Calibration of Interaction Energy between Bose and Fermi Superfluids

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In this letter we study the interaction energy in a mixture of Bose and Fermi superfluids realized in recent cold atom experiment. On the Bose-Einstein-condensate (BEC) side of a Feshbach resonance, the mean-field theory yields that the scattering length between fermion pairs (or dimers) equals $2a_s$. However, a precise four-body calculation gives a result of $0.6a_s$. This significant deviation suggests that it is necessary to include pair fluctuations in order to obtain a more accurate many-body description. Indeed, pair fluctuation theory can reduce this dimer scattering length to 0.

Few-body problems play many important roles in the study of cold atom gases, partly due to the diluteness condition which is generally fulfilled in the underlying systems. One of the most important examples is that few-body results, which can be numerically exact, can provide benchmark and calibration of many-body theories, where approximations are usually inevitable. For instance, in the study of BEC-BSC crossover of a Fermi superfluid around a Feshbach resonance, the mean-field approach. We also find that the multiple scattering between atom and dimer can account for such a deviation. Our results provide a calibration to the mean-field interaction energy, which can be verified by measuring the shift of collective oscillation frequency.

Described by

$$V = \frac{2\pi \hbar^2}{m_{bf}} \sum_{\sigma} \int d^3 \mathbf{r} \hat{b}^\dagger(\mathbf{r}) \hat{b}(\mathbf{r}) \hat{c}_\sigma^\dagger(\mathbf{r}) \hat{c}_\sigma(\mathbf{r}),$$

(1)

where $\hat{b}^\dagger$ and $\hat{c}_\sigma^\dagger$ are creation operators for bosons and fermions with spin $\sigma = \uparrow$ or $\downarrow$, respectively, and $m_{bf}$ is the reduced mass of boson and fermion. With Hatree-Fock mean-field decomposition, $\langle \hat{b}^\dagger \hat{b} \rangle = n_b$, and $\langle \hat{c}_\sigma^\dagger \hat{c}_\sigma \rangle = n_f$, this interaction energy density is naturally given by

$$\mathcal{E} = \frac{2\pi \hbar^2}{m_{bf}} n_b n_f.$$  

(2)

On the other hand, on the BEC side of the resonance, the Fermi superfluid can be viewed as a Bose condensate of dimers. The interaction energy between Bose and Fermi superfluids can then be considered as the boson-dimer interaction. We introduce $a_{ad}$ as the scattering length between bosonic atoms and dimers. In the dilute limit, the interaction energy density is given by

$$\mathcal{E} = \frac{2\pi \hbar^2}{m_{ad}} n_b n_d,$$

(3)

where $n_d$ is density of dimers, $n_d = n_f/2$, and $m_{ad}$ is the reduced mass of bosonic atom and dimer.

Eq. (2) and Eq. (3) are two different ways of representing the same interaction energy. Therefore, by equating these two expressions, we can obtain atom-dimer scattering length from a three-body calculation. Its deviation from Eq. (4) will be used as a calibration of the mean-field theory. Our calculation focuses on the resonance regime of Fermi superfluid with $a_{bf}/a_f \ll 1$ ($a_f$ denotes the scattering length between two fermionic components). Besides, we also retain ourself within the
is now known that this three-body parameter is of the systems [17–28]. The dimer scattering length has also been studied in other [12], from which 

A straightforward calculation employing Eqs. (5) and (6) is the three-body scattering state related to

\[
|\Psi\rangle = \lim_{\epsilon \to 0^+} \frac{i\epsilon}{-\frac{\hbar^2}{2m_{12}a_f^2} + i\epsilon - H}|\Psi_{\text{in}}\rangle. 
\]

A straightforward calculation employing Eqs. (5) and (6) lead to the Skorniakov–Ter-Martirosian (STM) equations [12], from which \(a_{ad}\) can be obtained [13]. The atom-dimer scattering length has also been studied in other systems [17,25].

We shall note that in the three-body calculation, a high-energy cutoff \(\Lambda e^{\eta}\) is required in order to regularize integrations, where \(\eta\) is usually very small. Since it is now known that this three-body parameter is of the order of the van der Waals length [29,35], and since for weak boson-fermion interaction, \(a_{bf}\) as a function of \(a_{bf}/a_{f}\) given by three-body calculation with mean-field approximation (purple dash-dotted line), zero-range pseudo potential (red solid line), single-pole approximation (black dash line), and three-body calculation with a separable potential suggested in Ref. [34] to incorporate the van der Waals effect (blue circle with solid line). Here we illustrate the results with \(a_{bf} = 40.8a_0\), \(\Lambda = 4/a_{bf}\), \(\eta = 0\), \(R_{\text{vdW}} = 31.26a_0\) for \(^6\text{Li}-^7\text{Li}\) interaction, and \(R_{\text{vdW}} = 32.49a_0\) for \(^6\text{Li}-^7\text{Li}\) interaction [33,34].

