanishes. This leads to the following important property of the eigenfunction $|\psi(\vec{r})\rangle_\mathrm{R}$ of H_R:

$$|\psi(\vec{r})\rangle_\mathrm{R} \propto \left(\frac{1}{r} - \frac{1}{a_\mathrm{R}}\right)|\mathrm{S}\rangle \quad (\text{for } r_* \lesssim r \ll r_s). \quad (28)$$

The result in Eq. (28) is proved as follows. In the region $r > r_*$ where $U_R(\vec{r})$ is negligible, the eigenequation of H_R reads

$$[\vec{p}^{\,2} - 2\lambda\vec{d}(\lambda\vec{r})\cdot\vec{p} + W(\vec{r})]|\psi(\vec{r})\rangle_\mathrm{R} = E|\psi(\vec{r})\rangle_\mathrm{R}. \quad (29)$$

As shown in Appendix B, in this region the wave function $|\psi(\vec{r})\rangle_\mathrm{R}$ can be expressed as

$$\begin{aligned} |\psi(\vec{r})\rangle_\mathrm{R} = \frac{C_{-1}}{r}|\mathrm{S}\rangle + \sum_{n=0}^{\infty} C_n r^n |\mathrm{S}\rangle \\ + \sum_{l=1}^{\infty}\sum_{m_l=-l}^{l}\sum_{n=0}^{\infty} r^n Y_{l,m_l}(\theta,\phi)|A_{l,m_l,n}\rangle, \end{aligned} \quad (30)$$

in the spherical coordinate (r,θ,ϕ). Here $Y_{l,m_l}(\theta,\phi)$ are the spherical harmonic functions, C_n $(n = -1,0,1,\ldots)$ is the coefficient of term $r^n|\mathrm{S}\rangle$, and $|A_{l,m_l,n}\rangle$ $(n = 0,1,\ldots)$ is the spin state with respect to $r^n Y_{l,m_l}(\theta,\phi)$. Substituting Eq. (30) into Eq. (29) and comparing the coefficient of the term r^{-2} on both sides, we find that because $d(\lambda\vec{r}) = O(\lambda r)$, one has $|A_{l,m_l,0}\rangle = 0$. Therefore, in the short-range region $|\psi(\vec{r})\rangle_\mathrm{R}$ behaves as in Eq. (28), with the scattering length a_R determined by both the potential $U_\mathrm{R}(\vec{r})$ and the operator $\vec{d}(\lambda\vec{r})$.

With Eq. (28) and following the procedure in the above section, we obtain the *modified* BP boundary condition for the general type of SO coupling as

$$\lim_{r\to 0}|\phi(\vec{r})\rangle \propto \left(\frac{1}{r}-\frac{1}{a_{\rm R}}\right)|{\rm S}\rangle - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|{\rm S}\rangle + O(r). \quad (31)$$

As in the previous section, the value of the scattering length $a_{\rm R}$ in general depends on the SO coupling. This dependence is also shown in Fig. 3 of Ref. [23] with a simple model where the potential $U(\vec{r})$ is modeled as a spin-independent spherical square well.

III. MODIFIED BP BOUNDARY CONDITION FOR ATOMS WITH ARBITRARY SPIN

Finally, we consider the general case: a system of two fermonic or bosonic atoms with any kind of SO coupling and arbitrary spin. The Hamiltonians for the single-atom motion and the relative motion of the two atoms are still given by Eqs. (19) and (20), respectively.

For simplicity, we first consider the case in which the interatomic interaction $U(\vec{r})$ (with scattering length a) is independent of the atomic spin. In this case, it can be shown that, without SO coupling, the low-energy eigenstate $|\psi(\vec{r})\rangle$ of the relative-motion Hamiltonian $(-\nabla^2 + U(\vec{r}) + Z^{(1)} + Z^{(2)})$ behaves as

$$|\psi(\vec{r})\rangle \propto \left(\frac{1}{r}-\frac{1}{a}\right)|\chi\rangle, \quad \text{for} \quad r_* \lesssim r \ll r_s. \quad (32)$$

This is very similar to Eq. (2), but now the $\vec{r}$-independent spin state $|\chi\rangle$ is not unique. Instead, $|\chi\rangle$ can be different for different eigenstates $|\psi(\vec{r})\rangle$.

