Few-body physics of one-dimensional ultracold atoms with spin-exchange interaction

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Motivated by recent progresses on ultracold alkaline-earth atoms towards the goal of simulating Kondo physics, in this work we exactly solve the few-body problem of one and two trapped fermions in one dimension interacting with a localized impurity under tunable spin-exchange interaction. It is found that depending on the sign of the spin-exchange coupling, ferromagnetic (FM) or antiferromagnetic (AFM), the attractive and repulsive branches can hold different magnetic structures. We demonstrate the Kondo screening effect for the attractive branch of three-body system with the AFM coupling, and show that such screening is absent for the ground state with FM coupling. Moreover, we find a sequence of FM upper branches in the AFM coupling side. These FM states are orthogonal to all other attractive branches and their wave functions feature a full spin-charge separation. The effect of an additional contact interaction and the extension of our results to many particles are also discussed. This work reveals the intriguing physics uniquely associated with the spin-exchange interaction in the few-body point of view, which are promisingly to be explored in the experiment of ultracold alkaline-earth atoms.

I. INTRODUCTION

Recent progresses on ultracold alkaline-earth atoms have opened the door for simulating Kondo physics$^{[1]}$. In these two-electron atoms, the metastable excited state $^3P_0$ as well as the ground state $^1S_0$ comprise the two-orbital system, and the high nuclear spin of these atoms serves as the spin degree of freedom. The spin-exchange interaction between different orbitals, as a crucial ingredient for Kondo physics, has been confirmed experimentally$^{[2–7]}$. The bare spin-exchange interaction is found to be ferromagnetic for $^{173}$Yb$^{[2–5]}$ and $^{87}$Sr$^{[6]}$, and antiferromagnetic for $^{171}$Yb$^{[7]}$. Using the confinement-induced resonance, the strength of spin-exchange interaction can be conveniently tuned in the low dimensions, as successfully demonstrated both theoretically$^{[8–13]}$ and experimentally$^{[14]}$. Furthermore, the Kondo model requires a local impurity, which can be implemented in alkaline-earth atoms by using a proper laser wavelength to selectively confine $^3P_0$ state while let $^1S_0$ state free$^{[15]}$. All these developments make the quantum simulation of Kondo physics quite promising in ultracold atomic systems.

Motivated by these developments, in this work we exactly solve the problems of a few fermions in one-dimension (1D) interacting with a local impurity under the spin-exchange interaction. Specifically, we consider the isotropic Heisenberg coupling between fermions and the impurity with a tunable coupling strength $J$. Previously, the 1D Kondo model describing the continuum fermions and a localized impurity was exactly solved by Bethe-ansatz method assuming a linear dispersion of fermions($\epsilon_k \propto k$)$^{[16]}$, which is thus expected to be applicable in weak coupling limit. Here, we obtain the exact solutions of a few fermions in a 1D harmonic trap interacting with a local impurity for an arbitrary coupling strength $J$. It is found that depending on the sign of $J$, namely, $J < 0$ for ferromagnetic (FM) coupling or $J > 0$ for anti-ferromagnetic (AFM) coupling, the attractive and repulsive branches of the system can hold different magnetic structures. For the attractive branches of three-body system, we demonstrate the Kondo screening effect under the AFM coupling, and show that such screening does not apply to the case of FM coupling. Moreover, we find a sequence of FM upper branches in the AFM coupling side, which are orthogonal to all other attractive branches and feature a full spin-charge separation. All these features are closely related to the spin-exchange nature of the interaction potential, and thus are very different from those under a pure contact interaction. The effect of an additional contact interaction and the extension of our results to many particles are also discussed in this work.

The rest of the paper is organized as follows. In section II, we present the formulism of exactly solving one and two fermions interacting with the impurity through the spin-exchange coupling. The results of two-body and three-body problem, as well as the extension to many particles are presented in section III. In section IV, we discuss the effect of an additional contact potential. Finally, we conclude our work in section V.
II. EXACT FORMALISM OF FEW-BODY PROBLEM WITH SPIN-EXCHANGE INTERACTION

A. Model

We consider the 1D harmonically trapped spin-1/2 fermions interacting with a local spin impurity (sitting at the trap center) with a spin-exchange coupling, which is described by Hamiltonian ($\hbar = 1$ throughout the paper):

$$H = H_0 + U,$$

$$H_0 = \sum_{i=1}^{N} \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + m\omega^2 \frac{x_i^2}{2}\right);$$

$$U = 2J \sum_{i=1}^{N} \delta(x_i) S_i \cdot S$$

Here $x_i$ is the coordinate of the $i$-th fermion; $S_i = (S_{ix_i}, S_{iy_i}, S_{iz_i})$ and $S = (S_x, S_y, S_z)$ are the spin operators for, respectively, the $i$-th fermion and the impurity. We rewrite (1) in the second quantized form:

$$H = \sum_{m} E_m C_{m\sigma}^\dagger C_{m\sigma} + \sum_{m,n} V_{mn}(C_{m\uparrow}^\dagger C_{n\downarrow} S_- + h.c.)$$