FIG. 1: (color online) The atom-dimer scattering length \(a_{ad}/a_{f}\) as a function of \(a_{bf}/a_{f}\) given by three-body calculation with mean-field approximation (purple dash-dotted line), zero-range pseudo potential (red solid line), single-pole approximation (black dash line), and three-body calculation with a separable potential suggested in Ref. [34] to incorporate the van der Waals effect (blue circle with solid line). Here we illustrate the results with \(a_{bf} = 40.8a_0\), \(\Lambda = 4/a_{bf}\), \(\eta = 0\), \(R_{\text{vdW}} = 31.26a_0\) for \(^6\text{Li}-^7\text{Li}\) interaction, and \(R_{\text{vdW}} = 32.49a_0\) for \(^6\text{Li}-^7\text{Li}\) interaction [33,34].

The results of \(a_{ad}\) for \(^6\text{Li}-^7\text{Li}\) mixture is shown by the red solid line in Fig. 1. Here we fix \(a_{bf}\) and calculate \(a_{ad}/a_{bf}\) with varying \(a_{bf}/a_{f}\). Comparing with the mean-field result shown by the horizontal dash-dotted line, one can see that the two approaches agree with each other only when \(a_{bf}/a_{f} \to 0\). For finite and positive \(a_{bf}/a_{f}\), the three-body result is always below the mean-field expectation. Specifically, the deviation is already about
ten percent for \(a_{bd}/a_t \approx 0.01\), and keeps increasing with \(a_{bd}/a_t\) until \(a_{bd}\) becomes comparable to \(a_t\) where Efimov physics starts to set in.

In Fig. 2 we investigate this deviation for other possible realizations of Bose-Fermi mixtures, including \(^{6}\)Li-\(^{87}\)Rb, \(^{6}\)Li-\(^{3}\)Li, \(^{6}\)Li-\(^{6}\)Li, \(^{40}\)K-\(^{2}\)Na, and \(^{40}\)K-\(^{3}\)Li. Here, we plot the relative derivation of the three-body result from the mean-field value as \((a_{0}^{0} - a_{bd})/a_{0}^{0}\). We find, on one hand, they all have qualitatively the same behaviors; and on the other hand, the deviation increases with enhanced boson-fermion mass ratio.

In the following, we would like to further understand two questions. First, what is the major physical process that causes such a significant deviation. Second, since \(a_{bd}\) is comparable to van der Waals length, whether a van der Waals potential will change this result obtained from zero-range models. The first question is to understand the underlying physics better, while the second question is crucial when comparing with experiments.

**Born and Single-Pole Approximations.** To understand more about the difference between \(a_{ad}\) and \(a_{0}^{0}\), we can rewrite Eq. \((6)\) as

\[
\langle \Psi_{in} | (V_{23} + V_{31}) | \Psi_{in} \rangle = \int dK |K| \langle \phi_{b} | (\beta + K^{2}/(2m_{ad})) | \phi_{r} \rangle,
\]

where \(G_{3} = (-\hbar^{2}/(2\pi m_{b} a_{f}^{2}) + i0^{+} - (T + V_{12})\) is the Green’s operator for a free boson and two interacting fermions, and expand Eq. \((5)\) as

\[
a_{ad} = 4\pi^{2} \hbar m_{ad} \langle \Psi_{in} | (V_{23} + V_{31}) | \Psi_{in} \rangle + 4\pi^{2} m_{ad} \langle \Psi_{in} | (V_{23} + V_{31}) G_{3} (V_{23} + V_{31}) | \Psi_{in} \rangle + \ldots
\]

\[(7)\]

If we take the 1st-order Born approximation by neglecting all higher order terms in Eq. \((7)\), it is straightforward to show that

\[
a_{ad} = 4\pi^{2} \hbar m_{ad} \langle \Psi_{in} | (V_{23} + V_{31}) | \Psi_{in} \rangle = \frac{2m_{ad}}{m_{bf}} a_{bf} = a_{ad}^{0}.
\]

\[(8)\]

This means that \(a_{ad}^{0}\) deduced from many-body mean-field treatment is equivalent to that obtained from a three-body calculation with 1st-order Born approximation. Thus, the difference between the exact \(a_{ad}\) and the mean-field \(a_{ad}^{0}\) is due to processes beyond the 1st-order Born approximation.

The higher order terms of Eq. \((7)\) correspond to the following two types of atom-dimer scattering processes: i) a dimer composed of two fermions remains in the bound state, and undergoes repeated collisions with bosons; ii) an incoming dimer first breaks into two fermions in the scattering state, and then they return to a bound state after the second collision. While the processes of the second type are difficult to incorporate, the ones of the first type can be integrated using a “single-pole” approximation. Within this approach, the three-body Green’s function \(G_{3}\) in Eq. \((7)\) is approximated as

\[
\int dK |K| \langle \phi_{b} | (\beta + K^{2}/(2m_{ad})) | \phi_{r} \rangle,
\]

where \(|K| \langle \phi_{b} | (\beta + K^{2}/(2m_{ad})) | \phi_{r} \rangle\) is the eigenstate of the relative momentum between atom 3 and the center-of-mass of atoms 1 and 2.