In the presence of SO coupling, the short-range behavior of the eigenfunction $|\psi(\vec{r})\rangle$ can be obtained via the same approach using the unitary transformation $\mathcal{R}(\vec{r})$ in Eq. (21). In particular, in the region $r \ll r_s$, it is sufficient to keep the lowest-order terms of $\vec{d}(\lambda\vec{r})$ and $W(\vec{r})$ defined in Eqs. (23)–(26). Thus, the rotated wave function $|\psi(\vec{r})\rangle_{\rm R} = \mathcal{R}(\vec{r})|\psi(\vec{r})\rangle$ satisfies the equation

$$[\vec{p}^{\,2} - 2\lambda\vec{g}(\lambda\vec{r})\cdot\vec{p} + W(0) + U(\vec{r})]|\psi(\vec{r})\rangle_{\rm R} = E|\psi(\vec{r})\rangle_{\rm R} (r \ll r_s), \quad (33)$$

where E is the eigenenergy. Here we have used $\vec{d}(0) = 0$ and the fact that $U_{\rm R}(\vec{r}) = U(\vec{r})$, which is because U is spin-independent. The operator $\vec{g} = (g_x, g_y, g_z)$ is defined as $g_i(\lambda\vec{r}) = \vec{r}\cdot[\nabla d_i(\lambda\vec{r})|_{\vec{r}=0}]$ with $i = x, y, z$. In Eq. (33) the term $-2\lambda\vec{g}\cdot\vec{p}$ couples the s-wave and d-wave components of $|\psi(\vec{r})\rangle_{\rm R}$. In the Schrödinger equation, the coupling terms are either independent of r or proportional to $r(\partial/\partial r)$, and thus they do not decrease the power of r in the wave function $|\psi(\vec{r})\rangle_{\rm R}$. The estimation with the semiclassical approximation $\partial|\psi(\vec{r})\rangle_{\rm R}/\partial r \lesssim \sqrt{-U(\vec{r})}|\psi(\vec{r})\rangle_{\rm R}$ shows that, in the short-range region $r_* \lesssim r \ll r_s$, the intensity of this coupling is much smaller than the centrifugal potential $6/r^2$, which is the energy gap between the s-wave and d-wave channels. In addition, for many systems this intensity is also much smaller than $6/r^2$ even when $r \lesssim r_*$. An example is a system with Lennard-Jones potential $U(\vec{r}) = -c_6/r^6 + c_{12}/r^{12}$. Therefore, for these systems we can neglect the SO coupling in the entire region $r \ll r_s$. Then one has

$$|\psi(\vec{r})\rangle_{\rm R} \propto \left(\frac{1}{r}-\frac{1}{a}\right)|\chi\rangle \quad (\text{for } r_* \lesssim r \ll r_s). \quad (34)$$

Note that a is still the scattering length of the potential $U(r)$. Accordingly, we have the modified BP boundary condition

$$\lim_{r\to 0}|\phi(\vec{r})\rangle \propto \left(\frac{1}{r}-\frac{1}{a}\right)|\chi\rangle - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|\chi\rangle + O(r). \quad (35)$$

The situation becomes more sophisticated if $U(\vec{r})$ is spin-dependent or the SO coupling cannot be neglected in H_R when $r \lesssim r_*$. In these cases, $1/a$ in the modified BP boundary condition (35) should be replaced by an operator $A_{\rm R}$ in the spin space, which is also determined by $U_{\rm R}(\vec{r})$ and $\vec{d}(\lambda\vec{r})$. The details are given in Appendix C.

We conclude this section by pointing out that, as in Sec. II, in the current experiments [14–20] for bosonic atoms with one-dimensional SO coupling, the rotated potential $U_{\rm R}$ is equivalent to the bare potential U_0 in the Schrödinger picture, and the operator $\vec{d}$ is zero. Then the operator $A_{\rm R}$ in the modified BP boundary condition is independent of the SO coupling. For instance, for the ultracold gases with spin-1 ^{87}Rb atoms, we have $A_{\rm R} = 1/a_0\mathcal{P}_{F=0} + 1/a_2\mathcal{P}_{F=2}$, 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 relevant projection operators.

IV. DISCUSSION

In this paper we derive the modified BP boundary condition for ultracold atomic gases with SO coupling. It is shown that the SO coupling brings a new anisotropic term to the BP boundary condition and may change the value of atomic scattering length.

