Stable Heteronuclear Few-Atom Bound States in Mixed Dimensions

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We study few-body problems in mixed dimensions with \( N \geq 2 \) heavy atoms trapped individually in parallel one-dimensional tubes or two-dimensional disks, and a single light atom travels freely in three dimensions. By using the Born-Oppenheimer approximation, we find three- and four-body bound states for a broad region of heavy-light atom scattering length combinations. Specifically, the existence of trimer and tetramer states persist to negative scattering lengths regime, where no two-body bound state is present. These few-body bound states are analogous to the Efimov states in three dimensions, but are stable against three-body recombination due to geometric separation. In addition, we find that the binding energy of the ground trimer and tetramer state reaches its maximum value when the scattering lengths are comparable to the separation between the low-dimensional traps. This resonant behavior is a unique feature for the few-body bound states in mixed dimensions.

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I. INTRODUCTION

One striking feature of few-body physics is the presence of universality under a resonant short-range interaction, where the low-energy behavior of the system does not depend on the details of its structure or interactions at short distances. Of particular interest is the existence of bound trimer states for three identical bosons in three dimensions with a resonant two-body interaction, as discussed in 1970 by Vitaly Efimov. At infinite scattering length, these three-body bound states form an infinite geometric spectrum with a constant ratio between two successive binding energies, indicating a discrete scaling symmetry. Besides, the bound trimer states persist rather counterintuitively to negative scattering length regime, where two-body bound states are not existent. After its original proposal, the Efimov physics has attracted great attention in multi-disciplinary systems, including atomic nuclei, \(^4\)He trimers, and other molecules. However, a direct evidence of such peculiar behavior was not achieved for more than three decades until its first observation in an ultracold gas of neutral atoms. Thanks to the extraordinary controllability of the mutual atomic interaction by tuning through a magnetic Feshbach resonance, signatures of trimer bound states have been observed in trapped atomic gases for both negative and positive scattering length regimes.

In addition to the original problem of identical bosons, the study of three-body physics has been extended to a variety of other three-particle systems, including three distinguishable particles with different scattering lengths and/or different masses, \(^3\)He trimers, \(^6\)He atoms, and the three-atom systems with with non-zero angular momentum. Of particular interest is the case of three distinguishable fermions in an ultracold gas of three-component \(^6\)Li atoms. In such a system, there exits a broad magnetic Feshbach resonance such that all three scattering lengths can be tuned around resonance simultaneously, leading to a promising candidate to observe the few-body universal behavior. Besides, the few-body problem has also been analyzed in ultracold gases of different atomic species by tuning the interaction across an interspecies Feshbach resonance.

Due to the multi-channel nature of the inter-atomic interaction, the Efimov states in the three-dimensional (3D) ultracold atomic gases are only metal-stable states. Through the three-body recombination process, two of the three atoms in an Efimov trimer can further form a deeply bound dimer and the third one would escape from the trap. In order to prepare stable trimer states, one has to figure out a mechanism to significantly reduce or even prevent three-body recombination. Since the three-body recombination process only occurs when three atoms all come to a close range, one possible route towards this goal is to use geometric confinement to separate atoms such that they can not travel to a same spot. For instance, if two of the three atoms are individually trapped in two spatially separated one-dimensional (1D) tubes or two-dimensional (2D) disks, and interact with each other via the third atom which is free in all three dimensions (3D), the three-body recombination is inherently forbidden and the trimer states are stable if they exist in this mixed dimensional configuration.

The few-body problem in mixed dimensions has been recently discussed by Nishida and Tan, where they consider two species of atoms confined in different dimensions and find trimer bound states for a certain range of mass ratio. However, since the atoms in lower dimensions are not geometrically separated, this configuration suffers the same problem of three-body recombination and the trimer states are unstable. Therefore, Nishida considers the problem of two atoms trapped in two separated 1D tubes or 2D layers, and interacts with the third atom...
which is free in 3D \( \mathbf{32, 36} \). This 1D-1D-3D or 2D-2D-3D mixture thus can support stable Efimov trimer states.