As a result, the wave function for relative motion between atoms 1 and 2 is forced in the bound state. With this approximation, process i) is fully taken into account, while process ii) is neglected, and the entire series of Eq. \((7)\) can be fully summed \(\sum_{i}\).

The result of \(a_{ad}\) from the single-pole approximation is shown as the black dash line in Fig. 1 for \(^{6}\)Li-\(^{6}\)Li mixture, which has the same qualitative behavior as the exact three-body calculation and also gives a large deviation from the mean-field value \(a_{ad}^{0}\). This suggests that processes of type i) is an important process which significantly reduces \(a_{ad}\) from \(a_{ad}^{0}\). This also inspires that in a more accurate many-body theory, it is necessary to include the ladder diagram to describe repeated scattering between fermion pairs and bosons. It is reminiscent of the ladder diagram between fermion pairs that reduces dimer-dimer scattering length significantly below its mean-field value on the BEC side of the Feshbach resonance\(\text{\textcopyright}\).

**Effect of van der Waals Potential.** To investigate the effect of van der Waals potential, we implement the separable potential proposed in Ref. \[\text{\textcopyright}\]. In this method, the interaction potential is modeled as \(V = \xi |\chi| \langle \chi \rangle\), which is designed to reproduce not only the zero-energy scattering length \(a_{s}\) but also the zero-energy wave function \(u(|r|)\) in a van der Waals potential \(-\alpha/|r|^{6}\). To meet this requirement, \(|\chi\rangle\) and \(\xi\) should be chosen as

\[
|\chi\rangle = (2\pi)^{-3/2} \{ 1 - q \int_{0}^{\infty} dq [1 - \frac{q}{\alpha} - u(q)] \sin(qr) \}^{1/2},
\]

\[
\xi = 4\pi \frac{1}{\alpha^{6}} - \frac{2}{\pi} \int_{0}^{\infty} dq |\langle q |\chi\rangle|^{2} - 1,
\]

respectively \(\text{\textcopyright}\). This separable potential naturally includes the length scale of the van der Waals length \(R_{vdW} = 1/2(\alpha/\hbar^{2})^{3/4}\)
through wave function $u(r)$. Besides, the three-body calculation with this potential does not require extra three-body parameters. Indeed, Ref. [34] used this model to show the three-body parameter depends on the van der Waals length universally. Here we use this separable potential, and following the same stratagem from Eq. [5] and Eq. [6], we calculate $a_{ad}$. Notice that in $^6$Li-$^7$Li mixture, $R_{ad}F$ between $^6$Li and $^7$Li is only slightly different from that between two spin components of $^6$Li [35,36]. The result of $a_{ad}$ from this separable potential is also shown in Fig. 1. We find that in the regime of our interests, the correction is visible but not significant.

Experimental Predictions. With three-body calculation of $a_{ad}$, we can provide a correction to the mean-field interaction energy between Bose and Fermi superfluids on the BEC side of the fermionic Feshbach resonance. This interaction energy has been extracted from a measurement of collective mode frequency shift in the underlying system[6], where the condensate of bosonic atoms with smaller particle number is embedded in a larger cloud of Fermi superfluid. So the effective trapping potential experienced by bosons should include contributions from both the harmonic trap $V(r) = (1/2)m\omega_r^2 r^2$ and the interaction energy between Bose and Fermi superfluids, leading to $V_{ef}(r) = V(r) + 2\pi\hbar^2 a_{ad}n_d(r)/m_{ad}$ on the BEC side of the Feshbach resonance. Here, since the number of fermions is much larger than that of bosons, we can safely assume that the fermion density distribution (i.e. dimer density distribution $n_d$) will not be affected by bosons and is solely determined by the equation of state of Fermi superfluid. Such an equation of state has been obtained quite accurately in previous experiment [39]. With local density approximation, we have $n_d(r) = n_d|mu - V(r)|$, where we have used the fact that $^6$Li and $^7$Li experience almost identical trapping potentials. Thus, for the dipole oscillation of bosons, its frequency $\omega_b$ will be shifted away from $\omega_b$, and the shift $\delta\omega_b = \omega_b - \omega_b$ is given by [6]

$$\frac{\delta\omega_b}{\omega_b} = \frac{\pi\hbar^2 a_{ad}}{m_{ad}} \left( \frac{dn_d}{d\mu} \right)_{r=0}. \quad (9)$$

In Ref. [6], this collective frequency has been measured in the unitary regime (with $1/(k_F a_f) < 1$), and fitted with a mean-field theory by replacing $a_{ad}$ with $a_{ad}^0$ in Eq. [6]. The experimental data points and the mean-field fitting are shown in Fig. 3. However, in this regime, the size of dimers is even larger than the inter-particle distance and the system can not be viewed as a boson-dimer mixture. Our expression of Eq. [9] should be applied to the regime with $1/(k_F a_f) > 1$, where the results for $\delta\omega_b/\omega_b$ with both zero-range and separable potential is shown in Fig. 3 and compared with mean-field prediction. Future experiments can perform more accurate measurements of frequency shift in the BEC regime, the difference between our result and the mean-field result can be distinguished.

