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Orbital Feshbach resonances with a small energy gap between open and closed channels

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Recently, a new type of Feshbach resonance, i.e., orbital Feshbach resonance (OFR), was proposed for the ultracold alkaline-earth-metal–like atoms and was experimentally observed in the ultracold gases of ^{173}Yb atoms. Unlike most of the magnetic Feshbach resonances of ultracold alkali atoms, when the OFR of ^{173}Yb atoms appears, the energy gap between the thresholds of the open channel (OC) and the closed channel (CC) is much smaller than the characteristic energy of the interatomic interaction, i.e., the van der Waals energy. In this paper we study the OFR in systems with a small CC-OC threshold gap. We show that in these systems the OFR can be induced by the coupling between the OC and either an isolated bound state of the CC or the scattering states of the CC. Moreover, we also show that in each case the two-channel Huang-Yang pesudopotential is always applicable for the approximate calculation of the low-energy scattering amplitude. Our results imply that in the two-channel theoretical calculations for these systems it is appropriate to take into account the contributions from the scattering states of the CC.

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I. INTRODUCTION

Feshbach resonance [1] exists in many kinds of ultracold gases and can be used as a power tool for controlling the interaction between ultracold atoms [2]. For instance, in the ultracold gases of alkali atoms, when the relative motional state of two atoms in the open channel (OC) is near resonant to a bound state of the closed channel (CC) with higher threshold energy, magnetic Feshbach resonance (MFR) can be induced by the short-range coupling between different channels [3]. With the help of this resonance effect, one can precisely control the scattering length between these two atoms by magnetically changing the interchannel energy difference. In almost all the current experiments of ultracold alkali atoms, when the MFR appears, the gap between the threshold energies of the OC and the CC is as high as 10^8–10^9 Hz [2]. As a result of this large energy gap, the resonance is usually induced by the coupling between the OC and a single bound state (or several bound states with similar energies) of the CC. The contribution of the scattering states of the CC to the resonance can be neglected.

For ultracold alkaline-earth-metal–like atoms, recently, we proposed a new type of Feshbach resonance, i.e., orbital Feshbach resonance (OFR) [4]. This resonance can occur in the scattering between two alkaline-earth-metal–like atoms in different electronic orbital and nuclear spin states. The OFR is a result of the spin-exchange interaction [5–7] and the Zeeman effect [8] in such a system and can be used for magnetically controlling the interaction between alkaline-earth-metal–like atoms. The OFR has been experimentally observed in ultracold ^{173}Yb atoms which are in the $^1S_0$ and $^3P_0$ electronic orbital states with different quantum numbers of nuclear spins [9,10]. In these experiments, when the OFR occurs, the energy gap between the thresholds of the CC and the OC is about 2×10^5 Hz [9,10]. This energy gap is not only much smaller than the CC-OC threshold gap of the MFR of ultracold alkali atoms but also much smaller than the characteristic energy (i.e., the van der Waals energy) of the interaction potential between these ^{173}Yb atoms, which is about 1.8×10^7 Hz [7].

This paper will address the effect of this small energy gap in OFR. Our results can be summarized as follows:

(i) For systems with a small CC-OC threshold gap, the effects contributed by the scattering states of the CC may be very important. As a result, the OFR can be induced by the coupling of either of the following two types: (A) the coupling between the OC and an isolated bound state of the CC or (B) the coupling between the OC and the scattering states of the CC [11,12].

(ii) In each of the above cases, the two-channel Huang-Yang pseudopotential [4,13] (i.e., the pseudopotential used in our previous work [4]) is always applicable for the approximate calculation of the low-energy scattering amplitude.

Our results imply that in the two-channel few-body or many-body calculations for systems with a small CC-OC threshold gap, it is appropriate to take into account the contributions of the scattering states of the CC.

This paper is organized as follows. In Sec. II, we derive the Hamiltonian for alkaline-earth-metal–like atoms with different orbitals and spins, and we introduce the OFR. In Sec. III we illustrate result (i) with a square-well model by analyzing three different cases. In Sec. IV we investigate the applicability of the two-channel Huang-Yang pseudopotential and derive result (ii). Some discussions are given in Sec. V. In the appendixes we show some of the details of our calculation and provide a brief explanation of the principle of the Feshbach resonance induced by the coupling between the OC and the scattering states of the CC [11,12].

II. OFR OF ALKALINE-EARTH-METAL–LIKE ATOMS

We consider the scattering of two fermionic alkaline-earth-metal–like atoms in the $^1S_0$ and $^3P_0$ electronic orbital states with different quantum numbers of nuclear spin. We denote the electronic states $^1S_0$ and $^3P_0$ for the ith atom ($i = 1,2$) as $|g\rangle_i^{(\mathrm{E})}$ and $|e\rangle_i^{(\mathrm{E})}$, respectively, and denote the nuclear spin states for the ith atom as $|\uparrow\rangle_i^{(\mathrm{N})}$ and $|\downarrow\rangle_i^{(\mathrm{N})}$ (Fig. 1). Here the

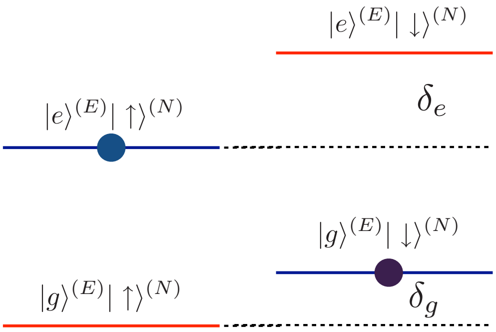

FIG. 1. Energy-level diagram of a single atom. Here δ_e is the Zeeman energy difference between states $|e\rangle^{(\mathrm{E})}|\downarrow\rangle^{(\mathrm{N})}$ and $|e\rangle^{(\mathrm{E})}|\uparrow\rangle^{(\mathrm{N})}$, and δ_g is the one between states $|g\rangle^{(\mathrm{E})}|\downarrow\rangle^{(\mathrm{N})}$ and $|g\rangle^{(\mathrm{E})}|\uparrow\rangle^{(\mathrm{N})}$. The Zeeman energy difference δ in Eq. (3) can be expressed as $\delta=\delta_e-\delta_g$. In our system with $\delta>0$, the open channel is the state $|o\rangle$ with one atom in $|e\rangle^{(\mathrm{E})}|\uparrow\rangle^{(\mathrm{N})}$ and one atom in $|g\rangle^{(\mathrm{E})}|\downarrow\rangle^{(\mathrm{N})}$.