+ $(C_{m\uparrow}^\dagger C_{n\downarrow} - C_{m\downarrow}^\dagger C_{n\uparrow})S_z$)

Here $C_{m\sigma}$ is the creation operator of a spin-$\sigma$($\uparrow, \downarrow$) fermion at the $m$-th harmonic oscillator level with energy $E_m = (m + \frac{1}{2})\omega$; $V_{mn} = J\phi_m(0)\phi_n(0)$ is the coupling matrix element, with $\phi_m(x)$ the eigenstate of the $m$-th harmonic oscillator level. The spin-exchange process is governed by the first two terms in the bracket of (4). Denoting $\uparrow$ and $\downarrow$ as the two spin states of the impurity, we then have $S_+ = |\uparrow\rangle\langle\downarrow|$, $S_- = |\downarrow\rangle\langle\uparrow|$, and $S_z = (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)/2$.

Next, we will present the formulism of exactly solving the two-body (one fermion plus the impurity) and the three-body (two fermions plus the impurity) problems.

B. Two-body solution

Because the Hamiltonian (4) preserves the spin-rotational symmetry, the two-body eigenstate can be classified into two cases with respect to the total spin $S_{tot}$: one is spin triplet with $S_{tot} = 1$, the other is spin singlet with $S_{tot} = 0$. We then have the effective interaction for each spin channel:

$$U_{s,t}(x_1) = \gamma_{s,t}\delta(x_1)$$

with effective coupling strengths $\gamma_{s} = \frac{3\gamma}{2}$ and $\gamma_{t} = \frac{\gamma}{2}$, respectively, for spin-singlet and spin-triplet channels.

To see the spin classification more clearly, we write down a general two-body ansatz in total zero magnetization ($S_{tot,z} = 0$) subspace:

$$|\Psi\rangle_2 = \sum_{m} \left(\phi_m^{\dagger} C_{m\uparrow}^\dagger |0\rangle \downarrow + \phi_m^{\dagger} C_{m\downarrow}^\dagger |0\rangle \uparrow\right)$$

By imposing the Schrodinger equation $H|\Psi\rangle_2 = E|\Psi\rangle_2$, we arrive at the following coupled equations:

$$(E - E_m)\phi_m^{\dagger} = \sum_{p} (V_{mp}\phi_p^2 - \frac{1}{2} V_{mp}\phi_p^{\dagger})$$

$$(E - E_m)\phi_m = \sum_{p} (V_{mp}\phi_p - \frac{1}{2} V_{mp}\phi_p^{\dagger})$$

We can see that above equations support two types of solutions. One is

$$\phi_m^\dagger = \phi_m^2 \propto \frac{\phi_m(0)}{E - E_m},$$

which represents a spin triplet, and the energy $E(= E_t)$ can be obtained from

$$\frac{1}{\gamma_t} = \sum_{m} \frac{|\phi_m(0)|^2}{E_t - E_m}.$$ (9)

The other is spin singlet solution with

$$\phi_m = -\phi_m^2 \propto \frac{\phi_m(0)}{E_s - E_m},$$

and the energy $E(= E_s)$ follows:

$$\frac{1}{\gamma_s} = \sum_{m} \frac{|\phi_m(0)|^2}{E_s - E_m}.$$ (10)

Eqs.(9,11) can be further simplified as

$$-2\sqrt{\pi} \kappa_{s,t} = B(-\frac{\rho_{s,t}}{2}, \frac{1}{2})$$ (12)

with $\kappa_{s,t} = \rho_{s,t}/\sqrt{m/\omega}$, $\rho_{s,t} = E_{s,t}/\omega - 1/2$ and $B(x,y)$ is the beta function.