FIG. 3: (color online) Frequency shift of dipole oscillation $\delta\omega_b$ for bosonic $^7$Li atoms as a function of $1/(k_F a_f)$. Dots with error bar are experimental data [6]. Blue dash line is prediction from mean-field theory. Red solid line is prediction based on $a_{ad}$ calculated with zero-range model, and black dash-dotted line is prediction based on $a_{ad}$ from separable potential including van der Waals effect. Here we have chosen $k_F = 4.6 \times 10^6 m^{-1}$. Other parameters take the same values as in Fig. 1.

In summary, our work studies the interaction energy between Bose and Fermi superfluids on the BEC side of the fermionic Feshbach resonance. Our result provides a striking example where mean-field theory can be qualitatively inaccurate even for quite weak interaction strength, and suggests a route to improve many-body theory in this system. This result can be easily verified in current experimental setup.

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SUPPLEMENTARY MATERIAL

In this supplementary material we introduce the Skorniakov–Ter-Martirosian (STM) equation and the single-pole approximation used in our manuscript.

I. STM EQUATIONS

In this section we show our STM-equation approach for the calculation of atom-dimer scattering length $a_{\text{sd}}$. We will first introduce a function $a(K, \varepsilon)$, and then prove that such a function satisfies the relation

$$\lim_{\varepsilon \to 0^+} a(0, \varepsilon) = a_{\text{sd}}.$$  \hspace{1cm} (10)

Namely, one can obtain $a_{\text{sd}}$ directly from $a(K, \varepsilon)$. At last we will derive the equation for $a(K, \varepsilon)$ with is called the STM equation for our system.

A. Function $a(K, \varepsilon)$

As shown in the main text, our system includes two fermionic atoms (labeled by 1 and 2) with same mass and different spins, and one bosonic atom (labeled by 3). In the following we use $|\cdot\rangle$ to denote the total quantum state of the relative motion of these three atoms, $|\cdot\rangle_{ij}$ for the state of the relative motion between atoms $i$ and $j$, and $|\cdot\rangle_{i,jk}$ for the state of the relative motion between the atom $i$ and the center-of-mass of atoms $j$ and $k$. We further denote the...
mass of the fermionic atom and bosonic atom as \( m_f \) and \( m_b \), respectively. In our calculation we use the natural unit \( \hbar = m_f = 1 \). We model the two-body interaction with Huang-Yang pseudo potential, i.e., the interaction operator \( V_{ij} \) for the atoms \( i \) and \( j \) satisfies

\[
 i_j \langle \mathbf{r} | V_{ij} | \Psi \rangle = \frac{2 \pi a_{ij}}{m_{ij}} \delta(\mathbf{r}) \left[ \frac{\partial}{\partial \mathbf{r}} \cdot (|\mathbf{r} \rangle \times i_j \langle \mathbf{r} | \Psi \rangle) \right], \tag{11}
\]

where \( |\mathbf{r} \rangle_{ij} \) is the eigenstate of the relative position between atoms \( i \) and \( j \) with eigenvalue \( \mathbf{r} \), \( m_{ij} \) and \( a_{ij} \) are the reduced mass and scattering length of these two atoms, respectively. As shown in the main text, here we assume \( a_{12} = a_f \) and \( a_{31} = a_{23} = a_{bf} \).

To introduce the function \( a(\mathbf{K}, \varepsilon) \), we first define state \( |\psi_3(\varepsilon)\rangle_{3-12} \) via the relation

\[
 |\psi_3(\varepsilon)\rangle_{3-12} = \delta(\mathbf{r}) |\psi_3(\varepsilon)\rangle_{3-12}, \tag{12}
\]

where \( |\Psi_+(\varepsilon)\rangle \) is defined as

\[
 |\Psi_+(\varepsilon)\rangle = \frac{i \varepsilon}{-a_f^{-2} + i \varepsilon - (T + V_{12} + V_{23} + V_{31})} |\Psi_{in}\rangle, \tag{13}
\]

with \( T \) the kinetic energy of the relative motion of these three atoms and \( |\Psi_{in}\rangle \) the incident state of the atom-dimer scattering process, as defined in the main text. We further define function \( \eta(\mathbf{K}, \varepsilon) \) as

\[
 \eta(\mathbf{K}, \varepsilon) = 3-12 \langle \mathbf{K} | \psi_3(\varepsilon) \rangle_{3-12}. \tag{14}
\]

With aid of Eqs. (12), (13) and (14), we can define the function \( a(\mathbf{K}, \varepsilon) \) via the equation

\[
 \eta(\mathbf{K}, \varepsilon) = \frac{\sqrt{2}}{\pi^{3/2} a_f^{1/2}} \left[ 2 \pi^2 \delta(\mathbf{K}) + \frac{a(\mathbf{K}, \varepsilon)}{\left( \frac{4M}{4M+2} \right)} i \varepsilon - K^2 \right], \tag{15}
\]

where \( M = m_b/m_f \) and \( |\mathbf{K}\rangle_{k-ij} \) is the eigenstate of the relative momentum between atom \( k \) and the center-of-mass of atoms \( i \) and \( j \), with eigenvalue \( \mathbf{K} \).