superscripts E and N denote the electronic orbital and nuclear spin degree of freedom, respectively. We further define $|o\rangle$ as the state where one atom is in $|g\rangle^{(\mathrm{E})}|\downarrow\rangle^{(\mathrm{N})}$ and the other one is in $|e\rangle^{(\mathrm{E})}|\uparrow\rangle^{(\mathrm{N})}$ and $|c\rangle$ as the state with one atom being in $|g\rangle^{(\mathrm{E})}|\uparrow\rangle^{(\mathrm{N})}$ and the other being in $|e\rangle^{(\mathrm{E})}|\downarrow\rangle^{(\mathrm{N})}$, i.e.,

$$\begin{aligned}|o\rangle \equiv |g,\downarrow;e,\uparrow\rangle \equiv \frac{1}{\sqrt{2}}\big[&|g\rangle_1^{(\mathrm{E})}|\downarrow\rangle_1^{(\mathrm{N})}|e\rangle_2^{(\mathrm{E})}|\uparrow\rangle_2^{(\mathrm{N})}\\ &-|e\rangle_1^{(\mathrm{E})}|\uparrow\rangle_1^{(\mathrm{N})}|g\rangle_2^{(\mathrm{E})}|\downarrow\rangle_2^{(\mathrm{N})}\big],\end{aligned} \tag{1}$$

$$\begin{aligned}|c\rangle \equiv |g,\uparrow;e,\downarrow\rangle \equiv \frac{1}{\sqrt{2}}\big[&|g\rangle_1^{(\mathrm{E})}|\uparrow\rangle_1^{(\mathrm{N})}|e\rangle_2^{(\mathrm{E})}|\downarrow\rangle_2^{(\mathrm{N})}\\ &-|e\rangle_1^{(\mathrm{E})}|\downarrow\rangle_1^{(\mathrm{N})}|g\rangle_2^{(\mathrm{E})}|\uparrow\rangle_2^{(\mathrm{N})}\big].\end{aligned} \tag{2}$$

The Hamiltonian of such a system can be written as ($\hbar=m=1$, with m being the single-atom mass)

$$\hat{H}=-\nabla_{\mathbf{r}}^2+\delta|c\rangle\langle c|+\hat{U}\equiv\hat{H}_0+\hat{U}, \tag{3}$$

where $\hat{H}_0$ and $\hat{U}$ are the free Hamiltonian for the two-atom relative motion and the interatomic interaction, respectively. Here $\mathbf{r}$ is the relative position of these two atoms, and δ is the Zeeman energy difference of states $|c\rangle$ and $|o\rangle$. It can be expressed as $\delta=(\Delta g)\mu_{\mathrm{B}}B(m_\downarrow-m_\uparrow)$, with B being the magnetic field, μ_{B} being the Bohr's magneton, Δg being the difference of the Landé g factors corresponding to states $|e\rangle^{(\mathrm{E})}$ and $|g\rangle^{(\mathrm{E})}$, and $m_\uparrow$ ($m_\downarrow$) being the quantum number of nuclear spin for states $|\uparrow\rangle^{(\mathrm{N})}$ ($|\downarrow\rangle^{(\mathrm{N})}$). Without loss of generality, we assume $\Delta g>0$ and thus $\delta>0$. In such a system the interatomic interaction $\hat{U}$ can be expressed as [5–7]

$$\hat{U}=U^{(+)}(r)|+\rangle\langle+|+U^{(-)}(r)|-\rangle\langle-|, \tag{4}$$

where states $|+\rangle$ and $|-\rangle$ are defined as

$$\begin{aligned}|\pm\rangle &\equiv \frac{1}{2}\big[|g\rangle_1^{(\mathrm{E})}|e\rangle_2^{(\mathrm{E})}\pm|e\rangle_1^{(\mathrm{E})}|g\rangle_2^{(\mathrm{E})}\big]\\ &\quad\otimes\big[|\uparrow\rangle_1^{(\mathrm{N})}|\downarrow\rangle_2^{(\mathrm{N})}\mp|\downarrow\rangle_1^{(\mathrm{N})}|\uparrow\rangle_2^{(\mathrm{N})}\big]\\ &=\frac{1}{\sqrt{2}}(|c\rangle\mp|o\rangle),\end{aligned} \tag{5}$$

respectively, and $U^{(\pm)}(r)$ is the potential curve with respect to state $|\pm\rangle$.

It is clear that the free Hamiltonian $\hat{H}_0$, which governs the physics in the long-distance region where the two atoms are far away from each other, is diagonal in the basis $|o\rangle$ and $|c\rangle$. On the other hand, the interaction potential $\hat{U}$, which is very important when the interatom distance is short, is diagonal in other bases $|+\rangle$ and $|-\rangle$. In the conventional treatment [2], we always take the same bases in the short-distance region as in the long-distance region, so that the kinetic energy takes the same form in each region. Therefore, we define the OC and CC as the scattering channels corresponding to $|o\rangle$ and $|c\rangle$, respectively. In these bases, the interaction potential is nondiagonal and can be reexpressed as

$$\hat{U}=\sum_{i,j=o,c}U_{ij}(r)|i\rangle\langle j|, \tag{6}$$

where

$$U_{oo}(r)=U_{cc}(r)=\tfrac{1}{2}[U^{(+)}(r)+U^{(-)}(r)] \tag{7}$$

and

$$U_{oc}(r)=U_{co}(r)=\tfrac{1}{2}[U^{(-)}(r)-U^{(+)}(r)]. \tag{8}$$

Here $U_{oo}(r)$ and $U_{cc}(r)$ can be viewed as the intrachannel potential for the OC and the CC, respectively, while $U_{oc}(r)$ and $U_{co}(r)$ can be viewed as the interchannel coupling between the OC and the CC.

We consider the scattering of two atoms in the OC and focus on the threshold scattering limit $E\rightarrow 0$, where E is the scattering energy. In this limit the scattering wave function $|\Psi(r)\rangle$ satisfies the equation $H|\Psi(r)\rangle=0$ and has the behavior

$$|\Psi(r\rightarrow\infty)\rangle\propto\left(\frac{1}{r}-\frac{1}{a_{\mathrm{s}}}\right)|o\rangle \tag{9}$$

in the long-range limit $r\rightarrow\infty$. Here a_{s} is the scattering length.