In this manuscript, we adopt another approach based on Born-Oppenheimer approximation (BOA) to study some few-body problems in mixed dimensions, and investigate the existence and properties of stable few-body bound states in a variety of configurations. For the three-body problems, we consider the systems with two heavy atoms trapped in two parallel 1D tubes (1D-1D-3D) or 2D disks (2D-2D-3D), plus one light atom moving freely in 3D (see Fig. 1 for illustration). We conclude that the light atom can induce an effective interaction between the two heavy atoms which are spatially separated by the low dimensional traps. Due to this effective interaction, the two heavy atoms can be bound with each other and lead to the formation of a three-body bound state in a very broad parameter region, including the regimes with negative s-wave scattering lengths between the light and the two heavy atoms, where two-body bound states are not present.

In addition to their existence in mixed dimensions, the universal three-body bound states also acquire some unique features due to the geometric confinement. Especially, we find that the two heavy atoms experience the strongest effective interaction when the scattering length between heavy and light atoms equals to the distance between the two low-dimensional traps. As a consequence of this resonance phenomenon, the binding energy of the ground trimer state takes a peak value around the resonance point, where the scattering length is of a finite value. We emphasis that, the BOA provides a very clear physical picture with which the new resonance phenomenon in the mixed-dimensional systems can be easily explored and clearly described.

We also compare our results with the exact expression \( \mathbf{32, 36} \) given by an effective field theory, and conclude that BOA works well even in systems with a mass ratio only about 6. This finding suggests that BOA is a powerful tool for the study of stable heteronuclear few-body bound states in mixed dimensions.

To demonstrate the usage of BOA for general few-body problems, we consider as an example the 1D-1D-3D geometry with three heavy atoms confined individually in parallel 1D tubes and a light atom in 3D free space. We find four-body bound states living in a wide range of scattering lengths. A similar resonance phenomenon is also observed when the scattering length becomes close to the mutual distances between 1D tubes, in which case the binding energy of the ground tetramer state takes largest value under the new resonance condition. Similar results of the 2D-2D-3D system are shown in Sec. IV. In Sec. V we extend the usage of BOA to the four-body problem in 1D-1D-1D-3D geometry, and discuss the existence and properties of bound tetramer states. In Sec. VI, we show the general scheme to apply BOA in problems with more than 3 atoms in arbitrary mixed dimensional geometries. Our main findings are concluded in Sec. VII, and the Bethe-Peierls boundary condition used in our BOA approach is derived in Appendix A.

**II. BOA FOR THREE-ATOM BOUND STATES IN 1D-1D-3D SYSTEMS**

In this section we present the Born-Oppenheimer approach for a three-body system with two heavy atoms individually trapped in two parallel 1D tubes and a light atom moving freely in the 3D space. The straightforward generalization to 2D-2D-3D systems will be given in Sec. IV, while the discussion for four-body problems in 1D-1D-1D-3D systems is given in Sec. V.

**A. System and Hamiltonian**

As shown in Fig. 1(a), the 1D-1D-3D system includes two heavy atoms \( A_1 \) and \( A_2 \), plus a light atom \( B \). The atoms \( A_1 \) and \( A_2 \) are trapped in two parallel 1D tubes centered along the lines \( x = \pm L/2, y = 0 \), while the light atom \( B \) moves freely in the 3D space. The quantum state of this system can be described by the wave function \( \Psi(\vec{r}_B; z_1, z_2) \), where \( z_1, z_2 \) are the \( z \)-coordinate of atoms \( A_{1,2} \) in the 1D tubes, and \( \vec{r}_B = (x_B, y_B, z_B) \) is the coordinate of atom \( B \) in 3D.