### B. Relation between \( a(\mathbf{K}, \varepsilon) \) and \( a_{ad} \)

Now we prove the relation of Eq. (10) which links the function \( a(\mathbf{K}, \varepsilon) \) defined in Eq. (15) with the atom-dimer scattering length \( a_{ad} \). To this end we re-write Eq. (13) as

\[
 |\Psi_+(\varepsilon)\rangle = |\Psi_{in}\rangle + G_3(\varepsilon)(V_{23} + V_{31}) |\Psi_+(\varepsilon)\rangle, \tag{16}
\]

where \( G_3(\varepsilon) = [-a_f^{-2} + i \varepsilon - (T + V_{12})^{-1} \right] \) is the Green’s operator for the free bosonic atom together with the two interacting fermionic atoms taking the form

\[
 G_3(\varepsilon) = \int d\mathbf{K} |\mathbf{K}\rangle_{3-12} \langle \mathbf{K} \otimes |\phi_b\rangle_{12} \langle \phi_b| + \int d\mathbf{K} d\mathbf{k} |\mathbf{K}\rangle_{3-12} \langle \mathbf{K} \otimes |\mathbf{k}+\rangle_{12} \langle \mathbf{k}+| \right] \left( \frac{\varepsilon}{\varepsilon - \frac{a_f^{-2} + i \varepsilon - \left( \frac{M+2}{4M} \right) K^2}{K^2 - \mathbf{k}^2} \right). \tag{17}
\]

Here \( |\mathbf{k}+\rangle_{12} \) is the scattering state of the relative motion between atoms 1 and 2 with incident momentum \( \mathbf{k} \), and \( |\phi_b\rangle_{12} \) is the bound state of these two atoms, as defined in our main text. By writing down Eq. (17), we have used the fact that \( T = p_{12}^2 + \left( \frac{M+2}{4M} \right) p_{3-12}^2 \), where \( p_{12} \) is the relative momentum operator between atoms 1 and 2, and \( p_{3-12} \) is the relative momentum operator of atom 3 and the center-of-mass of atoms 1 and 2. We have also used the eigen equations

\[
 (p_{12}^2 + V_{12}) |\phi_b\rangle_{12} = -\frac{1}{a_f} |\phi_b\rangle, \tag{18}
\]

\[
 (p_{12}^2 + V_{12}) |\mathbf{k}+\rangle_{12} = \mathbf{k}^2 |\mathbf{k}+\rangle \tag{19}
\]

satisfied by \( |\mathbf{k}+\rangle_{12} \) and \( |\phi_b\rangle_{12} \).
Now we are at the stage to calculate $\eta(K, \varepsilon)$. According to Eqs. (11) and (12), we have

$$\eta(K, \varepsilon) = 4\pi a_t \left\{ \frac{\partial}{\partial |r|} [ |r| \times 12 \langle r | (3-12(K)|\Psi_+(\varepsilon)) ] \right\}_{r=0}. \tag{20}$$

Substituting Eqs. (16) and (17) into Eq. (20), and using the results in two-body problems

$$
\begin{align*}
12 \langle r | \phi_b \rangle_{12} &= \frac{1}{\sqrt{2\pi a_t}} e^{-|r|/a_t}; \\
12 \langle r | k+ \rangle_{12} &= \frac{1}{(2\pi)^{3/2}} \left[ e^{ik-r} + \frac{1}{|i|\varepsilon + \frac{1}{a_t}} \right] e^{i|k||r|},
\end{align*}
$$

as well as the fact that $|\Psi_m\rangle = |\phi_b\rangle_{12}|0\rangle_{3-12}$ with $|0\rangle_{3-12}$ the eigenstate of $P_{3-12}$ with eigenvalue zero, we obtain

$$\eta(K, \varepsilon) = \frac{-2\sqrt{2\pi}}{\sqrt{a_t}} \int dK \frac{i a_t}{M+2} \left[ \langle k+ | (3-12(K)|V_{23} + V_{31})|\Psi_+(\varepsilon) \rangle \right] k^2 - K^2 - \frac{1}{\varepsilon - \left( \frac{M+2}{4M} \right) K^2 - k^2}. \tag{23}$$

Comparing Eq. (23) with the definition of $a(K, \varepsilon)$ Eq. (15), we find that $a(K, \varepsilon)$ can be re-expressed as

$$a(K, \varepsilon) = \left( \frac{8M\pi^2}{M+2} \right) \int dK \frac{i a_t^3/2}{M+2} \left[ \langle k+ | (3-12(K)|V_{23} + V_{31})|\Psi_+(\varepsilon) \rangle \right] \left( \frac{1}{\varepsilon - \frac{M+2}{4M} K^2 - k^2} \right). \tag{24}$$