Due to the coupling $U_{oc}(r)$ between the OC and the CC, in our system the scattering length a_{s} is a function of gap δ between the thresholds of these two channels. In some systems, a_{s} diverges when this threshold gap is tuned to some particular value. That is the OFR.

In this paper we consider the systems where the CC-OC threshold gap δ is much smaller than the characteristic energy E_* of the interaction potential, i.e., the systems with

$$\delta\ll E_*. \tag{10}$$

Here the characteristic energy E_* is defined as

$$E_*=\frac{1}{r_*^2}, \tag{11}$$

where r_* is the characteristic length of the interaction potential $U^{(\pm)}(r)$ and satisfies $U^{(\pm)}(r\gtrsim r_*)\approx 0$. For a realistic ultracold gas of alkaline-earth-metal–like atoms, r_* can be chosen as the van der Waals radius R_{vdW}, which is related to the asymptotic behavior of interaction by

$$U^{(\pm)}(r\rightarrow\infty)=-\frac{(2R_{\mathrm{vdW}})^4}{r^6}. \tag{12}$$

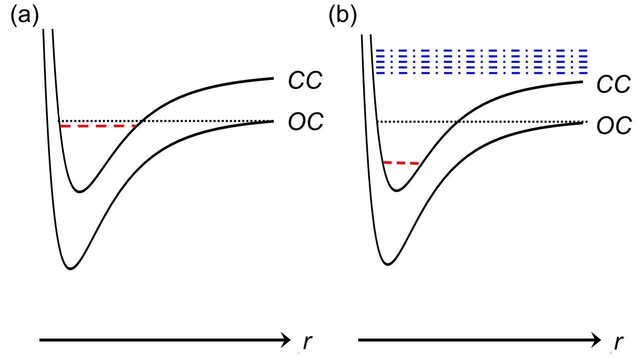

FIG. 2. Schematic diagram of the Feshbach resonances. Here r is the interatomic distance, the black solid lines are the potential curves of the OC and the CC, and the black dotted lines is the threshold of the OC. (a) The Feshbach resonance induced by the coupling between the OC and an isolated bound state (red dashed line) of the CC. (b) The Feshbach resonance induced by the coupling between the OC and the scattering states (blue dash-dotted lines) of the CC. In this case all the bound states (red dashed line) of the CC are far off resonant from the threshold of the OC.

III. OFR INDUCED BY COUPLINGS OF TYPES (A) AND (B)

In this section, using a simple square-well model [14–16], we illustrate that the OFR in the systems under condition (10) can be induced by the coupling between the OC and either the scattering states of the CC [Fig. 2(b)] [11,12] or an isolated bound state of the CC [Fig. 2(a)], i.e., the couplings of either type (A) or type (B) we introduced in Sec. I.

In our model $U^{(+)}(r)$ and $U^{(-)}(r)$ in Eq. (4) are square-well potentials which satisfy (Fig. 3)

$$U^{(\pm)}(r)=\begin{cases}-u^{(\pm)}, & r<b,\\ 0, & r>b,\end{cases} \tag{13}$$

where b is the range of the square-well potential. For simplicity, here we only consider the potentials $U^{(\pm)}(r)$ with at most two bound states. In this model we have $r_*=b$ and thus $E_*=b^{-2}$.

In this section we calculate the scattering length a_s between two atoms in the OC with both the exact numerical calculation and the single-pole approximation for the above square-well potential. In Appendix A we show the details of the approach of the exact numerical calculation. In the single-pole approximation, only the contribution from a single bound state of the CC, whose energy is closest to the threshold of the OC, is taken into account. The contributions from all the other bound states as well as the scattering states of the CC are neglected in this approximation. Under this approximation, the scattering length a_s is given by [3]

$$a_s=a_{bg}+\frac{2\pi^2|w|^2}{|\epsilon_b|-\delta-\epsilon_0}, \tag{14}$$

with

$$\epsilon_0=\int d\mathbf{r}d\mathbf{r}'\phi_b(\mathbf{r})^*U_{co}(r)G_{bg}(\mathbf{r},\mathbf{r}')U_{oc}(r')\phi_b(\mathbf{r}') \tag{15}$$

and

$$w=\int d\mathbf{r}\phi_b(\mathbf{r})^*U_{co}(r)\psi_{bg}(\mathbf{r}). \tag{16}$$

Here $\phi_b(\mathbf{r})$ and $|\epsilon_b|$ are the wave function and the binding energy of the isolated bound state of the CC, respectively, a_{bg} and $\psi_{bg}(\mathbf{r})$ are the scattering length and the threshold scattering wave function of the OC in the case without interchannel coupling, respectively, and

$$G_{bg}(\mathbf{r},\mathbf{r}')=\frac{1}{-[-\nabla_{\mathbf{r}}^2+U_{oo}(r)]}\delta(\mathbf{r}-\mathbf{r}') \tag{17}$$

is the Green's function for the OC in that case. It is clear that when the result from this single-pole approximation is close to the exact result, we can claim that the OFR is mainly due to the coupling between the OC and the isolated bound state ϕ_b.

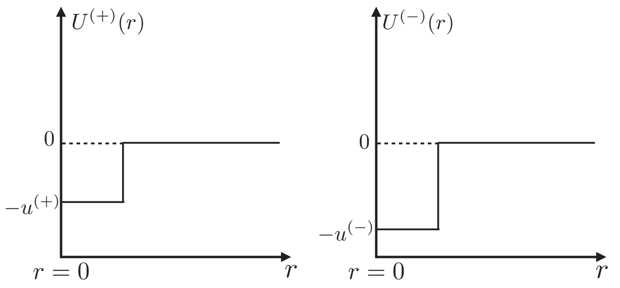

FIG. 3. The square-well model for the potentials $U^{(+)}(r)$ and $U^{(-)}(r)$.

In Figs. 4(a)–4(c) we illustrate our results for three typical cases.