In this manuscript, we use the natural units \( \hbar = m_B = L = 1 \), where \( m_B \) is the mass of atom \( B \). The Hamiltonian for the motion of the three atoms is

\[
H = \frac{1}{2} \nabla^2_B - \frac{1}{2m_1} \frac{\partial^2}{\partial z_1^2} - \frac{1}{2m_2} \frac{\partial^2}{\partial z_2^2} + V_{1B} + V_{2B},
\]

where \( m_{1,2} \) are the masses of atoms \( A_{1,2} \) in the natural unit, and \( V_{1B,2B} \) are the interaction potentials between \( A_{1,2} \) and \( B \), respectively. In this work we only consider the cases where the distance \( L \) between the two tubes is much larger than the characteristic length of the interaction potential between \( A_1 \) and \( A_2 \). Hence the \( A_1-A_2 \) interaction can be safely ignored.
interaction potentials \( V \) and wave scattering lengths between boundary conditions

\[ t \text{he 3D motion of all the three atoms} \]

\[ \text{tice that the Bethe-Peierls boundary conditions (4) and} \]

\[ \text{Here} \ r \ A \atoms \]

\[ \text{dimensional scattering lengths between} \ A \]

\[ \text{with fixed values of} \]

\[ \text{tion of the eigen-equation of the Hamiltonian of atom} \]

\[ \text{bound state can be approximated as a factorized form} \]

\[ \text{Therefore, the total wave function} \ \Psi \text{of the three-body} \]

\[ \text{BOA for three-body bound states} \]

\[ \text{The three-body bound state is given by the solution of} \]

\[ H \Psi = E \Psi. \tag{2} \]

\[ \text{When the masses of the heavy atoms} \ A_{1,2} \text{is much larger} \]

\[ \text{than the one of} \ B, \text{or} \ m_{1,2} \gg 1 \text{in the natural unit, the} \]

\[ \text{eigen-equation (2) can be solved with BOA. This approxi-} \]

\[ \text{mation is applicable when the motion of the heavy atoms} \]

\[ \text{A}_{1,2} \text{is slow enough such that the quantum transitions} \]

\[ \text{between different instantaneous eigen-states of the light} \]

\[ \text{atom} \ B \text{with fixed positions} \ z_{1,2} \text{of} \ A_{1,2} \text{are negligible.} \]

\[ \text{Therefore, the total wave function} \ \Psi \text{of the three-body} \]

\[ \text{bound state can be approximated as a factorized form} \]

\[ \Psi(\vec{r}_B; z_1, z_2) = \phi(z_1, z_2)\psi(\vec{r}_B, z_1, z_2), \tag{3} \]

\[ \text{where} \ \psi(\vec{r}_B, z_1, z_2) \text{is an instantaneous bound-state solution} \]

\[ \text{of the eigen-equation of the Hamiltonian of atom} \ B \]

\[ \text{with fixed values of} \ z_1 \text{and} \ z_2. \]

\[ \text{As shown in Appendix A, we can further replace the} \]

\[ \text{interaction potentials} \ V_{1B} \text{and} \ V_{2B} \text{with the Bethe-Peierls} \]

\[ \text{boundary conditions} \]

\[ \psi(r_{1B} \to 0) \propto \left(1 - \frac{a_1}{r_{1B}}\right) + \mathcal{O}(r_{1B}); \tag{4} \]

\[ \psi(r_{2B} \to 0) \propto \left(1 - \frac{a_2}{r_{2B}}\right) + \mathcal{O}(r_{2B}). \tag{5} \]

\[ \text{Here} \ r_{1B,2B} \text{are the relative distances between the heavy} \]

\[ \text{atoms} \ A_{1,2} \text{and the light atom} \ B, \text{a}_1,2 \text{are the mixed-} \]

\[ \text{dimensional scattering lengths between} \ A_{1,2} \text{and} \ B. \text{No-} \]

\[ \text{tice that the Bethe-Peierls boundary conditions (4) and} \]

\[ \text{are derived from the first-principle calculation where} \]

\[ \text{the 3D motion of all the three atoms} \ A_{1,2} \text{and} \ B \text{are} \]

\[ \text{taken into account. Then the mixed-dimensional scat-} \]

\[ \text{tering lengths} \ a_{1,2} \text{are determined by both the 3D} \]