When $K = 0$, in the limit $\varepsilon \to 0^+$ the right-hand side of Eq. (24) becomes zero. Therefore, we have

$$\lim_{\varepsilon \to 0^+} a(0, \varepsilon) = \left( \frac{8M\pi^2}{M+2} \right) \lim_{\varepsilon \to 0^+} \int dK \frac{i a_t^3/2}{M+2} \left[ \langle k+ | (3-12(K)|V_{23} + V_{31})|\Psi_+(\varepsilon) \rangle \right]. \tag{26}$$

On the other hand, according to Eqs. (5) and (6) in our main text, the atom-dimer scattering length $a_{ad}$ is given by

$$a_{ad} = \lim_{\varepsilon \to 0^+} \left( \frac{8M\pi^2}{M+2} \right) \int dK \frac{i a_t^3/2}{M+2} \left[ \langle k+ | (3-12(K)|V_{23} + V_{31})|\Psi_+(\varepsilon) \rangle \right]. \tag{27}$$

Here we have used the fact that in our natural unit with $m_t = 1$, the atom-dimer reduced mass is $2M/(M+2)$. With Eq. (27), we can re-write Eq. (26) as $\lim_{\varepsilon \to 0^+} a(0, \varepsilon) = a_{ad}$. That is the relation in Eq. (10).

C. STM equations

In the previous section, we show that the atom-dimer scattering length $a_{ad}$ can be obtained directly from the function $a(K, \varepsilon)$. Now we derive the equation for the function $a(K, \varepsilon)$, i.e., the STM equation. To this end, we first define states $|\psi_1(\varepsilon)\rangle_{1-23}$ and $|\psi_2(\varepsilon)\rangle_{2-31}$ via relations

$$
\begin{align*}
23 \langle r | V_{23} | \Psi_+(\varepsilon) \rangle &= \delta(r) |\psi_1(\varepsilon)\rangle_{1-23}, \tag{28} \\
31 \langle r | V_{31} | \Psi_+(\varepsilon) \rangle &= \delta(r) |\psi_2(\varepsilon)\rangle_{2-31}. \tag{29}
\end{align*}
$$

In our system, since atoms 1 and 2 has the same mass and scattering length with atom 3, it is easy to prove that $1-23 \langle K | \psi_1(\varepsilon) \rangle_{1-23} = 2-31 \langle K | \psi_2(\varepsilon) \rangle_{2-31}$. We further define the function $\zeta(K, \varepsilon)$ as

$$\zeta(K, \varepsilon) = -\left( \frac{2\pi^2}{\sqrt{a_t}} \right) \left( 2-31 \langle K | \psi_2(\varepsilon) \rangle_{2-31} \right). \tag{30}$$
As we have outlined in the previous section, it is easy to prove that

\[
\zeta(K, \epsilon) = -(2\pi)^{\frac{3}{2}} \frac{1}{a T} \alpha_{bf} \left\{ \frac{\partial}{\partial |r|} \left[ |r| \times 23 (r \cdot (1-23(K|\Psi_+|\epsilon))) \right] \right\}_{r=0}
\]

\[
= -(2\pi)^{\frac{3}{2}} \frac{1}{a T} \alpha_{bf} \left\{ \frac{\partial}{\partial |r|} \left[ |r| \times 31 (r \cdot (2-31(K|\Psi_+|\epsilon))) \right] \right\}_{r=0}
\]

by using Eqs. (11), (28), (29) and (30).

Now we rewrite Eq. (13) as

|\Psi_+|\epsilon) = i\epsilon G_0(\epsilon)|\Psi_in\rangle + G_0(\epsilon)(V_{12} + V_{23} + V_{31})|\Psi_+|\epsilon),

where

\[
G_0(\epsilon) = \frac{1}{-a T^2 + i\epsilon - T} = \int dK dK' \frac{|k|_{ij}}{-a T^2 + i\epsilon - |k|^2 + (\frac{M + 2}{4M}) K^2}],
\]

with |k|_{ij} the eigenstate of p_{ij} with eigenvalue k and K = |K|. Here (i, j, k) can take values (1, 2, 3), (2, 3, 1) or (3, 1, 2). Substituting Eq. (33) into Eq. (20), and using Eqs. (30), (31) and (32), we obtain

\[
\left( \frac{1}{a T} - \sqrt{\left( \frac{M + 2}{4M} \right) K^2 + \frac{1}{a T^2} - i\epsilon} \right) \eta(K, \epsilon) = \int \frac{dK'}{2\pi a T} \sqrt{\left( \frac{M + 1}{2M} \right) K^2 + K'^2 + K \cdot K' + \frac{1}{a T^2} - i\epsilon} \zeta(K', \epsilon)
\]

\[
+ \frac{2\sqrt{2\pi}}{a T} \left( \frac{1}{a T} - \sqrt{\frac{1}{a T^2} - i\epsilon} \right) \delta(K) = 0.
\]