Case (a). There is no bound state in CC, and thus, the OFR is induced by the scattering states of CC. In Fig. 4(a) we consider the system with $a^{(+)}=1000b$ ($u^{(+)}\approx 2.47b^{-2}$) and $a^{(-)}=0.5b$ ($u^{(-)}\approx -3.67b^{-2}$). Notice that here $U^{(-)}(r)$ is a repulsive square-well potential. According to the exact numerical calculation, the OFR can occur when $\delta\approx 4\times 10^{-6}b^{-2}$. Nevertheless, in this system the potentials $U_{cc}(r)=U_{oo}(r)=[U^{(+)}(r)+U^{(-)}(r)]/2$ for the OC and the CC are pure repulsive potentials. Thus, there is no bound state in the CC. Therefore, this OFR is completely induced by the coupling between the OC and the scattering states of the CC. The two-body physics of Feshbach resonance induced by this kind of coupling has been studied by Avishai *et al.* [11,12], and can be understood as a kind of shape resonance of the effective interaction in the OC. Acton *et al.* also discussed this kind of Feshbach resonance in the study of the many-body problem of Fermion-mediated BCS-BEC crossover [17]. In Appendix B we provide a brief explanation for this kind of Feshbach resonance.

Case (b). There are bound states of the CC, while the OFR is induced by the scattering states of the CC. In Fig. 4(b) we consider the system with $a^{(+)}=0.15b$ ($u^{(+)}\approx 19.8b^{-2}$) and $a^{(-)}=1000b$ ($u^{(-)}\approx 22.2b^{-2}$). According to the exact numerical calculation, the OFR of this system occurs when $\delta\approx 0.4\times 10^{-5}b^{-2}$, and the width of this OFR is of the order of $10^{-5}b^{-2}$. Moreover, in this system the binding energy $|\epsilon_b|$ of the shallowest bound state of the CC is as large as $14.5b^{-2}$. Therefore, when the OFR occurs, this bound state is far off resonant from the OC. Thus, the OFR in this system is mainly due to the coupling between the OC and the scattering

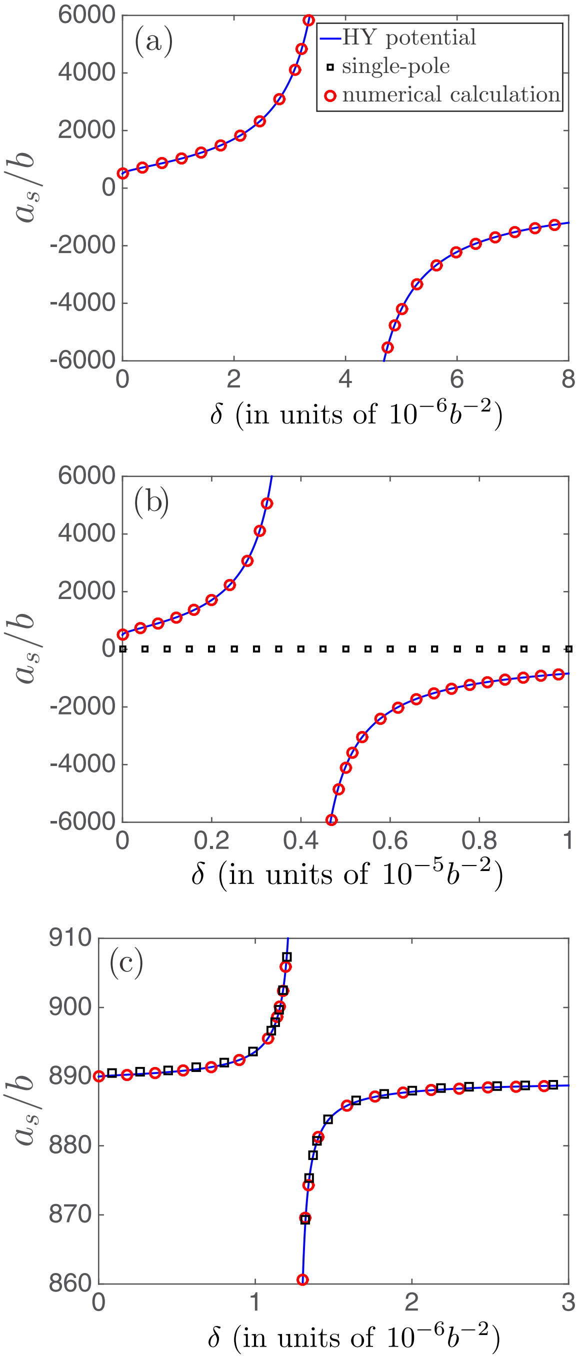

FIG. 4. The scattering length a_s of the square-well model. We show the results given by exact numerical calculation (red circles) and the two-channel Huang-Yang pseudopotential (blue solid lines). In (a) and (c) we also show the single-pole approximation (black squares). Here we consider the cases with (a) $a^{(+)} = 1000b$ ($u^{(+)} \approx 2.47b^{-2}$) and $a^{(-)} = 0.5b$ ($u^{(-)} \approx -3.67b^{-2}$), (b) $a^{(+)} = 0.15b$ ($u^{(+)} \approx 19.8b^{-2}$) and $a^{(-)} = 1000b$ ($u^{(-)} \approx 22.2b^{-2}$), and (c) $a^{(+)} = 870b$ ($u^{(+)} \approx 2.4697b^{-2}$) and $a^{(-)} = 910b$ ($u^{(-)} \approx 2.4696b^{-2}$).

states of the CC. This conclusion is further confirmed by our calculation with the single-pole approximation, which shows that the scattering length a_s given by this approximation is significantly different from the exact result and does not have any resonance behavior.

Case (c). The OFR is induced by the coupling between the OC and an isolated bound state of the CC. In Fig. 4(c) we consider the system with $a^{(+)} = 870b$ ($u^{(+)} \approx 2.47b^{-2}$) and $a^{(-)} = 910b$ ($u^{(-)} \approx 2.4696b^{-2}$). It is clear that for this system the results given by the single-pole approximation and the exact numerical calculation are quantitatively consistent with each other in the region around the OFR point. Thus, the OFR in this system is mainly due to the coupling between the OC and the isolated bound state of the CC.

Our results for the above cases show that the OFR with a small CC-OC threshold gap can be induced by coupling of either type (A) or type (B) defined in Sec. I. Here we point out that cases in Figs. 4(a) and 4(b) are essentially the same category; that is, in the region of the actual OFR there is no bound state of the CC, and the OFR is induced by coupling of type (B), i.e., the coupling between the OC and the scattering states of the CC.