\[ \text{s-wave scattering lengths between} \ A_{1,2} \text{and} \ B, \text{as well as} \]

\[ \text{the intensity of the transverse confinements of the 1D} \]

\[ \text{traps. Thus,} \ a_{1,2} \text{can be tuned either through a 3D mag-} \]

\[ \text{netic Feshbach resonance [33] or via a mixed-dimensional} \]

\[ \text{confinement-induced resonance [31].} \]

\[ \text{With the Bethe-Peierls boundary conditions, the wave} \]

\[ \text{function} \ \psi(\vec{r}_B, z_1, z_2) \text{is determined by} \]

\[ -\frac{1}{2}\nabla_B^2 \psi(\vec{r}_B, z_1, z_2) = V_{\text{eff}}(z_1, z_2) \psi(\vec{r}_B, z_1, z_2), \tag{6} \]

\[ \text{through which the shape of the wave function} \]

\[ \psi(\vec{r}_B, z_1, z_2) \text{and the relevant eigen-energy} \ V_{\text{eff}}(z_1, z_2) \]

\[ \text{can be determined for a given value of} \ z_{1,2}. \]

\[ \text{In the approach of BOA, the instantaneous energy} \ V_{\text{eff}}(z_1, z_2) \]

\[ \text{of the light atom} \ B \text{serves as an effective potential between the two} \]

\[ \text{slowly moving heavy atoms. Then the wave function} \ \phi(z_1, z_2) \]

\[ \text{in Eq. (4) satisfies the Schrödinger equation} \]

\[ \left[ \frac{1}{2m_1} \frac{\partial^2}{\partial z_1^2} + \frac{1}{2m_2} \frac{\partial^2}{\partial z_2^2} + V_{\text{eff}}(z_1, z_2) \right] \phi(z_1, z_2) = E \phi(z_1, z_2), \tag{7} \]

\[ \text{where} \ E \text{is the total energy of the trimer state defined in} \]

\[ \text{Eq. (2). In this manuscript, we focus only on the} \]

\[ \text{ground state of the three-body eigen-equation (2), which is} \]

\[ \text{consisted of the ground-state solutions} \ \psi \text{and} \ \phi \text{of (4) and (7), respectively.} \]

\[ \text{In summary, to derive the three-body bound state with} \]

\[ \text{BOA, we should first find the ground-state solution} \ \psi \]

\[ \text{of the instantaneous eigen-equation (6) of the light atom} \]

\[ \text{B, and then solve the effective eigen-equation (7) of the} \]

\[ \text{heavy atoms} \ A_{1,2} \text{where the instantaneous eigen-energy} \]

\[ V_{\text{eff}}(z_1, z_2) \text{of} \ \psi \text{plays a role as interaction potential be-} \]

\[ \text{tween} \ A_1 \text{and} \ A_2. \text{Therefore, the BOA provides a simple and} \]

\[ \text{clear physical picture for the three-body problem, i.e., the} \]

\[ \text{light atom} \ B \text{induces an effective interaction between} \]

\[ \text{the two heavy atoms, which determines the prop-} \]

\[ \text{erties of the three-body bound state. With this picture, one} \]

\[ \text{can perform not only quantitative calculations but also} \]

\[ \text{qualitative discussions for the appearance and fea-} \]

\[ \text{tures of the trimer states when the potential function} \]

\[ V_{\text{eff}}(z_1, z_2) \text{is known from (6). This is a major advantage of} \]

\[ \text{the BOA approach.} \]

\[ \text{In the end of this subsection we emphasize that, since} \]

\[ \text{in BOA the transitions between different solutions of the} \]

\[ \text{instantaneous eigen-equation (6) is neglected, this app-} \]

\[ \text{proximation can only be used when the gap between} \]

\[ V_{\text{eff}}(z_1, z_2) \text{and other eigen-energies of (6) [with boundary} \]

\[ \text{conditions (4) and (5)] is large enough. In the cases where} \]