Here we have used the relations

\[
\frac{1}{12} |r|_{22}^3 = \int dK' \frac{\zeta(K', \epsilon)}{(2\pi)^3} \eta(K, \epsilon) = \int \frac{dK'}{2\pi a T} \sqrt{\left( \frac{M + 1}{2M} \right) K^2 + K'^2 + K \cdot K' + \frac{1}{a T^2} - i\epsilon} \zeta(K', \epsilon)
\]

\[
+ \frac{1}{\pi} \sqrt{\frac{1}{a T^2}} \left( |k|^2 + \frac{1}{a T^2} \right).
\]

Substituting Eq. (15) into Eq. (35), we obtain

\[
\frac{1}{a T} + \sqrt{\left( \frac{M + 2}{4M} \right) K^2 + \frac{1}{a T^2} - i\epsilon} + \int \frac{dK'}{(2\pi)^3} \sqrt{\left( \frac{M + 1}{2M} \right) K^2 + K'^2 + K \cdot K' + \frac{1}{a T^2} - i\epsilon} \zeta(K', \epsilon) = 0.
\]

On the other hand, substituting Eq. (33) into Eq. (31) and using similar techniques as above, we obtain

\[
\left[ \frac{1}{a T^2} - \sqrt{2M(M + 1)} \left( \frac{M + 2}{2(M + 1)} K^2 + \frac{1}{a T^2} - i\epsilon \right) \right] \zeta(K, \epsilon) + \frac{(M + 1)}{(2\pi)^2 M} \int \frac{dK'}{(2\pi)^3} \sqrt{\left( \frac{M + 1}{2M} \right) K^2 + K'^2 + K \cdot K' + \frac{1}{a T^2} - i\epsilon}
\]

\[
- \frac{2\pi(M + 1)}{M} \int \frac{dK'}{(2\pi)^3} \sqrt{K'^2 - 4 \frac{M+1}{M+2} \epsilon} \left( \frac{M + 1}{2M} K^2 + K \cdot K' + \frac{1}{a T^2} - i\epsilon \right)
\]

\[
+ \frac{2\pi(M + 1)}{M} \frac{2\pi(M + 1)i\epsilon}{M} - \frac{2\pi(M + 1)i\epsilon}{M} \left( K^2 + \frac{1}{a T^2} - i\epsilon \right) = 0.
\]
Equations \((38)\) and \((39)\) are the integral equations satisfied by \(a(K, \varepsilon)\) and \(\zeta(K, \varepsilon)\). We can further express \(a(K, \varepsilon)\) and \(\zeta(K, \varepsilon)\) as \(a(K, \varepsilon) = \sum_{l,m} a_{l,m}(K, \varepsilon) Y_l^m(K)\) and \(\zeta(K, \varepsilon) = \sum_{l,m} \zeta_{l,m}(K, \varepsilon) Y_l^m(K)\), where \(K\) is the unit vector along the direction of \(K\), and \(Y_l^m\) is the spherical harmonic with degree \(l\) and order \(m\). Then we can obtain equations of \(a_{l,m}(K, \varepsilon)\) and \(\zeta_{l,m}(K, \varepsilon)\). It is easy to prove that the equations for different values of \((l, m)\) are decoupled with each other. Furthermore, the inhomogeneous term only appears in equations for \(a_{0,0}(K, \varepsilon)\) and \(\zeta_{0,0}(K, \varepsilon)\). As a result, we have \(a_{l,m}(K, \varepsilon) = \zeta_{l,m}(K, \varepsilon) = 0\) for \(l > 0\). Therefore, the solution of Eqs. \((38)\) and \((39)\) is independent on the direction of \(K\), and thus can be expressed as

\[
a(K, \varepsilon) = a(K, \varepsilon), \quad \zeta(K, \varepsilon) = \zeta(K, \varepsilon).
\]

Using this result, Eqs. \((38)\) and \((39)\) can be simplified as

\[
\frac{M''}{M} a(K, \varepsilon) + \frac{1}{\pi^2} \int dK' K' \ln \left[ \frac{M'}{2\pi} K^2 - K' K + \frac{\gamma_K}{M'} \right] \zeta(K', \varepsilon) = 0;
\]

\[
\left[ \frac{1}{\alpha_{bf}} - \sqrt{\frac{2M''}{M'}} \frac{M'' K^2}{2M'} + \frac{1}{\alpha_{f}} - i\varepsilon \right] \zeta(K, \varepsilon) - \frac{2M'}{M} \int dK' K' \ln \left[ \frac{M'' K^2}{2M'} + K' K + \frac{\gamma_K}{M'} \right] a(K', \varepsilon) + \frac{M'}{2\pi} \int dK' K' \ln \left[ \frac{M''(K^2 + K'^2)}{2M'} + \frac{1}{\alpha_{f}} - i\varepsilon \right] \zeta(K', \varepsilon) = \frac{2\pi M'}{M} \left[ \frac{i\varepsilon}{\gamma_K(\gamma_K + i\varepsilon)} - \frac{1}{\gamma_K} \right],
\]

with \(M' = M + 2\), \(M'' = M + 2\) and \(\gamma_K = K^2 + a_{f}^2 - i\varepsilon\).