We further emphasize that, as shown in Figs. 4(a)–4(c), in the simple square-well model the OFR is usually induced by coupling of type (A) or type (B) when the scattering lengths $a^{(+)}$ and $a^{(-)}$ are very close or significantly different from each other, respectively. Nevertheless, in ultracold gases of alkaline-earth-metal–like atoms, e.g., ultracold gases of ^{173}Yb atoms, the realistic interatomic interaction potential curve is much more complicated than the square-well model. For these ultracold gases, to know which type of coupling induces the OFR, one requires not only the values of $a^{(\pm)}$ but also the short-range details of the potential curves $U^{(\pm)}(r)$.

IV. TWO-CHANNEL HUANG-YANG PSEUDOPOTENTIAL

In the section above we illustrate that the OFR of systems under condition (10) can be induced by coupling of two different types. In this section we show that in each of these two cases, the two-channel Huang-Yang pseudopotential [4,13] is always applicable for the approximate calculation of the low-energy scattering amplitude.

To this end, we consider the two-atom scattering wave function $|\psi(\mathbf{r})\rangle$ of our system, which can be expanded as

$$|\psi(\mathbf{r})\rangle = \psi_+(\mathbf{r})|+\rangle + \psi_-(\mathbf{r})|-\rangle. \tag{18}$$

This wave function satisfies the Schrödinger equation

$$\hat{H}|\psi(\mathbf{r})\rangle = E|\psi(\mathbf{r})\rangle, \tag{19}$$

with E being the scattering energy, as well as the outgoing boundary condition. As in the above discussions, we consider systems under condition (10). We further focus on the low-energy scattering processes where the scattering energy is much smaller than the characteristic energy E_* of the interaction potential, i.e.,

$$E \ll E_*. \tag{20}$$

It is clear that conditions (10) and (20) imply $1/\sqrt{E} \gg r_*$ and $1/\sqrt{\delta} \gg r_*$, where r_* is the characteristic length of the interaction potential $U^{(\pm)}(r)$, as defined in Sec. II.

When $\delta = 0$, the low-energy scattering wave function $|\psi(\mathbf{r})\rangle$ has the short-range behavior

$$\psi_\pm(\mathbf{r}) \propto \left(\frac{1}{r} - \frac{1}{a_s^{(\pm)}}\right), \quad r_* \lesssim r \ll \frac{1}{\sqrt{E}}, \tag{21}$$

where $a_s^{(\pm)}$ is the s-wave scattering length with respect to the potential $U^{(\pm)}(r)$.

Furthermore, when δ is finite, the behavior of the wave function in the region $r \ll 1/\sqrt{\delta}$ is almost unchanged. Therefore, under conditions (10) and (20) we have

$$\psi_\pm(\mathbf{r}) \propto \left(\frac{1}{r} - \frac{1}{a_s^{(\pm)}}\right), \; r_* \lesssim r \ll \mathrm{Min}\left(\frac{1}{\sqrt{E}}, \frac{1}{\sqrt{\delta}}\right). \tag{22}$$

Due to this fact, in our calculation we can approximately replace the real interaction potential $U^{(\pm)}(r)$ with the Bethe-Peierls boundary condition [18]

$$\lim_{r\to 0} \psi_\pm(\mathbf{r}) \propto \left(\frac{1}{r} - \frac{1}{a_s^{(\pm)}}\right) \tag{23}$$

or the two-channel Huang-Yang pseudopotential [4,13]

$$\hat{U}_{\mathrm{HY}} = 4\pi\left[a_s^{(+)}|+\rangle\langle+| + a_s^{(-)}|-\rangle\langle-|\right]\delta(\mathbf{r})\left(\frac{\partial}{\partial r} r\right), \tag{24}$$

which is mathematically equivalent to boundary condition (23). Thus, we know that for our system two-channel Huang-Yang pseudopotential $\hat{U}_{\mathrm{HY}}$ can always be used for the approximate calculation of the low-energy two-body problems, regardless of whether OFR is induced by coupling of type (A) or (B).

To illustrate this result, we calculate the scattering length of two atoms incident from the OC with the two-channel Huang-Yang pseudopotential $\hat{U}_{\mathrm{HY}}$. To this end we consider the threshold scattering with $E = 0$. In this case the scattering wave function given by $\hat{U}_{\mathrm{HY}}$ can be expressed as

$$|\psi(\mathbf{r})\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}}\left[\left(1 - \frac{a_s^{(\mathrm{HY})}}{r}\right)|o\rangle + B\frac{e^{-\sqrt{\delta}r}}{r}|c\rangle\right], \tag{25}$$

where the scattering length $a_s^{(\mathrm{HY})}$ is the scattering length given by $\hat{U}_{\mathrm{HY}}$. The values of $a_s^{(\mathrm{HY})}$ and the factor B can be obtained via the Schrödinger equation

$$(\hat{H}_0 + \hat{U}_{\mathrm{HY}})|\psi(\mathbf{r})\rangle = 0. \tag{26}$$

With straightforward calculation, we can obtain

$$a_s^{(\mathrm{HY})} = \frac{-a_{s0} + \sqrt{\delta}\left(a_{s0}^2 - a_{s1}^2\right)}{a_{s0}\sqrt{\delta} - 1}, \tag{27}$$

where a_{s0} and a_{s1} are defined as

$$a_{s0} = \tfrac{1}{2}\left[a_s^{(+)} + a_s^{(-)}\right], \; a_{s1} = \tfrac{1}{2}\left[a_s^{(-)} - a_s^{(+)}\right]. \tag{28}$$

In Figs. 4(a)–4(c) we compare $a_s^{(\mathrm{HY})}$ with the scattering length given by the exact numerical calculation. Notice that according to the exact numerical calculation, for these cases when the OFR occurs, the low-energy condition (10) is satisfied very well ($\delta \sim 10^{-6}b^{-2} - 10^{-5}b^{-2}$). As shown in Figs. 4(a)–4(c), in all of these cases $a_s^{(\mathrm{HY})}$ is very close to the result from the exact numerical calculation, regardless of whether the OFR is induced by the coupling between the bound or scattering states of the CC.