\[ V_{\text{eff}}(z_1, z_2) \text{is close to the lower bound of the continuous} \]

\[ \text{spectrum, the application of BOA may be questionable.} \]

\[ \text{C. Effective interaction between the two heavy} \]

\[ \text{atoms} \]

\[ \text{In the discussion above we outline the procedure for the} \]

\[ \text{derivation of the three-body bound states with BOA. In} \]

\[ \text{FIG. 1: (color online) (a) The 1D-1D-3D system with two} \]

\[ \text{heavy atoms} \ A_1 \text{and} \ A_2 \text{confined in two 1D tubes and the} \]

\[ \text{light atom} \ B \text{moving freely in 3D. (b) The 2D-2D-3D system} \]

\[ \text{with two heavy atoms} \ A_1 \text{and} \ A_2 \text{confined in two 2D planes} \]

\[ \text{and the light atom} \ B \text{moving freely in the 3D space.} \]
In this subsection we solve Eqs. (10) to calculate the instantaneous eigen-state $\psi(\vec{r}_B, z_1, z_2)$ of the light atom $B$, and the light-atom-induced effective potential $V_{\text{eff}}(z_1, z_2)$ between the two heavy atoms.

A straightforward calculation shows that the lowest ground state solution $\psi$ (up to a normalization factor) of Eq. (6) and the corresponding energy $V_{\text{eff}}(z_1, z_2)$ are given by

$$\psi(\vec{r}_B, z_1, z_2) = \frac{e^{-\kappa r_{1B}}}{r_{1B}} + \xi(r_{12}) \frac{e^{-\kappa r_{2B}}}{r_{2B}}, \quad V_{\text{eff}}(z_1, z_2) = -\frac{\kappa^2(r_{12})}{2},$$

where $r_{12} = \sqrt{1 + (z_1 - z_2)^2}$ is the distance between $A_1$ and $A_2$.

Substituting the expression of $\psi(\vec{r}_B, z_1, z_2)$ into the Bethe-Peierls boundary conditions (4) and (5), one can derive the values of $\kappa$ and $\xi$ in terms of the distance $(z_1 - z_2)$, and then obtain expressions for $\psi(\vec{r}_B, z_1, z_2)$ and $V_{\text{eff}}(z_1, z_2)$. Notice that, as a bound state, the wave function $\psi(\vec{r}_B, z_1, z_2)$ must approach zero in the limit $r_{1B} \to \infty$ or $r_{2B} \to \infty$. Therefore, the condition $\kappa > 0$ must be satisfied when we solve the equations of $\kappa$ and $\xi$.

According to Eq. (9), the effective potential $V_{\text{eff}}(z_1, z_2)$ is a function of distance $z_{12} = z_1 - z_2$ between the two heavy atoms along the axial direction of 1D tubes. Then the wave function $\phi(z_1, z_2)$ in the total wave function (8) is also a function of $z_{12}$, indicating the translational symmetry along the $z$-axis. From now on, we rewrite $V_{\text{eff}}(z_1, z_2)$ as $V_{\text{eff}}(z_{12})$, and $\phi(z_1, z_2)$ as $\phi(z_{12})$, and write Eq. (8) as

$$\left[-\frac{1}{2m_a} \frac{\partial^2}{\partial z_{12}^2} + V_{\text{eff}}(z_{12})\right] \phi(z_{12}) = E\phi(z_{12}), \quad (10)$$

where $m_a = m_1 m_2 / (m_1 + m_2)$ is the reduced mass of the two heavy atoms. From Eq. (10), we can see clearly that $V_{\text{eff}}$ serves as an effective interaction between the two heavy atoms $A_{1,2}$, and determines the existence and behavior of the three-body bound states. Next, we discuss the feature of $V_{\text{eff}}$ in different parameter regions.

