Orbital Feshbach Resonance in Alkali-Earth Atoms

Ren Zhang,1 Yanting Cheng,1 Hui Zhai,1 and Peng Zhang2,3,*

1Institute for Advanced Study, Tsinghua University, Beijing, 100084, China
2Department of Physics, Renmin University of China, Beijing, 100872, China
3Beijing Key Laboratory of Opto-electronic Functional Materials & Micro-nano Devices, 100872 (Renmin University of China)
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For a mixture of alkali-earth atomic gas in the long-lived excited state $^3P_0$ and ground state $^1S_0$, in addition to nuclear spin, another “orbital” index is introduced to distinguish these two internal states. In this letter we propose a mechanism to induce Feshbach resonance between two atoms with different orbital and nuclear spin quantum numbers. Two essential ingredients are inter-orbital spin-exchanging scattering and orbital dependence of the Landé g-factors. Here the orbital degrees of freedom plays similar role as electron spin degree of freedom in magnetic Feshbach resonance in alkali-metal atoms. This resonance is particularly accessible for $^{173}$Yb system. The BCS-BEC crossover in this system requires two fermion pairing order parameters, and displays significant difference comparing to that in alkali-metal system.

Magnetic Feshbach resonance (MFR) is a powerful tool to tune interaction between atoms to strongly interacting regime, and plays a crucial role in cold atom physics [1]. For instance, for alkali atoms, each atom has an electronic spin $S = 1/2$. The interaction between two atoms have different potentials depending on whether the total electronic spin is singlet or triplet. Thus, one can utilize the Zeeman energy to control their relative energy and to reach a scattering resonance. However, alkali-earth atom (like Sr) or alkali-earth-like atom (like Yb) has fully occupied outer shell, and their total spin is zero. Thus, it is conventional wisdom that there is no MFR in alkali-earth atoms at ground state. Instead, one can tune interaction by optical Feshbach resonance [2], but such a scheme suffers from strong atomic loss and heating.

Another significant feature of alkali-earth atom is the existence of a long-lived excited state $^3P_0$, in which one electron is excited to $p$-orbital and the total electronic spin $S = 1$. The dipole transition to ground state $^1S_0$ is “spin-forbidden” and therefore its lifetime can be as long as a few seconds, which is used for atomic clock transition. Considering an atomic gas mixture of $^3P_0$ (denoted by $|e\rangle$) and $^1S_0$ (denoted by $|g\rangle$) states, in addition to nuclear spin degree of freedom, one introduces another so-called “orbital” degree of freedom to label the internal state of atoms [3,4]. Previously attentions have been paid to MFR between $^3P_2$ state and $^1S_0$ state due to anisotropic interactions, but these resonances are generally quite narrow [5]. Moreover, since $J = 0$ for $^3P_0$, even such a MFR is not found between $^3P_0$ and $^1S_0$.

In this letter we propose an alternative mechanism that can lead to Feshbach resonance (FR) between atoms in $|e\rangle$ and $|g\rangle$. Though this FR is also controlled by magnetic field, the mechanism of how it works is quite different from MFR in alkali atoms. Two essential ingredients are inter-orbital (nuclear-)spin-exchanging interactions, which has been observed in recent experiments [3,4,5], and the small difference in the nuclear Landé g-factor $\delta g$ between different orbital states ($|e\rangle$ and $|g\rangle$) [6]. We there-