C. Three-body solution

For a three-body system consisting of two fermions and the impurity, we can have the total spin $S_{tot} = 3/2$ or $S_{tot} = 1/2$. Considering the general case with total magnetization $S_{tot,z} = 1/2$, we can write down the following three-body ansatz:

$$|\Psi\rangle_3 = \sum_{mn} \left(\phi_m^{\dagger} C_{m\uparrow} C_{n\uparrow}^\dagger |0\rangle \downarrow + \phi_m^{\dagger} C_{m\downarrow} C_{n\downarrow}^\dagger |0\rangle \uparrow\right)$$ (13)

Here we should take care of the anti-symmetry property of $\phi_m^{\dagger}$, i.e., $\phi_m^{\dagger} = -\phi_m^{\dagger}$. Again by imposing the Schrodinger equation, we obtain the following coupled equations:
$$\phi_{mn}^{1} = \frac{1}{E - E_{m} - E_{n}} \cdot \frac{1}{2} \sum_{p} -V_{mp}\phi_{np}^{2} + V_{np}\phi_{mp}^{2} + V_{np}\phi_{pm}^{1} - V_{mp}\phi_{pn}^{1}$$

$$\phi_{mn}^{2} = \frac{1}{E - E_{m} - E_{n}} \sum_{p} V_{np}\phi_{mp}^{1} - V_{np}\phi_{pm}^{1} + \frac{1}{2} V_{mp}\phi_{pm}^{2} - \frac{1}{2} V_{np}\phi_{mp}^{2} \tag{14}$$

To solve these coupled equations, we introduce three series of variables $F_{m}^{1}, F_{m}^{2}, F_{m}^{3}$:

$$F_{n}^{1} = \sum_{p} \phi_{p}(0)\phi_{np}^{1}$$

$$F_{n}^{2} = \sum_{p} \phi_{p}(0)\phi_{np}^{2} \tag{15}$$

$$F_{n}^{3} = - \sum_{p} \phi_{p}(0)\phi_{pn}^{2}$$

Then we can multiply both sides of (14) by $\phi_{n}(0)$ and sum over $m$ to obtain the coupled equations of $F_{m}^{n}$. To see more clearly the physical meaning of the variables in (15), we can alternatively perform a linear transformation of them to a different set of variables:

$$\tilde{F}_{n}^{1} = - \frac{3}{2} F_{n}^{1} + \frac{3}{4} F_{n}^{2}$$

$$\tilde{F}_{n}^{2} = \frac{1}{2} F_{n}^{1} + \frac{1}{4} F_{n}^{2} \tag{16}$$

$$\tilde{F}_{n}^{3} = \frac{1}{2} F_{n}^{3}$$

Then we find that $\{\tilde{F}_{n}^{1,2,3}\}$ are exactly the atom-dimer amplitudes in the three-body wave function:

$$|\Psi_{3}\rangle = \sum_{m} \tilde{F}_{m}^{1} |m \uparrow\rangle |d_{m}^{00}\rangle + \tilde{F}_{m}^{2} |m \uparrow\rangle |d_{m}^{10}\rangle + \tilde{F}_{m}^{3} |m \downarrow\rangle |d_{m}^{01}\rangle \tag{17}$$

with the dimer states:

$$|d_{m}^{11}\rangle = \sum_{p} \frac{\phi_{p}(0)}{E - E_{m} - E_{p}} |p \uparrow\rangle |p \uparrow\rangle$$

$$|d_{m}^{10}\rangle = \sum_{p} \frac{\phi_{p}(0)}{E - E_{m} - E_{p}} |p \uparrow\rangle |p \downarrow\rangle$$

$$|d_{m}^{01}\rangle = \sum_{p} \frac{\phi_{p}(0)}{E - E_{m} - E_{p}} |p \downarrow\rangle |p \uparrow\rangle$$

Denoting $\tilde{F}^{i} = (\tilde{F}_{i}^{1}, \tilde{F}_{i}^{2}, ...)^{T}$, finally we arrive at the following matrix equation from (14):

$$\begin{pmatrix}
\frac{1}{2} (\epsilon - 2q) & \frac{3}{2} e \\
\frac{1}{2} e & -\frac{1}{2} (\epsilon - 2q) & \frac{3}{2} e \\
\frac{1}{2} e & \frac{3}{2} e & -\frac{1}{2} (\epsilon - 2q)
\end{pmatrix}
\begin{pmatrix}
\tilde{F}^{1} \\
\tilde{F}^{2} \\
\tilde{F}^{3}
\end{pmatrix} = \frac{1}{J}
\begin{pmatrix}
\tilde{F}^{1} \\
\tilde{F}^{2} \\
\tilde{F}^{3}
\end{pmatrix} \tag{18}$$

where $e$ and $q$ are all matrices with elements $e_{mn} = \phi_{m}(0)\phi_{n}(0)$ and $q_{mn} = \delta_{mn} \sum_{p} \phi_{p}(0)^{2}$. The $q$-matrix is due to the interaction between one fermion and the impurity (forming a dimer), while $e$-matrix is due to interaction between the dimer and the other fermion. In practical simulation, we find convergent results can be reached with cutoff $N_{e} = 100$ for the element indices of $e$- and $q$-matrixes. Accordingly, (18) is a $3N_{e} \times 3N_{e}$ matrix.