Our result can be used for the research of both few-body and many-body problems in SO-coupled ultracold gases. For instance, for N spin-1/2 fermonic atoms with the Hamiltonian

$$H_T = \sum_{i=1}^{N} H_{1\rm b}(i) + \sum_{i=1}^{N} V_{\rm trap}^{(i)} + \sum_{i<j}^{N} U(\vec{r}_{ij}) \equiv H_F + \sum_{i<j}^{N} U(\vec{r}_{ij}), \quad (36)$$

one can replace the interaction potential $U(\vec{r}_{ij})$ by the modified BP boundary condition

$$\lim_{|\vec{r}_{ij}|\to 0}\langle\vec{r}_{ij}|\Phi\rangle \propto \left[\left(\frac{1}{|\vec{r}_{ij}|}-\frac{1}{a_{\rm R}}\right)|{\rm S}\rangle_{ij} - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}_{ij}}{|\vec{r}_{ij}|}\right)|{\rm S}\rangle_{ij}\right] \times|\Phi'\rangle + O(r_{ij}). \quad (37)$$

In Eq. (36) $V_{\rm trap}^{(i)}$ is the trap potential for the ith atom and $\vec{r}_{ij}$ is the relative position between the ith and jth atoms; in Eq. (37) $|\Phi\rangle$ is the N-atom state, $|\vec{r}_{ij}\rangle$ is the eigenstate of the relative motion of the (i, j) pair, $|{\rm S}\rangle_{ij}$ is the singlet spin state for the two atoms, and $|\Phi'\rangle$ is a quantum state for other atoms. The limit in Eq. (37) is taken for fixing the positions of other atoms as well as the mass center of the (i, j) pair. In the region $|\vec{r}_{ij}| \gtrsim r_*$, the solution of the Schrödinger equation with the free Hamiltonian H_F under the boundary condition (37) has

the same behavior as the solution of the Schrödinger equation with the total Hamiltonian H_T.

Our result is also useful in the current experiments of ultracold gases with one-dimensional SO coupling and far away from the Feshbach resonance point. As shown in Secs. II and III, the scattering lengths in these systems are independent of the SO coupling, and thus all the terms in the modified BP boundary condition can be fully determined with the known parameters.

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APPENDIX A: SHORT-RANGE BEHAVIOR OF SCATTERING WAVE FUNCTION

In this Appendix we prove Eq. (3) for the short-range behavior of the wave function $|\psi(\vec{r})\rangle$ in the cases without SO coupling. Without loss of generality, here we consider the case in which $|\psi(\vec{r})\rangle$ is the scattering wave function and then satisfies the Lippmman-Schwinger equation [49]

$$|\psi(\vec{r})\rangle = |\psi^{(0)}(\vec{r})\rangle + \int d\vec{r}\,' g_0(E,\vec{r},\vec{r}\,')U(\vec{r}\,')|\psi(\vec{r}\,')\rangle, \quad \text{(A1)}$$

where E is the eigenenergy of H in Eq. (2) with respect to $|\psi(\vec{r})\rangle$, and $|\psi^{(0)}(\vec{r})\rangle$ is the incident state and satisfies $(\vec{p}^{\,2}+B)|\psi^{(0)}(\vec{r})\rangle = E|\psi^{(0)}(\vec{r})\rangle$. For our system with two fermonic atoms, $|\psi^{(0)}(\vec{r})\rangle$ is antisymnetric with respect to the permutation of the two atoms. In Eq. (A1) the Green's operator $g_0(E,\vec{r},\vec{r}\,')$ is defined as

$$\begin{aligned} g_0(\eta,\vec{r},\vec{r}\,') &= \frac{1}{\eta + i0^+ - (\vec{p}^{\,2}+B)}\delta(\vec{r}-\vec{r}\,') \\ &= -\sum_n \frac{e^{i\sqrt{\eta-\varepsilon_n}|\vec{r}-\vec{r}\,'|}}{\pi|\vec{r}-\vec{r}\,'|}|n\rangle\langle n| \end{aligned} \quad \text{(A2)}$$

with ε_n and $|n\rangle$ the nth eigenvalue and eigenstate of the operator B, respectively.