![FIG. 1: (a) Original energy level diagram. $\Delta E$ denotes the excitation energy between $|e\rangle$ and $|g\rangle$. $\delta_e = B_{eg} \mu_B$ and $\delta_g = B_{egr} \mu_B$ are Zeeman energies of $|g\rangle$ and $|e\rangle$ states, respectively. Two states in open channel are occupied. Arrows indicate an inter-orbital (nuclear-) spin exchanging scattering process, which couples open channel $|g\downarrow; e\uparrow\rangle$ and closed channel $|g\uparrow; e\downarrow\rangle$. $\delta = \delta_e - \delta_g = B(\delta g) \mu_B$ is the Zeeman energy difference between two channels and $\delta g = g_e - g_g$ is the difference in Landé g-factor. (b) Reorganized energy level diagram for many-body Hamiltonian, in which open channel states appear in lower energy.](cond-mat.quant-gas)
of freedom forms a singlet or triplet. For s-wave scattering we introduce two anti-symmetrized bases
\[ |\pm\rangle = \frac{1}{2} (|e\rangle \pm |g\rangle)(|\uparrow\rangle \mp |\downarrow\rangle) = \frac{1}{\sqrt{2}}(|c\rangle \mp |o\rangle), \]
the Huang-Yang pseudo-potential is diagonal in this bases with two different scattering lengths \( a_s^+ \) and \( a_s^- \),
\[ \hat{V} = \left( \frac{4\pi\hbar^2}{m} \sum_{i=\pm} a_i \delta(|i\rangle \langle i|) \right) \delta(r) \frac{\partial}{\partial r} (r). \]

One can write the interaction potential \( \hat{V} \) in the \(|o\rangle\) and \(|c\rangle\) bases, which becomes
\[ \hat{V} = \hat{V}_0 \left(|o\rangle \langle o| + |c\rangle \langle c|\right) + \hat{V}_1 \left(|o\rangle \langle o| + |c\rangle \langle c|\right), \]
where \( V_j = \frac{4\pi\hbar^2}{m} a_{s0} \delta(r) \frac{\partial}{\partial r} (r) \), and \( a_{s0} \) denotes \((a_s^+ + a_s^-)/2\), and \( a_{s1} \) denotes \((a_s^- - a_s^+)/2\). The \( \hat{V}_1 \) term describes an inter-orbital spin exchanging process, as illustrated in Fig. 1, which couples the open and closed channels. \( a_{s0} \) can be viewed as the background scattering length of both open and closed channels. Since \( a_{s0} \) is positive, it supports a bound state with energy \( \varepsilon_b = -\hbar^2/(ma_{s0}^2) \). Therefore, when \( \delta \sim \varepsilon_b \), one will expect a scattering resonance in the open channel.

The two-body wave function can be generally written as
\[ \psi = [e^{ikr + f_o(k) \frac{e^{ikr}}{r}} |o\rangle + f_c(k) e^{-\sqrt{m\delta/\hbar^2 - k^2} r} |c\rangle]. \]
Solving the Schrödinger equation \( (\hat{H}_0 + \hat{V})\psi = E\psi \) with \( E = \hbar^2 k^2/m \), one can find
\[ (1 + i a_{s0}) f_o(k) - a_{s1} \sqrt{\frac{m\delta}{\hbar^2} - k^2} f_c(k) + a_{s0} = 0; \]
\[ i a_{s1} f_o(k) + \left( 1 - a_{s0} \sqrt{\frac{m\delta}{\hbar^2} - k^2} \right) f_c(k) + a_{s1} = 0. \]

Straightforward calculation yields the scattered length \( a_s \) in the open channel as
\[ a_s = -f_o(k = 0) = \frac{-a_{s0} + \sqrt{m\delta/\hbar^2 (a_{s0}^2 - a_{s1})}}{a_{s0} \sqrt{m\delta/\hbar^2 - 1}}. \]

Two-body Problem with Finite Range Potential. Furthermore, we can consider a coupled two-channel model with finite range \( r_0 \). When \( r > r_0 \), two atoms are non-interacting, and the zero-energy s-wave wave function \( \psi = u(r)/r \) with
\[ u(r) = \alpha \exp\left(-\sqrt{\frac{m\delta}{\hbar^2}} |c\rangle + \beta (r - a_s)|o\rangle \right). \]