### III. RESULTS

In this section, we present the results of two-body and three-body problems based on the formalism shown in previous section. Given the even parity of interaction potential ($x \leftrightarrow -x$), we only present the few-body results associated with even-parity wave functions but neglect the odd-parity ones which are not affected by the interaction.

#### A. Two-body

In Fig.1, we show the energy spectra for both spin-triplet ($E_{t}$) and spin-singlet ($E_{s}$) states, obtained by solving, respectively, (9) and (11).

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**FIG. 1.** (Color online). Energy spectrum of one fermion and one impurity in $S_{tot,z} = 0$ subspace. The blue dashed (red dotted) lines show $E_{t}$ ($E_{s}$) for spin-triplet (singlet) eigenstates. The black solid line shows the asymptotic fitting to (19) in strong coupling limit. Here the units of $E$ and $J$ are respectively $\omega$ and $\sqrt{\omega/m}$. For the spin-singlet (AFM) case, as the effective coupling is given by $\gamma_{s} = -3J/2$, therefore the bound states will be supported at $J > 0$. As shown in Fig.1, as increasing $J$ from zero to $\infty$, the singlet dimer becomes deeper
and deeper, and the energy approaches \( E_s \to -9J^2/8 \) in large \( J \) limit. This is the so-called lower attractive branches. Meanwhile, we also see another sequence of eigenstates with energies approaching finite values when \( J \to \infty \). These branches are well above the attractive branch in the spectrum, therefore called the repulsive upper branches. For these types of branches, one can carry out an effective perturbation theory in terms of small value 1/\( J \to 0 \). As shown in Appendix A, the \( n \)-th upper branch energy approaches

\[
E_{s,n} \simeq (2n + 1)\omega - \frac{\phi_{2n+1}(0)^2}{m^2\gamma_s},
\]

(19)

here \( \phi'_n = d\phi_n(x)/dx \) is the first derivative of single-particle state \( \phi_n \). Accordingly, the zero-th order wave function is [18]:

\[
|\Psi\rangle_{s,n} = \phi_{2n+1}(x)\text{sgn}(x)|\uparrow\downarrow - \downarrow\uparrow\rangle,
\]

(20)

with the sign function \( \text{sgn}(x) = 1 \) (−1) for \( x > 0 \) (<0).

For the spin-triplet (FM) state, the analysis is similar, except now the effective coupling is \( \gamma_t = J/2 \). Therefore the spin-triplet bound state is supported at \( J < 0 \) side, with the binding energy approaches \( E_t \to -J^2/8 \) in large \( |J| \) limit. The asymptotic behavior of upper branches follows the form of (19) by replacing \( E_t, \gamma_s \) with \( E_t, \gamma_t \). The according zero-th order wave function follows the spin-charge separation form of (20) with the spin part replaced by \( |\uparrow\downarrow + \downarrow\uparrow\rangle \).

One thus can summarize that for the two-body problem, once considering the effective coupling for each spin channel, the resulted spectrum is quite similar to the case of a pure contact potential, as solved originally by T. Busch et al. However, for the three-body problem, we will show below that the resulted spectrum is very rich due to the spin-exchange interaction, which is very different from the case of a pure contact potential.

B. Three-body

In Fig.2, we show the energy spectrum of three-body system in the \( S_{tot,z} = 1/2 \) subspace. In particular, we mark the FM state (\( S_{tot} = 3/2 \)) with red color, and the rest are all with \( S_{tot} = 1/2 \).

Compared to the three-body system with a contact interaction, we can see from Fig.2 that the current system with spin-exchange interaction displays very rich spectrum. Here we would like to highlight three properties that are uniquely associated with the spin-exchange interaction.

First, many branches of bound states appear in both \( J > 0 \) and \( J < 0 \) sides (see 2(a)), which are respectively associated with the AFM and FM bound states. For large and positive \( J \), the energies of three-body bound states are dominated by the AFM dimer (composed by the impurity and one fermion, with energy \( \sim -9J^2/8 \)), and the residue interaction between the dimer and the other fermion only contributes constant energies (e.g., \( 1.5\omega, 3.5\omega \ldots, \) see Fig.2(b1,c1)), which are much smaller than the dimer binding energy. Therefore, the impurity appears to be nearly screened through the formation of AFM dimer with the first fermion, which cannot further attract the other fermion. This resembles the Kondo screening effect in metals, where the magnetic spin of the localized impurity is screened by forming a spin singlet with conduction electrons [19]. On the contrary, the lowest bound state in \( J < 0 \) side is not simply dominated by a single FM dimer; rather, the impurity can attract both fermions to produce a deep trimer with binding energy \( E_3 \approx -1.395J^2 (< E_t = -J^2/8), \) see Fig.2(h2)). This means that the impurity cannot be screened by forming a FM dimer with a fermion, opposite to the AFM coupling case. This is because the FM dimer is magnetic, and the other fermion can still interact with this dimer to form an