1. $a_1 = a_2 = a > 0$

In this case the two heavy atoms $A_{1,2}$ have the same positive scattering length with the light atom $B$. Since $\psi$ is the ground-state solution of Eq. (6), a straightforward calculation shows that in this symmetric case we have $\xi = 1$ and $\kappa$ given by the equation

$$-\kappa + \frac{e^{-\kappa r_{12}}}{r_{12}} = \frac{1}{a}. \quad (11)$$

This equation can be solved analytically, leading to,

$$\kappa = \frac{1}{a} + \frac{W(e^{-r_{12}/a})}{r_{12}}, \quad (12)$$

where $W(z)$ is Lambert $W$ function or the principle root of equation $z = We^W$. Substituting the result (12) into Eq. (10), we finally obtain an analytic expression of the effective interaction between the two heavy atoms:

$$V_{\text{eff}}(z_{12}) = U(a; z_{12}) - \frac{1}{2a^2}, \quad (13)$$

where the regularized part $U(a; z_{12})$ is given by

$$U(a; z_{12}) = -\frac{1}{2} \frac{W(e^{-\sqrt{1+z_{12}^2}/a})^2}{1 + z_{12}^2}, \quad -\frac{1}{a} \frac{W(e^{-\sqrt{1+z_{12}^2}/a})}{\sqrt{1 + z_{12}^2}}, \quad (14)$$

which approaches zero in the limit $|z_{12}| \to \infty$. Therefore, the characters of bound states are essentially determined by the behavior of $U(a; z_{12})$.

With the knowledge of the $W$ function, we can easily find that when $a > 0$, $U(a; z_{12})$ is a pure symmetric potential well with

$$U(a; z_{12}) = U(a, -z_{12}) < 0. \quad (15)$$

In Fig. 2 we plot $U(a; z_{12})$ for a set of typical values of scattering lengths. It is clearly shown that $U(a; z_{12})$ provides a simple 1D potential well for the two heavy atoms. This behavior guarantees that there exists at least one bound-state solution $\phi$ of Eq. (10), and then the total system has at least one three-body bound state.

Intuitively speaking, one would expect that the atom-atom interaction effect be most significant when the scattering length takes infinite value. However, we find from Fig. 2 that the depth of the effective interaction $U(a; z_{12})$ takes a maximum value when $a = 1$ in our natural unit,
As a consequence, when the scattering length \( a \) takes a maximum value at \( a = 1 \), indicating a new resonance behavior for mixed dimensional systems.

This resonance effect can also be proved analytically with the character of the \( W \) function. For any given value of \( a \), the potential \( U (a, z_{12}) \) has only one minimum point, which is localized at the origin \( z_{12} = 0 \). Thus, the depth of the potential well takes the form

\[
D (a) \equiv - U (a, 0) = \frac{1}{2} W \left( e^{-1/a} \right)^2 + \frac{1}{a} W \left( e^{-1/a} \right). \tag{16}
\]

It is easy to show that \( D (a) \) takes the maximum value when \( a = 1 \). In Fig. 3 we plot the potential depth as a function of \( 1/a \), exhibiting the resonance signature at \( a = 1 \).

2. \( a_1 = a_2 = a < 0 \)

In this case, by substituting Eq. (8) into the Bethe-Peierls boundary conditions (4) and (5), we also get \( \xi = 1 \) and \( \kappa \) given by Eqs. (11) and (12) for \( r_{12} < |a| \). However, for \( r_{12} > |a| \), there is no positive solution of Eq. (11) for \( \kappa \). This suggests that the Schrödinger equation (8) with Bethe-Peierls boundary conditions (4) and (5) do not support any instantaneous bound state \( \psi \) of the light atom \( B \), and then one cannot derive any effective interaction for the two heavy atoms \( A_{1,2} \) within BOA. As a consequence, when the scattering length \( |a| < 1 \), there would be no three-body bound state since the condition \( r_{12} > |a| \) is satisfied with arbitrary 1D distance \( z_{12} \) between the two heavy atoms.