For \( r < r_0 \), the Hamiltonian is written as
\[ \hat{H} = \sum_{i=\pm} \left( -\frac{\hbar^2}{m} \nabla^2 + V^i(r) \right) |i\rangle \langle i|, \]
where we have assumed that \( \delta \) is much smaller than energy scale of van der Waal potential \( V^i(r) \) such that it can be safely ignored in this regime. Each \( V^i(r) \) \((i = +, -)\) corresponds to an s-wave scattering length \( a_s^i \), that is, to say, the wave function \( \psi = u^i(r)/r \) in \( r < r_0 \) regime satisfies the boundary condition \( u^i(r)/u^i(r)|_{r=r_0} = 1/(r_0 - a_s^i) \). In \( r < r_0 \) regime the wave function can be written in a general form
\[ u(r) = u^+(r)|+\rangle + A u^-(r)|-\rangle \]
\[ = \frac{u^+(r) + A u^-(r)}{\sqrt{2}} |c\rangle + \frac{u^+(-r) + A u^-(r)}{\sqrt{2}} |o\rangle. \]

By matching boundary conditions between wave functions Eq. 9 and Eq. 11 at \( r = r_0 \) for \(|o\rangle\) and \(|c\rangle\) channels independently, and utilizing the boundary condition for each \( u^i \), one can obtain \( A \) and \( a_s \), where
\[ a_{s} = \frac{-a_{s0} + \sqrt{m\delta/\hbar^2 (a_{s0}^2 - a_{s1}^2) - r_0 a_{s0}}}{\sqrt{m\delta/\hbar^2 (a_{s0} - r_0) - 1}}. \]

In the limit \( r_0 \rightarrow 0 \), Eq. 12 recovers the result of Eq. 8. Thus we have demonstrated, from both pseudo-potential and finite-range model, that \( a_{s0} \) of open channel can be strongly modified by \( \delta \). Eq. 8 and Eq. 12 also show that the difference between \( a_s^- \) and \( a_s^+ \), i.e. \( a_{s1} \neq 0 \), is crucial, as \( a_s \) becomes a constant as \( a_{s1} = 0 \) in Eq. 8 and Eq. 12.

Orbital Feshbach Resonance. Eq. 12 shows that \( a_{s0} \) diverges when
\[ \delta = \delta_{as} = \frac{\hbar^2}{m(a_{s0} - r_0)} \]

FIG. 2: Scattering length \( a_s \) between \(|e\rangle\) and \(|g\rangle\) as a function of magnetic field for \(^{173}\text{Yb} \) atom. Blue dashed line and red dash-dotted line is the real and imaginary part of \( a_{s0} \) obtained from the zero-range pseudo-potential. Solid line and red dotted line are \( a_{s1} \) obtained from the finite range potential. Here we take \((\delta g)_{13} = 2\pi \hbar \times 112\text{Hz}/G, a_{s1}^2 = 219.5a_0, a_{s1} = 3300a_0 + 0.78a_0 \) [4, 5] and \( r_0 \) is taken as van der Waal length, which equals to \( 84.8a_0 \) [8], with \( a_0 \) the Bohr’s radius.
much high magnetic field ($10^3 - 10^4$G for $^{87}$Sr) to reach this resonance.

Here we would like to contrast the OFR in alkali-earth atom with MFR in alkali-metal atom. In MFR, two atoms stay in hyperfine eigenstate when they are far separated; while in OFR two atoms are in $|g\downarrow;e\uparrow\rangle$ or $|g\uparrow;e\downarrow\rangle$ states. When two atoms interact at short distance, for MFR, the interaction potential are different for total electronic spin singlet and triplet, while for OFR, the interaction potentials are distinguished by orbital singlet or triplet. Finally in MFR, due to hyperfine interaction, electronic singlet and triplet states are not hyperfine eigenstate, and therefore, two channels are coupled. While in OFR, orbital dependent Landé g-factor can be viewed as coupling between orbital and nuclear spin, because of which orbital singlet and triplet are also not eigenstate at large distance, and consequently, two channels are coupled. In this analogy, orbital degree of freedom in OFR plays the same role as electronic spin degree of freedom in MFR.