![Fig. 2](image)

(a) Energy spectrum of two fermions and one impurity in \( S_{tot,z} = 0 \) subspace. The FM states with \( S_{tot} = 3/2 \) are highlighted by red color, and the rest are all with total spin \( S_{tot} = 1/2 \). (b1) Energies of deep bound states for large and positive \( J \), shifted by the AFM dimer energy \( -9J^2/8 \). All shifted energies saturate to a finite value, signifying the Kondo screening effect (see text). (b2) Energies of deep bound states for large and negative \( J \), shifted by the FM dimer energy \( -J^2/8 \). The lowest bound state does not saturate as in (b1), showing the absence of screening effect for FM coupling. (c1,2) show zoomed shaded region in (b1,2) illustrating the asymptotic behavior towards odd harmonic levels. The units of \( E \) and \( J \) are respectively \( \omega \) and \( \sqrt{\omega/m} \).
even deeply bound trimer as ground state. The situation is different for the higher excited branches. As shown in Fig.2(c2), the energies of these excited branches are still dominated by the FM dimer energy.

Second, a sequence of full FM states (with spin $S_{\text{tot}} = 3/2$) can be found in upper branches of the AFM coupling ($J > 0$) side, as marked by red color in the spectrum in Fig.2(a). Since the attractive branches in $J > 0$ side are all associated with a spin-singlet dimer, thus have total spin $S_{\text{tot}} = 1/2$, they are all orthogonal to the FM branches. Therefore, once an initial state is prepared in the FM branch, it will always stay on this branch due to zero-coupling with other branches. Another interesting feature of these FM branches is that their wave functions all feature a full spin-charge separation. This is because in a full FM state, any two particles will form a triplet pair. Therefore, the interaction potential can be simplified as $U_{\text{i}}(x_i) = \gamma \psi(x_i)$, which is only relevant to the charge part. As a result, one can construct the FM wave function of three-body system as:

$$\Psi_{3,FM}(x_1, x_2) = \left| \psi_1(x_1) \right| \psi_1(x_2) \left| \psi_2(x_2) \right| (| \uparrow \downarrow \uparrow \rangle + | \downarrow \uparrow \uparrow \rangle + | \uparrow \uparrow \downarrow \rangle) \left(21\right)$$

where $\psi_{1,2}$ is any of the triplet eigenstates for two-body system (one fermion plus the impurity), and the spin part is a full FM state. One can see clearly this wave function is an eigen-state of the Hamiltonian of three-body system, with eigen-energy $E = E_1 + E_2$ ($E_{1,2}$ is the eigen-energy of $\psi_{1,2}$ for two-body system). Note that these FM branches should be distinguished from those in the pure contact interaction case[20], where the FM states do not feel any s-wave interaction and the energy are always static as changing coupling strength. The asymptotic expansion of the energies of FM states and the other branches will be presented in Appendix A 2.

Third, in the weak coupling limit $J \to 0^\pm$, we see that the ground state energy of the three-body system exhibits a quadratic scaling as $E(J) \sim -cJ^2$, instead of a linear one in the case of contact potential. This is because in the non-interaction limit, the two fermions form a spin singlet with the same orbital wave function (at the lowest harmonic oscillator level). It then follows that the expectation value of the spin-exchange interaction in this state is zero. This means that there is no mean-field contribution to the interaction energy, and the lowest level of energy correction comes from the second-order process (leading to $E \propto J^3$), which involves excitations to higher orbitals (or higher harmonic oscillator levels). Note that this is different from the two-body case, where there is only one fermion and the mean-field contribution does exist and give the energy linearly depending on $J$ in weak coupling limit.

We would like to remark here that the three features discussed above, including the Kondo screening effect, the FM upper branches, and the quadratic energy scaling, are all closely related to the spin-exchange nature of the interaction, which cannot exist in the system with pure contact interaction. These features can be generalized to many-fermion system as discussed below.

### C. Extension to many-body

The two- and three-body solutions have provided us an important insight to the properties of many-body system, where many spin-1/2 fermions (with number $N$) interact with a localized impurity with spin-exchange coupling $J$. These properties include:

First, the Kondo screening effect is expected to be applicable to the bound states in the AFM coupling ($J > 0$) side, which tells that the impurity is essentially screened by forming a singlet dimer with one fermion (at the Fermi surface). Indeed, we note in literature, a simple variational ansatz, which assumed an AFM dimer and an perturbed Fermi sea, was employed to estimate the Kondo temperature in metals[19]. On the other hand, our three-body calculation also suggests a finite residue interaction energy between the rest fermions and the dimer, so they are not completely independent. How this residue interaction affects the Fermi sea atoms and the Kondo physics surely needs further investigation, which are beyond the scope of this work.