On the other hand, when \( |a| > 1 \), the BOA can give the effective interaction potential

\[
V_{\text{eff}} (z_{12}) = - \frac{1}{2} \left[ \frac{1}{a} + \frac{\sqrt{1 + z_{12}^2/a}}{\sqrt{1 + z_{12}^2}} \right]^2, \tag{17}
\]

provided that \( |z_{12}| < \sqrt{a^2 - 1} \) or \( r_{12} < |a| \). In the outer region of \( |z_{12}| > \sqrt{a^2 - 1} \), the potential takes zero value as \( V_{\text{eff}} (z_{12}) = 0 \). In Fig. 2 we also show \( V_{\text{eff}} (z_{12}) \) with negative scattering length.

We would like to emphasize that BOA can only be used when \( V_{\text{eff}} \) is well-separated from the continuous spectrum of the Schrödinger equation (9). This criteria is actually broken in the region \( r_{12} \sim |a| \) or \( z_{12} \sim \sqrt{a^2 - 1} \), where we have \( V_{\text{eff}} (r_{12}) \sim 0 \). Then the effective potential is not applicable in these regions. Fortunately, if the potential is deep enough, the ground-state wave function \( \phi \) of the heavy atoms \( A_{1,2} \) would be mainly localized in the region \( z_{12} \sim 0 \) or \( r_{12} \ll |a| \), where BOA is applicable. Thus, the ground-state wave function and its corresponding binding energy obtained from BOA is still reliable. Notice that in this negative scattering length regime, \( A_{1,2} \) and \( B \) cannot form any two-body bound state, hence the appearance of a three-body bound state is a non-trivial universal phenomenon.

3. \( 0 < a_1 < a_2 \) or \( a_2 < 0 < a_1 \)

Now we consider the general cases where the scattering lengths \( a_1 \) and \( a_2 \) are different. In these cases one can also derive the values of \( \xi \) and \( \kappa \) by substituting the expression (8) into the Bethe-Peierls boundary conditions (4) and (5). When \( 0 < a_1 < a_2 \) or \( a_2 < 0 < a_1 \), we know that in the limit \( r_{12} \to \infty \), that is the two heavy atoms are far away from each other, the instantaneous ground state of the light atom \( B \) is the two-body bound state of \( B \) and \( A_1 \). Considering the expression (8) of the instantaneous bound state, we have

\[
\xi (r_{12} \to \infty) = 0. \tag{18}
\]

With the help of this condition, we obtain the result

\[
\xi = - \Delta + \sqrt{\Delta^2 + 4e^{-2\kappa r_{12}/r_{12}^2}} / 2, \tag{19}
\]

where

\[
\Delta \equiv \frac{1}{a_1} - \frac{1}{a_2} > 0. \tag{20}
\]

Then the value of \( \kappa \) is given by

\[
- \kappa + \frac{- \Delta + \sqrt{\Delta^2 + 4e^{-2\kappa r_{12}/r_{12}^2}}}{2} = \frac{1}{a_1}. \tag{21}
\]

By solving Eqs. (19) and (21) numerically, we can obtain the values of \( \xi \) and \( \kappa \), and then the effective potential.
it is easy to show that $V_{\text{eff}} < 0$ for all values of $z_{12}$. Therefore, there is also at least one three-body bound state. When $a_2 < a_1$, although the atoms $A_1$ and $B$ can form a two-body bound state, there is no two-body bound state for $A_2$ and $B$. In this sense the existence of a three-body bound state is also a non-trivial phenomenon.

4. $a_1 < a_2 < 0$

In this case a straightforward calculation shows that the values of $\xi$ and $\kappa$ are also determined by Eqs. (19) and (21). Nevertheless, similar to the case of $a_1 = a_2 = a < 0$, there are also some regions where the instantaneous bound state $0$, there are also some regions where the instantaneous bound state $\psi$ does not exist. Specifically, we can define a critical distance $r_{12}^{*}$ as

$$r_{12}^{*} = 2 \left( \left( \Delta - 2 \frac{a}{a_1} \right)^2 - \Delta^2 \right)^{-1/2}$$