**Two Order-Parameters BCS-BEC Crossover.** Since $(\delta g)\mu_B$ is five orders of magnitude smaller than the $g_e\mu_B$, comparing OFR at $\sim 60$G with a MFR in about the same magnetic field regime, the energy separation between open and closed channel is much larger in the MFR case than that in the OFR case. In a MFR case, this energy separation is a few orders of magnitude larger than the Fermi energy. Therefore, in a BCS-BEC crossover theory studied before in alkali-metal atoms [9], one can either start with a single-channel model only, or with a two-channel model but only including the bound state of one channel are never important.

However, the situation in the OFR case is dramatically different. Considering a typical density of Fermi gas, one can estimate that $\delta$ is comparable or can be even smaller than the Fermi energy. Thus, we have to take into account scattering states in both open and closed channels. This requires introducing two self-consistent paring order parameters for open and closed channels, respectively. Below we shall present such a formalism for crossover across an OFR.

We consider the situation that in the non-interacting limit, total $N$ fermions are equally populated in the two states in the open channel ($|e\uparrow\rangle$ and $|g\downarrow\rangle$). We note that both $N_e = N_{e\uparrow} + N_{e\downarrow}$ and $N_t = N_{g\uparrow} + N_{g\downarrow}$ are good quantum numbers. Subtracting the Hamiltonian with a constant term $(\Delta E/2)N_e - (\delta_e + \delta_g)N_t/2$, one can show the level diagram can be reorganized as shown in Fig. 3(b), such that the two states in the open channel appear in the lower energy, with an energy separation of $\delta/2$ below the two states in the closed channel. Then in the non-interacting limit (say, $\delta = \delta_0$), $\delta/2$ is larger than the Fermi energy so that only open channel is equally populated. The many-body Hamiltonian can be written

\[
\delta = \delta_0 = \frac{\hbar^2}{m(a_{s0} - r_0 - a_{s1}/a_{s0})^2}.
\]
as
\[
\hat{H} = \hat{H}_{\text{ho}} + \hat{H}_{\text{fc}} + \frac{g_a}{2} \hat{A}_+ \hat{A}^\dagger + \frac{g_o}{2} \hat{A}_- \hat{A}^\dagger ,
\]
where \( \varepsilon_k = \hbar^2 k^2/(2m) - \mu \), and
\[
\hat{A}_+ = \sum_k (c_{g\uparrow \bar{k}} c_{g\downarrow k} - c_{g\downarrow \bar{k}} c_{g\uparrow k}) ,
\]
\[
\hat{A}_- = \sum_k (c_{g\uparrow \bar{k}} c_{g\downarrow k} + c_{g\downarrow \bar{k}} c_{g\uparrow k}) .
\]

Now we defined two order parameters as \( \Delta_+ = g_o \langle \hat{A} \rangle/2 \) and \( \Delta_- = g_a \langle \hat{A} \rangle/2 \), and we can perform mean-field decoupling of the interaction term which leads to
\[
\hat{H}_{\text{MF}} = \hat{H}_{\text{ho}} + \hat{H}_{\text{fc}} + (\Delta_+ \hat{A}_+ + \text{h.c.}) + (\Delta_- \hat{A}_- + \text{h.c.}) - \frac{2|\Delta_+|^2}{g_o} - \frac{2|\Delta_-|^2}{g_a} .
\]