Equations \((41)\) and \((42)\) are the STM equations in our system. As shown in the main text, in our problem the 3-body boundary condition in the region where all the three atoms are close with each other is necessary. Such condition is provided by the momentum cut-off \(\Lambda_{\text{c}}\) in the integrations in the left-hand side of Eqs. \((41)\) and \((42)\). We then numerically solve these two equations and obtain the atom-dimer scattering length via relation Eq. \((10)\).

### II. SINGLE-POLE APPROXIMATION

In this section we show our calculation of atom-dimer scattering length with single-pole approximation. As we have discussed before, the atom-dimer scattering length is given by Eq. \((27)\):

\[
a_{\text{ad}} = \lim_{\varepsilon \to 0^+} \frac{8M^2\pi^2}{M + 2} \langle 31-12 | \phi_0 | 31-12 \rangle |V_{23} + V_{31}| \Psi_+ (\varepsilon),
\]

with \(\Psi_+ (\varepsilon)\) given by Eq. \((16)\):

\[
|\Psi_+ (\varepsilon)\rangle = |\Psi_{1a}\rangle + G_3 (\varepsilon) (V_{23} + V_{31}) |\Psi_+ (\varepsilon)\rangle.
\]

Here the Green’s function \(G_3 (\varepsilon)\) is defined in Eq. \((17)\), and the states and operators are defined as before.

As shown in main text, in the single-pole approximation, we have

\[
G_3 (\varepsilon) \approx \int dK |K|_{31-12} |K| \otimes |\phi_0|_{12} |\phi_0|, \frac{i\varepsilon}{\gamma_K(\gamma_K + i\varepsilon)} - \frac{1}{\gamma_K}.
\]

Substituting Eq. \((45)\) into Eq. \((44)\), we find that under the single-pole approximation there is

\[
|\Psi_+ (\varepsilon)\rangle = |\phi_0|_{12} |\psi\rangle_{3-12},
\]

where \(|\psi\rangle_{3-12}\) satisfies the relation

\[
3-12 \langle K | \psi \rangle_{3-12} = \delta (K) + \frac{T(K, \varepsilon)}{i\varepsilon - \left( \frac{M + 2}{4M} \right) K^2},
\]

with

\[
T(K, \varepsilon) = \int dK' \langle 3-12 | K_{12} (\phi_0 | V_{23} + V_{31} | \Psi_+ (\varepsilon))
\]

\[
= \int dK' [3-12 (\phi_0 | (V_{23} + V_{31}) | \phi_0)_{12} | K' \rangle_{3-12} \times (3-12 (K' | \psi \rangle_{3-12})].
\]
According to Eqs. (43) and (47), we have

\[ a_{ad} = \lim_{\varepsilon \to 0^+} \left( \frac{8M\pi^2}{M+2} \right) T(0, \varepsilon). \]  

(49)

On the other hand, substituting Eq. (48) into Eq. (46), we can obtain the integral equation for \( 3 - 12 \langle K|\psi\rangle_{3-12} \), from which an integral equation for \( T(K, \varepsilon) \) can be derived. Using the similar analysis as in the paragraph before Eq. (40), we can find that the solution of such an equation is independent on the direction of \( K \), i.e., we have \( T(K, \varepsilon) = T(K, \varepsilon) \), and the integral equation can be simplified as

\[ T(K, \varepsilon) + \frac{8(M+1)a_{bf}}{(M+2)\pi^2a_f} \int dK' \mathcal{F}(K, K', \varepsilon) T(K', \varepsilon) = \frac{(M+1)a_{bf}}{M\pi^3a_f} \int_0^\infty \frac{k'dk'}{K(k'^2 + a_f^{-2} - i\varepsilon)} \log \left[ \frac{4 + a_f^2(K + 2k'^2 - 4i\varepsilon)}{4 + a_f^2(K - 2k'^2 - 4i\varepsilon)} \right]. \]  

(50)

where

\[ \mathcal{F}(K, K', \varepsilon) = \int_{-1}^1 du \int_0^\infty dk' \frac{k'}{\sqrt{K^2 - 2uKK' + K'^2(k'^2 + a_f^{-2} - i\varepsilon)}} \log \left[ \frac{4 + a_f^2(\sqrt{K^2 - 2uKK'} + K'^2 + 2k'^2 - 4i\varepsilon)}{4 + a_f^2(\sqrt{K^2 - 2uKK'} - K'^2 - 2k'^2 - 4i\varepsilon)} \right]. \]  

(51)

By numerically solving Eq. (50), we obtain the atom-dimer scattering length via Eq. (49) under the single-pole approximation.

[1] P. Naidon, and M. Ueda, Comptes Rendus Physique 12, 13 (2011).