Since the potential $U(\vec{r})$ is negligible in the region $r > r_*$, the integration in Eq. (A1) is only effective in the region $r' \leqslant r_*$. In the low-energy cases, when $r \to \infty$ and $r' \leqslant r_*$, the function $g_0(E,\vec{r},\vec{r}\,')$ becomes very steady 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

$$|\psi(\vec{r})\rangle = |\psi^{(0)}(\vec{r})\rangle + g_0(E,\vec{r},0)|\chi\rangle, \quad \text{(A3)}$$

where the spin state $|\chi\rangle$ is related to $|\psi(\vec{r})\rangle$ via the equation $|\chi\rangle = \int d\vec{r}\,'U(\vec{r}\,')|\psi(\vec{r}\,')\rangle$. Furthermore, because $P_{12}|\psi(\vec{r})\rangle = -|\psi(\vec{r})\rangle$ and $P_{12}U(\vec{r})P_{12} = U(\vec{r})$ with P_{12} the permutation operator of the two atoms, one finds that $P_{12}U(\vec{r})|\psi(\vec{r})\rangle = -U(\vec{r})|\psi(\vec{r})\rangle$. This result yields

$$|\chi\rangle = |\mathrm{S}\rangle \int d\vec{r}\,'U(r')\langle \mathrm{S}|\psi(\vec{r}\,')\rangle. \quad \text{(A4)}$$

On the other hand, since $|\psi(\vec{r})\rangle$ is an eigenstate of H and the potential $U(\vec{r})$ is negligible in the region $r > r_*$, in such a region the wave function $|\psi(\vec{r})\rangle$ satisfies the equation

$$(\vec{p}^{\,2}+B)|\psi(\vec{r})\rangle = E|\psi(\vec{r})\rangle. \quad \text{(A5)}$$

Therefore, the behavior of the wave function $|\psi(\vec{r})\rangle$ in the region $r \gtrsim r_*$ is determined by Eq. (A5) and the boundary condition (A3) in the limit $r \to \infty$. Considering Eq. (A4), one can easily prove that the function

$$|\psi(\vec{r})\rangle = |\psi^{(0)}(\vec{r})\rangle + \Lambda_0 g_0(E,\vec{r},0)|\mathrm{S}\rangle \quad \text{(A6)}$$

with Λ_0 a constant satisfies both of the two conditions. Therefore, $|\psi(\vec{r})\rangle$ satisfies Eq. (A6) in the whole region of $r \gtrsim r_*$.

To obtain the short-range behavior of $|\psi(\vec{r})\rangle$, one can expand Eq. (A6) as a series of r, and then neglect the high-order terms. Using Eq. (A2) and the fact that $P_{12}|\psi^{(0)}(\vec{r})\rangle = -|\psi^{(0)}(\vec{r})\rangle$, we immediately get the result in Eq. (3):

$$|\psi(\vec{r})\rangle \propto \left(\frac{1}{r}-\frac{1}{a}\right)|\mathrm{S}\rangle \quad \text{for } r_* \lesssim r \ll 1/\sqrt{\varepsilon}. \quad \text{(A7)}$$

APPENDIX B: PROOF OF EQ. (30)

Now we prove Eq. (30) for the behavior of $|\psi(\vec{r})\rangle_{\mathrm{R}}$ in the region $r \gtrsim r_*$. To this end, we first consider the behavior of the unrotated eigenfunction $|\psi(\vec{r})\rangle$ of Hamiltonian H defined in Eq. (20). Without loss of generality, here we consider the case in which $|\psi(\vec{r})\rangle$ is the scattering wave function. Using the approach in Appendix A, we can prove that when $r \gtrsim r_*$ we have

$$|\psi(\vec{r})\rangle = |\psi^{(0)}(\vec{r})\rangle + \Lambda_0 g(E,\vec{r},0)|\mathrm{S}\rangle, \quad \text{(B1)}$$

where E is the eigenenergy of H with respect to $|\psi(\vec{r})\rangle$, and $|\psi^{(0)}(\vec{r})\rangle$ is the incident state and satisfies $H_0|\psi^{(0)}(\vec{r})\rangle = E|\psi^{(0)}(\vec{r})\rangle$ with H_0 defined in Eq. (20). The Green's operator $g(E,\vec{r},\vec{r}\,')$ is defined as

$$g(\eta,\vec{r},\vec{r}\,') = \frac{1}{\eta + i0^+ - H_0}\delta(\vec{r}-\vec{r}\,'). \quad \text{(B2)}$$