We also do a calculation for the ^{173}Yb atoms with our square-well model and the two-channel Huang-Yang pseudopotential. In our calculation we take $b = R_{\mathrm{vdW}} = 84.84a_0$ [7], $a^{(+)} = 1900a_0 \approx 22.4b$ ($u^{(+)} \approx 2.56b^{-2}$), and $a^{(-)} = 200a_0 \approx 2.34b$ ($u^{(-)} \approx 3.76b^{-2}$) [9,10]. We illustrate our results in Fig. 5. It is shown that although we can still approximately derive the scattering length a_s with the Huang-Yang pseudopotential $\hat{U}_{\mathrm{HY}}$, there is a relative error of 10% in this approximation. This fact can be understood by the following analysis. For ^{173}Yb atoms, the OFR occurs when $\delta \sim 10^{-2}b^{-2}$. Thus, in this system the low-energy condition (10) is not satisfied as perfectly as in the examples in Figs. 4(a)–4(c). As a result, the relative error of the pseudopotential approximation is larger. Our result implies that to obtain a more accurate theoretical result for ^{173}Yb atoms, we need to include more details about the interaction $U^{(\pm)}(r)$ in our calculation.

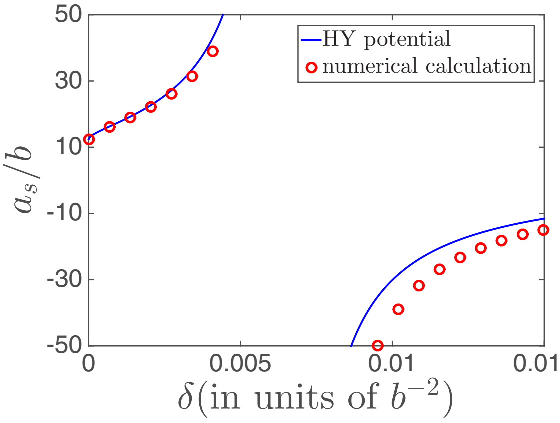

FIG. 5. The scattering length a_s of the square-well model. We show the results given by exact numerical calculation (red circles) with the approach in Appendix A and the two-channel Huang-Yang pseudopotential (blue solid lines). Here we consider the cases with $a^{(+)} = 22.4b$ ($u^{(+)} \approx 2.56b^{-2}$) and $a^{(-)} = 2.34b$ ($u^{(-)} \approx 3.76b^{-2}$).

V. DISCUSSION

In this paper we show that the OFR in systems where the CC-OC threshold gap δ is much smaller than the characteristic energy E_* can be induced by the coupling between the OC and either an isolated bound state or the scattering states of the CC. In any case, the two-channel Huang-Yang pseudopotential $\hat{U}_{\mathrm{HY}}$ can always be used as a good approximation for the interatomic interaction potential in the region $\delta \ll E_*$. We illustrate these conclusions with a simple square-well model.

According to Eq. (27), the scattering length $a_s^{(\mathrm{HY})}$ given by the Huang-Yang pseudopotential diverges when

$$\delta = \frac{1}{a_{s0}^2}, \tag{29}$$

with a_{s0} defined in Eq. (28). Therefore, the OFR can occur in systems with $\delta \ll E_*$ only when $1/a_{s0}^2 \ll E_*$; that is, a_{s0} should be much larger than the characteristic length r_* of the interaction potential. According to Eqs. (11) and (28), this condition yields that either of the two scattering lengths $a_s^{(+)}$ and $a_s^{(-)}$ for channels $|+\rangle$ and $|-\rangle$ should be positive and much larger than r_*. Therefore, when an OFR occurs under the condition $\delta \ll E_*$, there must be a shallow bound state in channel $|+\rangle$ or $|-\rangle$, although there may not be a shallow bound state in the CC $|c\rangle$.

Here we also would like to make a comment about the scattering length of the CC itself. Naively, by projecting the two-channel Huang-Yang pseudopotential $\hat{U}_{\rm HY}$ on the CC, one can obtain

$$\langle c|\hat{U}_{\rm HY}|c\rangle = 4\pi a_{\rm s0}\delta(\mathbf{r})\left(\frac{\partial}{\partial r}r\right). \tag{30}$$

Thus, it seems that the scattering length of the CC is just $a_{\rm s0} = (a_{\rm s}^{(+)} + a_{\rm s}^{(-)})/2$. However, this conclusion is incorrect. The real interaction potential of the CC is

$$\langle c|U|c\rangle = U_{cc}(r) = \tfrac{1}{2}[U^{(+)}(r) + U^{(-)}(r)]. \tag{31}$$

It is clear that the scattering length of this real potential, which can be denoted as $a_{\rm sc}$, is determined by not only the scattering length $a_{\rm s}^{(\pm)}$ of the potential curves $U^{(\pm)}(r)$ but also the short-range details $U^{(\pm)}(r)$. The value of $a_{\rm sc}$ can be either significantly different from $a_{\rm s0}$ or close to $a_{\rm s0}$. Accordingly, although the complete two-channel Huang-Yang pseudopotential $\hat{U}_{\rm HY}$ is always applicable in a two-channel problem under conditions (10) and (20), that does not mean that we can directly use the projection $\langle c|\hat{U}_{\rm HY}|c\rangle$ to study the single-channel physics for the CC itself.

As shown above, the OFR can occur in the region $\delta \ll E_*$ in a system with $a_{\rm s0} > 0$ and $1/a_{\rm s0}^2 \ll E_*$. In such a system, if the value of the scattering length $a_{\rm sc}$ of the CC is close to the value of $a_{\rm s0}$, then there exists a shallow bound state in the CC with binding energy close to $1/a_{\rm s0}^2$. When the OFR occurs, i.e., $\delta \approx 1/a_{\rm s0}^2$, this bound state is near resonant to the threshold of the OC and thus makes a significant contribution to the OFR. On the other hand, if the value of $a_{\rm sc}$ is negative or much smaller than $a_{\rm s0}$, then when the OFR occurs, all the bound states of the CC are far off resonant from the threshold of the OC. In that system the OFR may be mainly induced by the coupling between the OC and the scattering states of the CC.

It is also pointed out that, in principle, the Feshbach resonance induced by the coupling between the OC and the scattering states of the CC can also occur in systems where the CC-OC threshold gap is comparable to or larger than the characteristic energy [11,12]. However, in these systems that kind of Feshbach resonance usually requires extremely strong CC-OC coupling [11,12], which is very difficult to generate in the realistic systems. Therefore, the Feshbach resonances in realistic ultracold gases with a large CC-OC threshold gap, e.g., the MFR of ultracold alkali atoms, are usually induced by the coupling between the OC and one or several isolated bound states of the CC.