Second, a sequence of FM upper branches with total spin $S_{\text{tot}} = (N + 1)/2$ should exist in the AFM coupling ($J > 0$) side, which are orthogonal to all other branches in this regime. The wave functions of FM states feature a full spin-charge separation:

$$\Psi_{N+1,FM}(x_1, x_2, ... x_N) = \left| \psi_1(x_1) \right| \psi_1(x_2) \left| \psi_2(x_2) \right| (| FM \rangle) \left(22\right)$$

where $\psi_i$ is a triplet eigenstate for two-body system with eigen-energy $E_i$, and $\{FM\}$ is the FM spin state with $S_{\text{tot}} = (N + 1)/2$ and a specific $S_z$. The total energy of $\Psi_{N+1,FM}$ is $E = \sum_{i=1}^{N} E_i$.

Third, the coupling dependence of ground state energy in the weak coupling limit $J \to 0^\pm$ will depend on whether the fermion number $N$ is even or odd. When $N$ is even, then in non-interacting limit the fermions are composed of $N/2$ pairs of spin singlet, and there is no mean-field contribution because the expectation value of the spin-exchange interaction in this state is zero. In this case, $E$ scales quadratically as $E(J) \sim J^2$. When $N$ is odd, then the single fermion at the Fermi surface will contribute to the mean-field energy as $E(J) \sim J$. However, in the thermodynamic limit ($N \to \infty$), the energy per particle $E/N$ will be dominated by quadratic term $\sim J^2$ in $J \to 0$ regime regardless of even or odd $N$, because the coefficient of linear dependence (for odd $N$) approaches zero when divided by $N$. This is different from the pure contact interaction case, where the energy per particle is always dominated by the mean-field contribution ($\sim J$) in weak coupling regime.
IV. EFFECT OF AN ADDITIONAL CONTACT INTERACTION

In this section, we discuss the effect of an additional contact interaction between fermion and the impurity, $U(x) = U \delta(x)$. The full Hamiltonian then reads

$$\hat{H} = \sum_{m\sigma} E_m C^\dagger_{m\sigma} C_{m\sigma} + \sum_{m,n} V_{mn} (C^\dagger_{m\uparrow} C_{n\downarrow}) S^z + h.c.$$ 

$$+ (C^\dagger_{m\uparrow} C_{n\uparrow} - C^\dagger_{m\downarrow} C_{n\downarrow}) S_z) + U_{mn} (C^\dagger_{m\uparrow} C_{n\uparrow} + C^\dagger_{m\downarrow} C_{n\downarrow})$$

with $U_{mn} = U \phi_m(0) \phi_n(0)$. (23)

Therefore, the AFM bound states are supported at $J > 2U/3 \ (\gamma_s < 0)$, and the FM bound states are supported at $J < -2U \ (\gamma_t < 0)$.

The three-body bound states also have similar properties, in that the presence of contact $U$ will change the parameter regime to support AFM or FM bound states. The formalism of solving three-body problem based on the Hamiltonian (23) is given in Appendix B. In Fig.3 we show the spectrum for three typical values of $U/J$. One can see that as changing $U/J$ across $-0.5$, the original bound states in $J < 0$ regime gradually vanish since the effective FM coupling strength $\gamma_t$ changes from negative to positive. Similarly, we expect the vanishing of AFM bound states (originally in $J > 0$ regime) will occur when increasing the contact interaction to $U > 3J/2$. Our results may be probed in quasi-1D alkali-earth atoms, where the ratio $U/J$ can be conveniently tuned from negative to positive across resonance by using the confinement-induced resonance[8].

V. CONCLUSION

In this work, we have exactly solved few-body problem of one and two fermions in a 1D harmonic trap interacting with a local impurity for an arbitrary spin-exchange coupling strength $J$. It is found that the spin-exchange interaction can lead to a number of unique phenomena that cannot be achieved by pure contact interaction. These phenomena include the Kondo screening effect, the full FM upper branches in the AFM coupling regime, and the quadratic energy scaling in the weak coupling regime. These unique properties can be extended to many-body system with spin-exchange interaction. Moreover, we also discuss the effect of an additional contact interaction, which effectively changes the parameter regime to support bound states with different magnetic structures. These unique features of spin-exchange interaction may be explored in future experiments of ultracold alkaline-earth atoms.