Following the standard BCS theory to diagonalized \( \hat{H}_{\text{MF}} \) with the Bogoliubov transformation and minimizing the ground state energy with respect to both \( \Delta_+ \) and \( \Delta_- \), we reach two coupled gap equations
\[
\left[ \frac{\Delta_+}{4 \hbar^2 a_o^2} - 1 + \frac{\Delta_+}{\frac{4 \hbar^2 a_o^2}{m}} \right] \sum_k \frac{1}{\varepsilon_k + \frac{\delta}{2} + |\Delta_+|^2} - \frac{m}{\hbar^2 k^2} ,
\]
\[
\left[ \frac{\Delta_-}{4 \hbar^2 a_o^2} - 1 + \frac{\Delta_-}{\frac{4 \hbar^2 a_o^2}{m}} \right] \sum_k \frac{1}{\varepsilon_k + \frac{\delta}{2} + |\Delta_-|^2} - \frac{m}{\hbar^2 k^2} ,
\]
where \( \Delta_o = \Delta_- - \Delta_+ \) and \( \Delta_c = \Delta_- + \Delta_+ \) are pairing order parameters in the open and closed channels, respectively. We note here, in contrast to usual BCS-BEC crossover where scattering length is the tunable control parameter, here both \( a_o^+ \) and \( a_o^- \) are fixed. Instead, \( \delta \) is the tunable parameter to control the crossover. Moreover, the number equation also includes contribution from both channels
\[
N = \sum_k \left( 2 - \frac{\varepsilon_k}{\varepsilon_k + |\Delta_o|^2} - \frac{\varepsilon_k + \frac{\delta}{2}}{\varepsilon_k + \frac{\delta}{2} + |\Delta_c|^2} \right) .
\]

Solving gap equation Eq. [21] with Eq. [22] we determine both \( \Delta_o \), \( \Delta_c \) and \( \mu \) as a function of \( \delta \), as shown in Fig. [3]. We find (i) when \( \delta \gg \delta_{\text{res}} \), the system is away from OFR. In this case we find small \( \Delta_o/\Delta_c \), \( \Delta_o/\Delta_c \) and \( \mu \rightarrow \mu_F \), which is the typical behavior in the BEC regime. (ii) As \( \delta \rightarrow \delta_{\text{res}} \), both \( \Delta_o \) and \( \Delta_c \) increase rapidly toward the same order as \( \mu \rightarrow \mu_F \) and meanwhile, \( \mu \) decreases. This feature is qualitatively consistent with a crossover from BCS to the unitary regime. (iii) While when \( \delta < \delta_{\text{res}} \) and \( \delta \rightarrow 0 \), both pairing gaps saturate instead of continuously increasing toward deep BEC limit. This is consistent with that \( a_o \) finally saturates to \( a_o^0 \).

We also plot the ratio \( \Delta_o/\Delta_c \) in the inset of Fig. [3] a), we find when \( \delta \gg \delta_{\text{res}} \), this ratio decreases toward zero, and thus the L.H.S. of Eq. [21] diverges as it depends on \( \Delta_o/\Delta_c \). Effectively, if one compares Eq. [21] with a single-channel BCS-BEC gap equation [10], this is equivalent to that an open channel scattering length decreases toward zero. When \( \delta \rightarrow \delta_{\text{res}} \), \( \Delta_o/\Delta_c \rightarrow (a_o^- - a_o^+)/(a_o^- + a_o^+) \) (∼ 0.875 for 173Yb case). The L. H. S. of Eq. [21] approaches zero, indicating an divergent effective scattering length. Finally when \( \delta \rightarrow 0 \), two channels become essentially degenerate and thus this ratio approaches unity. We remark that this mean-field calculation does not use the results from two-body calculation above. It is an independent many-body calculation, while the results are qualitatively consistent with two-body results.

On the other hand, the quantitative behavior is quite different from usual single channel BCS-BEC crossover. We perform a single-channel mean-field calculation, in which we only keep the two states in the open channel and use open channel scattering length \( a_o \) given by two-body result of Eq. [8]. The result is shown by the dotted line in Fig. [3] and compared with the two-gap theory presented above. Remarkably, we find that in the BCS regime, the pairing in the two-gap theory is stronger than that in the single channel model.

**Outlook.** Our predication of OFR opens an avenue for studying strongly interacting physics in alkali-earth atomic gases. The two-gap Fermi superfluid is reminiscent of two-gap superconductor and displays a series of novel features which can be investigated in the future. Moreover, by coupling \( |e \uparrow \rangle \) and \( |g \downarrow \rangle \) states with a laser, one can create spin-orbit coupling between them, which avoids heating from spontaneous emission as in Raman scheme. Our OFR increases attractive interaction between them and can help to reach a topological superfluid phase in this system.

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