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APPENDIX A: EXACT CALCULATION OF $a_{\rm s}$ FOR THE TWO-CHANNEL SQUARE-WELL MODEL

In this appendix we show our approach for the exact calculation of the scattering length $a_{\rm s}$ for the two-channel square-well model. In this model the total Hamiltonian $\hat{H}$ for the two-atom relative motion can be expressed as in Eq. (3), with the interaction potential $\hat{U}$ being given by Eqs. (6), (7), (8), and Eq. (13). As shown in the main text, we consider the scattering of two atoms in the OC $|o\rangle$ with zero scattering energy. Thus, the scattering wave function $|\Psi(r)\rangle$ satisfies the Schrödinger equation

$$\hat{H}|\Psi(r)\rangle = 0. \tag{A1}$$

It is clear that in the region $r > b$, with b being the width of the square well, the Hamiltonian $\hat{H}$ can be written as

$$\hat{H} = -\nabla_{\mathbf{r}}^2 + \delta|c\rangle\langle c|. \tag{A2}$$

Thus, in this region the solution of Eq. (A1) can be expressed as

$$|\Psi(r > b)\rangle = \frac{1}{r}\big[\phi_o^{(\rm out)}(r)|o\rangle + \phi_c^{(\rm out)}(r)|c\rangle\big], \tag{A3}$$

where

$$\phi_o^{(\rm out)}(r) = r - a_{\rm s}, \tag{A4}$$

$$\phi_c^{(\rm out)}(r) = f_c e^{-\sqrt{\delta}r}, \tag{A5}$$

with $a_{\rm s}$ being the scattering length and f_c being a constant coefficient which can be obtained later.

On the other hand, according to Eqs. (6), (7), (8), and (13), in the region $r < b$ the Hamiltonian $\hat{H}$ can be written as

$$\hat{H} = -\nabla_{\mathbf{r}}^2 - \hat{B}, \tag{A6}$$

where

$$\hat{B} = \sum_{i,j=o,c} B_{ij}|i\rangle\langle j| \tag{A7}$$

is an r-independent operator with matrix elements

$$B_{cc} = -\delta + \tfrac{1}{2}[u^{(+)} + u^{(-)}], \tag{A8}$$

$$B_{oo} = \tfrac{1}{2}[u^{(+)} + u^{(-)}], \tag{A9}$$

$$B_{oc} = B_{co} = \tfrac{1}{2}[u^{(-)} - u^{(+)}]. \tag{A10}$$

Here $u^{(+)}$ and $u^{(-)}$ are defined in Eq. (13) of the main text. We can further derive the eigenvalue λ_i ($i = 1,2$) and eigenstate $|\lambda_i\rangle$ of operator $\hat{B}$, which satisfies

$$\hat{B}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle\ (i = 1,2). \tag{A11}$$

The direct calculation yields

$$\lambda_1 = \frac{(B_{oo} + B_{cc}) + \sqrt{(B_{oo} - B_{cc})^2 + 4B_{oc}^2}}{2}, \tag{A12}$$

$$\lambda_2 = \frac{(B_{oo} + B_{cc}) - \sqrt{(B_{oo} - B_{cc})^2 + 4B_{oc}^2}}{2}, \tag{A13}$$

and

$$|\lambda_1\rangle = \alpha|c\rangle + \beta|o\rangle, \tag{A14}$$

$$|\lambda_2\rangle = -\beta|c\rangle + \alpha|o\rangle, \tag{A15}$$

with

$$\alpha = \frac{\lambda_1 - B_{oo}}{\sqrt{(\lambda_1 - B_{oo})^2 + B_{oc}^2}}, \tag{A16}$$

$$\beta = \frac{B_{oc}}{\sqrt{(\lambda_1 - B_{oo})^2 + B_{oc}^2}}. \tag{A17}$$

Therefore, the solution of the Schrödinger equation (A1) in the region $r < b$ can be written as

$$|\Psi(r < b)\rangle = \frac{1}{r}[A_1 \sin(\sqrt{\lambda_1}r)|\lambda_1\rangle + A_2 \sin(\sqrt{\lambda_2}r)|\lambda_2\rangle], \tag{A18}$$

with $A_{1,2}$ being constant coefficients. Here for $z < 0$ we define $\sqrt{z} = i\sqrt{|z|}$. Using Eqs. (A12)–(A15), we can rewrite this result as

$$|\Psi(r < b)\rangle = \frac{1}{r}\big[\phi_o^{(\mathrm{in})}(r)|o\rangle + \phi_c^{(\mathrm{in})}(r)|c\rangle\big], \tag{A19}$$

where

$$\phi_o^{(\mathrm{in})}(r) = A_1\beta \sin(\sqrt{\lambda_1}r) + A_2\alpha \sin(\sqrt{\lambda_2}r), \tag{A20}$$

$$\phi_c^{(\mathrm{in})}(r) = A_1\alpha \sin(\sqrt{\lambda_1}r) - A_2\beta \sin(\sqrt{\lambda_2}r). \tag{A21}$$

So far we have obtained the forms (A3) and (A19) for the scattering wave function in the regions $r > b$ and $r < b$, respectively. Since the scattering wave function $|\Psi(r)\rangle$ and its first-order derivative should be continuous at the point $r = b$, we have the equations

$$\phi_o^{(\mathrm{in})}(r = b) = \phi_o^{(\mathrm{out})}(r = b), \tag{A22}$$

$$\phi_c^{(\mathrm{in})}(r = b) = \phi_c^{(\mathrm{out})}(r = b), \tag{A23}$$

$$\frac{d}{dr}\phi_o^{(\mathrm{in})}(r)\bigg|_{r=b} = \frac{d}{dr}\phi_o^{(\mathrm{out})}(r)\bigg|_{r=b}, \tag{A24}$$

$$\frac{d}{dr}\phi_c^{(\mathrm{in})}(r)\bigg|_{r=b} = \frac{d}{dr}\phi_c^{(\mathrm{out})}(r)\bigg|_{r=b}, \tag{A25}$$

with $\phi_{o,c}^{(\mathrm{out})}(r)$ being defined in Eqs. (A4) and (A5) and $\phi_{o,c}^{(\mathrm{in})}(r)$ being defined in Eqs. (A20) and (A21). By solving Eqs. (A22)–(A25), we can obtain the values of the scattering length a_{s} as well as the coefficients f_c and $A_{1,2}$.