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Appendix A: Asymptotic energy expansion in strong coupling limit

1. Two-body

In the strong coupling regime, the energies of upper-branch two-body states take the form of:

\[ E_m \simeq (2m + 1)\omega - \frac{A_m}{\gamma} \]  \hspace{1cm} (A1)

where \( m \) is the level index, \( \gamma \) is the effective coupling in the spin-singlet or triplet channel, and coefficient \( A_m \) can be calculated as:

\[
A_m = \lim_{\gamma \to \infty} \frac{\partial E(\gamma)}{\partial \frac{1}{\gamma}} \\
= \lim_{\gamma \to \infty} \int dx \gamma \psi_\gamma(x) \delta(x) \gamma \psi_\gamma(x)  \hspace{1cm} (A2)
\]

By using the boundary condition \( \gamma \psi_\gamma(0) = \frac{\psi_\gamma(0)}{m} \), we can arrive at the expansion form of Eq.(19) in the main text.

2. Three-body

We take the eigen-states saturating at \( E = 5\omega \) for example. In Fig 2, we see that there are three upper branches saturating at \( E = 5\omega \) as \( |J| \to \infty \). It can be shown that these upper branches can be divided into two classes. The first class of upper branch has coupling with the attractive lower branches, and therefore there will be an avoided level crossing when they meet in the spectrum. The second class of upper branch is orthogonal to all attractive lower branches, which leads to a direct level crossing when they meet.

From the knowledge of two-body spectrum, the lowest two-body eigen-energies for the upper branches are \( E = 1.5, 3.5\omega \) in the strong coupling regime \( |J| = \infty \). When adding one more fermion, the strong fermion-impurity interaction requires the boundary condition:

\[
\psi(x_1\sigma_1, x_2\sigma_2) = 0 \quad \text{if} \quad x_i = 0 \hspace{1cm} (A3)
\]

Combining with fermion exchange anti-symmetry, we construct the following wave functions for three degenerate eigen-states:

\[
|\psi^1_{\text{deg}}\rangle = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_3(x_2) - \psi_3(x_1)\psi_1(x_2)) |\uparrow\uparrow\downarrow\rangle
\]

\[
|\psi^2_{\text{deg}}\rangle = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_3(x_2) |\uparrow\downarrow\uparrow\rangle) - \frac{1}{\sqrt{2}}(\psi_3(x_1)\psi_1(x_2) |\uparrow\downarrow\uparrow\rangle)
\]

\[
|\psi^3_{\text{deg}}\rangle = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_3(x_2) |\uparrow\uparrow\downarrow\rangle) - \frac{1}{\sqrt{2}}(\psi_3(x_1)\psi_1(x_2) |\uparrow\uparrow\downarrow\rangle)
\]

(A4)

with \( \psi_n(x) = \phi_n(x) \cdot \text{sign}(x) \), where \( \phi_n(x) \) is nth-eigenfunction of harmonic trap.

For large but finite coupling \( (1/J \neq 0) \), the above degeneracy will be lifted and the three energy levels split as:

\[
E_m(J) = E_0 - \frac{\kappa_m}{J} \quad \text{with} \quad m = 1, 2, 3  \hspace{1cm} (A5)
\]

Accordingly, the zero-th order eigenstates can be a linear combination of \( |\psi^m_{\text{deg}}\rangle \) as:

\[
|\psi^m_{\text{J}}\rangle = \sum_n a_{mn} |\psi^m_{\text{deg}}\rangle,  \hspace{1cm} (A6)
\]

which can be reorganized as

\[
|\psi^m_{\text{J}}\rangle = |\psi^m_{J_1}|\uparrow\uparrow\downarrow\rangle + |\psi^m_{J_2}|\uparrow\downarrow\uparrow\rangle + |\psi^m_{J_3}|\uparrow\uparrow\downarrow\rangle \equiv (|\psi^m_{J_1}\rangle, |\psi^m_{J_2}\rangle, |\psi^m_{J_3}\rangle)  \hspace{1cm} (A7)
\]

Eqs.(A6,A7) determine the relation between \( \{ |\psi^m_{J_n}\rangle \} \) and \( \{ a_{mn} \} \).

From the definition in Eq.(A5), we have

\[
\kappa_m \delta_{mn} = \lim_{J \to \infty} \langle \psi^m_J | \frac{\partial \hat{H}}{\partial \frac{1}{J}} | \psi^m_J \rangle  \\
= \lim_{J \to \infty} \langle \psi^m_J | 2J^2(\delta(x_1)\hat{S}_1 \cdot \hat{S}_0 + \delta(x_2)\hat{S}_2 \cdot \hat{S}_0) | \psi^m_J \rangle  \\
= \lim_{J \to \infty} \int dx_1 \Psi^m_J(x_1,0) 2J^2 \hat{S}_1 \cdot \hat{S}_0 \Psi^m_J(x_1,0)  \\
+ \int dx_2 \Psi^m_J(x_1,0) 2J^2 \hat{S}_2 \cdot \hat{S}_0 \Psi^m_J(x_1,0)  \hspace{1cm} (A8)
\]