Now we expand the right-hand side of Eq. (B1) as a power series of r. To this end, we first consider the operator $F(\vec{k}) \equiv \lambda\vec{c}\cdot\vec{k} + B(\vec{K})$, with $\vec{k}$ a constant operator and λ, $\vec{c}$, and $B(\vec{K})$ defined in Sec. II. For each given vector $\vec{k}$, $F(\vec{k})$ is an operator in the four-dimensional spin space. We denote the αth ($\alpha = 1,2,3,4$) eigenenergy and eigenstate $F(\vec{k})$ as $\mathcal{E}(\alpha,\vec{k})$ and $|\alpha(\vec{k})\rangle$, respectively. Therefore, the incident wave function $|\psi^{(0)}(\vec{r})\rangle$, which is an eigenfunction of H_0 defined in Eq. (20), takes the form

$$|\psi^{(0)}(\vec{r})\rangle = \frac{1}{2(2\pi)^{3/2}}(1-P_{12})e^{i\vec{k}\cdot\vec{r}}|\alpha(\vec{k})\rangle, \quad \text{(B3)}$$

with P_{12} the permutation operator for both the spin and the spatial motion of the two atoms. Equation (B3) leads to the result that

$$|\psi^{(0)}(\vec{r})\rangle = O(r^0). \quad \text{(B4)}$$

Now we consider the expansion of the Green's function $g(E,\vec{r},0)$. By using the fact that

$$\delta(\vec{r}-\vec{r}\,') = \int d\vec{k}\,\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{(2\pi)^3}\left(\sum_\alpha |\alpha(\vec{k})\rangle\langle\alpha(\vec{k})|\right), \quad \text{(B5)}$$

it is easy to show that

$$g(E,\vec{r},0) = \sum_\alpha \int d\vec{k}\,\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^3}\frac{|\alpha(\vec{k})\rangle\langle\alpha(\vec{k})|}{E+i0^+-[\vec{k}^2+\mathcal{E}(\alpha,\vec{k})]}. \quad \text{(B6)}$$

Equation (B6) and the completeness relationship $\sum_\alpha |\alpha(\vec{k})\rangle\langle\alpha(\vec{k})| = 1$ lead to the result

$$\begin{aligned} &g(E,\vec{r},0) \\ &= \int d\vec{k}\,\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^3}\frac{1}{E+i0^+-\vec{k}^2} + \sum_\alpha \int d\vec{k}\,\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^3}|\alpha(\vec{k})\rangle \\ &\quad\times\langle\alpha(\vec{k})|\left(\frac{1}{E+i0^+-[\vec{k}^2+\mathcal{E}(\alpha,\vec{k})]}-\frac{1}{E+i0^+-\vec{k}^2}\right). \quad \text{(B7)} \end{aligned}$$

It is pointed out that, in the limit $r\to 0$, the integration on the right-hand side of Eq. (B7) converges to a constant operator in the spin space. On the other hand, we also have

$$\int d\vec{k}\,\frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^3}\frac{1}{E+i0^+-\vec{k}^2} = -\frac{e^{i\sqrt{E}r}}{\pi r}. \quad \text{(B8)}$$

Due to these facts, we have $g(E,\vec{r},0)\propto 1/r + O(r^0)$. Substituting this result and Eq. (B4) into Eq. (B1) and using the relation $|\psi(\vec{r})\rangle_{\rm R} = \mathcal{R}(\vec{r})|\psi(\vec{r})\rangle$ with $\mathcal{R}(\vec{r})$ defined in Eq. (21), we can find that

$$|\psi(\vec{r})\rangle_{\rm R} \propto \frac{1}{r}|{\rm S}\rangle + O(r^0). \quad \text{(B9)}$$

Namely, $|\psi(\vec{r})\rangle_{\rm R}$ takes the form of Eq. (30).

APPENDIX C: THE MODIFIED BP BOUNDARY CONDITION FOR ATOMS WITH SPIN-DEPENDENT INTERACTION

In Sec. III of our main text, we derive the modified BP boundary condition for atoms with arbitrary spin and SO coupling. Our result in Eq. (35) is based on the following two assumptions: (a) the interatomic interaction is spin-independent; (b) in the rotated frame, the influence of the SO coupling or the term $-2\vec{g}\cdot\vec{p}$ is negligible in the region $r\lesssim r_*$. In this Appendix we go beyond these two assumptions and derive the general type of modified BP boundary condition for atoms with arbitrary spin and SO coupling.