We numerically solve Eqs. (A22)–(A25) for the cases discussed in Sec. III and Sec. IV of the main text and obtain the exact values of the scattering length a_{s} for these cases. These results are illustrated by the red circles of Figs. 4(a)–4(c) and 5.

APPENDIX B: FESHBACH RESONANCE INDUCED BY THE SCATTERING STATES OF THE CC

In this appendix we show that the Feshbach resonance induced by the coupling between the OC and the scattering states of the CC can be understood as a shape resonance of the effective interaction in the OC. For convenience, here we also consider the OFR system discussed in the main text. Nevertheless, our result is applicable to the general two-channel scattering problems of two atoms.

As shown in Sec. II, the Hamiltonian of our system can be expressed as

$$\begin{aligned}\hat{H} &= \big(-\nabla_{\mathbf{r}}^2 + \delta\big)|c\rangle\langle c| + \big(-\nabla_{\mathbf{r}}^2\big)|o\rangle\langle o| + \hat{U}\\ &\equiv \hat{H}_0 + \hat{U},\end{aligned} \tag{B1}$$

where the interaction potential $\hat{U}$ can be written as $\hat{U} = \sum_{i,j=o,c} U_{ij}(r)|i\rangle\langle j|$, with $U_{oo}(r)$ and $U_{cc}(r)$ being the intrachannel interaction potential of the OC and CC, respectively, and $U_{oc}(r) = U_{co}(r)^*$ being the interchannel coupling.

In our system the scattering wave function can be expressed as

$$|\psi(\mathbf{r})\rangle = \psi^{(o)}(\mathbf{r})|o\rangle + \psi^{(c)}(\mathbf{r})|c\rangle \tag{B2}$$

and satisfies the Schrödinger equation

$$\hat{H}|\psi(\mathbf{r})\rangle = E|\psi(\mathbf{r})\rangle, \tag{B3}$$

with E being the scattering energy. Furthermore, when $E = 0$, we have

$$\lim_{r\to\infty} \psi^{(o)}(\mathbf{r}) \propto \left(1 - \frac{a_{\mathrm{s}}}{r}\right), \tag{B4}$$

where a_{s} is the scattering length of two atoms incident from the OC. Therefore, to obtain the scattering length a_{s}, we should first calculate the component $\psi^{(o)}(\mathbf{r})$ of the scattering wave function for the case with $E = 0$. In this case, Eq. (B3) can be rewritten as

$$\begin{aligned}&-\nabla_{\mathbf{r}}^2\psi^{(c)}(\mathbf{r}) + \delta\psi^{(c)}(\mathbf{r}) + U_{cc}(r)\psi^{(c)}(\mathbf{r}) + U_{co}(r)\psi^{(o)}(\mathbf{r})\\ &= 0,\end{aligned} \tag{B5}$$

$$-\nabla_{\mathbf{r}}^2\psi^{(o)}(\mathbf{r}) + U_{oo}(r)\psi^{(o)}(\mathbf{r}) + U_{oc}(r)\psi^{(c)}(\mathbf{r}) = 0. \tag{B6}$$

Using these two equations, we can obtain the effective interaction potential of the OC via the projection operator technique. To this end we first solve Eq. (B5) and obtain

$$\psi^{(c)}(\mathbf{r}) = \int d\mathbf{r}' g(\delta,\mathbf{r},\mathbf{r}')U_{co}(r')\psi^{(o)}(\mathbf{r}'), \tag{B7}$$

where $g(\delta,\mathbf{r},\mathbf{r}')$ is the Green's function of the CC and is defined as

$$g(\delta,\mathbf{r},\mathbf{r}') = \frac{1}{-\big[-\nabla_{\mathbf{r}}^2 + U_{cc}(r) + \delta\big]}\delta(\mathbf{r} - \mathbf{r}'). \tag{B8}$$

We assume all the bound states of the CC are far off resonant from the threshold of the OC. Thus, in the calculation of $g(\delta,\mathbf{r},\mathbf{r}')$ we can neglect the contributions from the bound states of the CC. Then we obtain

$$g(\delta,\mathbf{r},\mathbf{r}') \approx \int d\mathbf{k}\frac{\psi_{\mathbf{k}}^*(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}')}{-\delta - k^2}, \tag{B9}$$

where $\psi_{\mathbf{k}}(\mathbf{r})$ is the scattering state of the CC with incident momentum $\mathbf{k}$. Substituting Eq. (B7) into Eq. (B6), we obtain the equation for $\psi^{(o)}(\mathbf{r})$:

$$-\nabla_{\mathbf{r}}^2\psi^{(o)}(\mathbf{r}) + \mathcal{V}_{\mathrm{eff}}(\delta)\psi^{(o)}(\mathbf{r}) = 0. \tag{B10}$$

Here $\mathcal{V}_{\rm eff}(\delta)$ is the effective interaction of the OC. It is nondiagonal in the $\mathbf{r}$ representation, and satisfies

$$\mathcal{V}_{\rm eff}(\delta)\psi^{(o)}(\mathbf{r}) = U_{oc}(r)\int d\mathbf{r}' g(\delta,\mathbf{r},\mathbf{r}')U_{co}(r')\psi^{(o)}(\mathbf{r}') + U_{oo}(r)\psi^{(o)}(\mathbf{r}), \tag{B11}$$

with $g(\delta,\mathbf{r},\mathbf{r}')$ given by Eq. (B9).

Equations (B10) and (B4) show that we can obtain the wave function $\psi^{(o)}(\mathbf{r})$ and the scattering length a_s of our two-channel scattering problem by solving the single-channel scattering problem with effective interaction $\mathcal{V}_{\rm eff}(\delta)$, which changes with the CC-OC threshold gap δ. Although in $\mathcal{V}_{\rm eff}(\delta)$ we have ignored all the contributions from the bound states of the CC, it is still possible that a shape resonance for $\mathcal{V}_{\rm eff}(\delta)$ can appear when δ is tuned to a particular value δ_0 ($\delta_0 > 0$). In this case, we would have $a_s = \infty$. It is clear that this resonance is nothing but the Feshbach resonance induced by the coupling between the OC and the scattering states of the CC.

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