Given the Schrodinger equation \( \hat{H} |\psi^m_J\rangle = E_m(J) |\psi^m_J\rangle \), we can integrate over \( x_1, x_2 \) separately and get the boundary conditions as:

\[
\frac{\hbar^2}{2m} \frac{\partial}{\partial x_1} \Psi^m_J(x_1, x_2)|_{x_1=0}^{x_1=0^+} = 2J\hat{S}_1 \cdot \hat{S}_0 \Psi^m_J(0, x_2)  \hspace{1cm} (A9)
\]

\[
\frac{\hbar^2}{2m} \frac{\partial}{\partial x_2} \Psi^m_J(x_1, x_2)|_{x_2=0}^{x_2=0^+} = 2J\hat{S}_2 \cdot \hat{S}_0 \Psi^m_J(x_1, 0)
\]

Use above boundary conditions we can simplify (A8) as:
\[
\kappa_m \delta_{mn} = \left( \frac{\hbar^2}{2m_t} \right)^2 \int dx_2 \partial_x \Psi_{m_1}^* (x_1, x_2) \big| x_1 = 0^+ \frac{1}{2S_1} \left( \Psi_{m_1}^* (x_1, x_2) \big| x_1 = 0^+ \right) + \left( \frac{\hbar^2}{2m_t} \right)^2 \int dx_1 \partial_x \Psi_{m_2}^* (x_1, x_2) \big| x_2 = 0^+ \frac{1}{2S_1} \left( \Psi_{m_2}^* (x_1, x_2) \big| x_2 = 0^+ \right)
\]

with the same definition of \( \tilde{\phi} = \frac{1}{\sqrt{2}} \phi_1(0) \psi_3(x) \), and in the last step we have used \( \int dx A^2 = \frac{1}{\sqrt{\pi}} \), \( \int dx B^2 = \frac{3}{\sqrt{\pi}} \) and \( \int dx AB = 0 \).

Finally we diagonalize the matrix and obtain the eigen vector of \( a_{mn} \) (without normalization temporarily):

\[
\begin{pmatrix}
1 \\
1 \\
(1/2 \ (\sqrt{7} - 3)) \\
1/2 \ (1 - \sqrt{7}) \\
1/2 \ (\sqrt{7} + 1)
\end{pmatrix}
\]

(A11)

Note that the first state is the full FM state. The corresponding coefficients for the three states are:

\[
\kappa_m = \frac{10}{\sqrt{\pi}} \cdot \frac{2}{3\sqrt{\pi}} \left( 2\sqrt{7} + 5 \right) \cdot \frac{2}{3\sqrt{\pi}} \left( 5 - 2\sqrt{7} \right)
\]

(A12)

We have checked that the coefficients are consistent with our numerical fitting of the spectrum in the strong coupling regime.

**Appendix B: Formulism of three-body problem with an additional contract interaction**

After adding the contact interaction term \( U \delta(x) \), Eq.(14) in the main text then changes to:

\[
\phi^1_{mn} = \frac{1}{E - E_m - E_n} \cdot \frac{1}{2} \sum_p -V_{mp} \phi^2_{np} + V_{np} \phi^2_{mp} + V_{mp} \phi^1_{pm} - V_{mp} \phi^1_{pm} + 2U_{mp} \phi^1_{pm} - 2U_{mp} \phi^1_{pm}
\]

\[
\phi^2_{mn} = \frac{1}{E - E_m - E_n} \sum_p V_{mp} \phi^2_{mp} - V_{np} \phi^2_{pm} + \frac{1}{2} V_{mp} \phi^2_{pm} - \frac{1}{2} V_{np} \phi^2_{pm} + U_{mp} \phi^2_{pm} + U_{np} \phi^2_{mp}
\]

(B1)

With the same definition of \( F^i \) in the main text, we obtain the following matrix equation:

\[
\begin{pmatrix}
\frac{1}{4}(e - 2q)(3 - 2U) \\
\frac{1}{2}e(1 + 2U) \\
\frac{1}{2}e(3 - 2U) - \frac{1}{2}q(1 + 2U)
\end{pmatrix}
\begin{pmatrix}
\frac{1}{4}(-3)e(1 + 2U) \\
\frac{1}{2}e(1 + 2U) \\
\frac{1}{2}q(1 + 2U)
\end{pmatrix} = \frac{1}{J} \begin{pmatrix}
\hat{F}^1 \\
\hat{F}^2 \\
\hat{F}^3
\end{pmatrix}
\]

(B2)

with \( U_{mn} = U \phi_m \phi_n \), which can be diagonalized to obtain the spectrum for various ratios \( \frac{U}{J} \).

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