We first go beyond assumption (a) and consider the case of atoms with spin-dependent interaction $U(\vec{r})$. When there is no SO coupling, the eigenfunction $|\psi(\vec{r})\rangle$ of the two-atom relative Hamiltonian satisfies

$$[-\nabla^2 + U(\vec{r}) + Z^{(1)} + Z^{(2)}]|\psi(\vec{r})\rangle = E|\psi(\vec{r})\rangle. \quad \text{(C1)}$$

We assume the spin space of the two atoms is n dimensional, and we denote the eigenstates of $Z^{(1)}+Z^{(2)}$ as $|j\rangle$ $(j=1,\ldots,n)$. We further define

$$|\Psi(\vec{r})\rangle = r|\psi(\vec{r})\rangle.$$

Then $|\Psi(\vec{r})\rangle$ satisfies the boundary condition $|\Psi(0)\rangle = 0$.

We first consider that $U(\vec{r})$ is spherical. Thus, $|\Psi(\vec{r})\rangle$ can be written as

$$|\Psi(\vec{r})\rangle = \sum_{j=1}^{n}\Psi_j(r)|j\rangle. \quad \text{(C2)}$$

Then, Eq. (C1) can be reexpressed as the equation for $|\Psi(\vec{r})\rangle$. We define $|\Phi^{(\alpha)}(r)\rangle$ as the s-wave solution of this equation, with component $\Phi_j^{(\alpha)}(r)$ satisfying the boundary conditions $\Phi_j^{(\alpha)}(0)=0$ and

$$\frac{d}{dr}\Phi_j^{(\alpha)}(r)\Big|_{r=0} = \begin{cases} 1, & \text{for } \alpha = j, \\ 0, & \text{for } \alpha \neq j. \end{cases} \quad \text{(C3)}$$

Therefore, the states $|\phi^{(\alpha)}(\vec{r})\rangle = |\Phi^{(\alpha)}(\vec{r})\rangle/r$ are n special solutions of Eq. (C1). In the short-range region, the low-energy wave function $|\phi^{(\alpha)}(\vec{r})\rangle$ behaves as

$$|\phi^{(\alpha)}(\vec{r})\rangle = \frac{1}{r}|M_\alpha\rangle - |T_\alpha\rangle \quad \text{(C4)}$$

with $|M_\alpha\rangle$ and $|T_\alpha\rangle$ as states of atomic spin.

Furthermore, any s-wave solution $|\psi(\vec{r})\rangle$ of Eq. (C1) can be written as the linear combination of $|\phi^{(\alpha)}(\vec{r})\rangle$ and then expressed as

$$|\psi(\vec{r})\rangle = \sum_{\alpha=1}^{n} b_\alpha\left[\frac{1}{r}|M_\alpha\rangle - |T_\alpha\rangle\right] \qquad \text{for } r_*\lesssim r\ll r_s. \quad \text{(C5)}$$

In addition, the low-energy solutions of Eq. (C1) with high partial waves are negligible in the short-range region. Therefore, Eq. (C5) is actually satisfied by all the low-energy solutions of Eq. (C1).

When the states $|M_\alpha\rangle$ with different α are linearly independent of each other, we can define an operator A which satisfies $A|M_\alpha\rangle = |T_\alpha\rangle$. (In particular, when the interaction U is independent of the atomic spin, we have $A = 1/a$.) With this definition, the behavior (C5) of $|\psi(\vec{r})\rangle$ can be rewritten as

$$|\psi(\vec{r})\rangle \propto \left(\frac{1}{r}-A\right)|\chi\rangle \qquad \text{for} \qquad r_*\lesssim r\ll r_s. \quad \text{(C6)}$$

As in Sec. III, the $\vec{r}$-independent state $|\chi\rangle$ in the spin space is not unique. Finally, it can be proved that in the low-energy limit the above result is also correct when $U(\vec{r})$ becomes anisotropic.

In the presence of SO coupling, with Eq. (C6) and the approach in our main text we can obtain the modified BP boundary condition

$$\lim_{r\to 0}|\phi(\vec{r})\rangle \propto \left(\frac{1}{r}-A_{\rm R}\right)|\chi\rangle - i\frac{\lambda}{2}\vec{c}\cdot\left(\frac{\vec{r}}{r}\right)|\chi\rangle + O(r) \quad \text{(C7)}$$

with the operator $A_{\rm R}$ determined by both the potential $U_{\rm R}(\vec{r})$ and the operator $\vec{d}(\lambda\vec{r})$.

Finally, if we go beyond assumption (b) and consider the case in which the SO coupling cannot be neglected when $r\lesssim r_*$, we can also follow the above approach, and we obtain the modified BP boundary condition which has the form in Eq. (C7).

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