with $\Delta$ defined in (20). It is apparent that when $r_{12} > r_{12}^{*}$, we cannot find any real $\kappa$ which satisfies Eq. (21). In this sense, $r_{12}^{*}$ can be understood as the range of the effective interaction between $A_1$ and $A_2$. When this range is smaller than the distance between the two 1D tubes, i.e. $r_{12} < 1$, the two heavy atoms are always separated far enough such that the BOA does not give any effective mutual interaction. On the other hand, when $r_{12} > 1$ the effective potential of the two heavy atoms can be defined as

$$V_{\text{eff}} = \begin{cases} -\kappa^2/2; & 1 \leq r_{12} \leq r_{12}^{*} \\ 0; & r_{12} > r_{12}^{*} \end{cases}$$

This potential is also not reliable in the region $r_{12} \sim r_{12}^{*}$ where the condition for BOA is broken. However, as shown blow, this approach could lead to the existence of a bound state wave function $\psi$ which takes negligible value in this questionable region, such that the discussion within BOA remains valid. Since the negative scattering lengths do not support any two-body bound states, the existence of such a three-body bound state in this region is of great interest.

III. THREE-BODY UNIVERSAL BOUND STATES IN 1D-1D-3D SYSTEMS

In the previous section, we have obtained the instantaneous bound-state wave function $\psi$ of the light atom $B$ and the effective interaction potential $V_{\text{eff}}$ between the two heavy atoms. We have shown that $V_{\text{eff}}$ is most significant when the two-body scattering length is resonant with the distance between the two 1D tubes. In this section we derive the wave functions and binding energies of the relevant three-body bound states, and further confirm the observation of this new resonance effect.

In Fig. 4 the binding energy $E_{3b}$ of the ground trimer state is plotted as a function of $1/a_1$ and $1/a_2$ with heavy-atom reduced masses $m_a = 3.33$ and 9.5 in the natural unit. These values correspond to the cases of $(A_1 = A_2 = ^{40}\text{K}, \ B = ^{6}\text{Li})$ and $(A_1 = A_2 = ^{133}\text{Cs}, \ B = ^{7}\text{Li})$, respectively. Here, the binding energy $E_{3b}$ is defined as the energy gap between the three-body ground state $E$ and the threshold of the effective interaction, i.e.

$$E_{3b} = V_{\text{eff}}(\infty) - E. \ (24)$$

From Fig. 4 we notice that a three-body bound state exists for a wide range of positive and negative scattering length combinations, as discussed in the previous section. Nevertheless, the binding energy reaches a peak value when the two scattering lengths $a_1$ and $a_2$ are close with each other, especially in the region around $a_1 \sim a_2 \sim 1$. This observation is consistent with the expectation outlined in the previous section, which shows that when $a_1 = a_2 = a$, the effective potential well for $A_1 - A_2$ interaction is deepest as the scattering lengths are resonant with the distance between the two 1D tubes $a = 1$. 
FIG. 6: (color online) The binding energy $E_{3b}$ of the ground trimer state as a function of the reduced mass $m_*$ with $a_1 = a_2 = a = 1$ (blue solid line with open triangle) and $a_1 = a_2 = a = \infty$. In Fig. 7, we compare our BOA results of the ground trimer state energy with the exact solution of the Schrödinger equation. In this case, the instantaneous energy of $\psi$ serves as an effective 2D interaction between the two heavy atoms, and can be obtained by replacing the argument $z_1 - z_2$ in $V_{\text{eff}}(z_1 - z_2)$ with $\rho = \sqrt{(y_1 - y_2)^2 + (z_1 - z_2)^2}$. Following the same procedure as outlined in Sec. II, we can show that in the case of $a_1 = a_2 = a$, the depth of the 2D effective potential also takes its maximal value when $a = 1$ in the natural unit. This observation indicates that the resonance phenomenon also exists in the 2D-2D-3D configuration.

Notice that the 2D-2D-3D geometry is invariant under a rotation along the $x$-axis. This SO(2) symmetry thus leads to the conservation of the $x$-component angular momentum of $A_1$-$A_2$ relative motion. Therefore, the wave function $\phi$ in the three-body bound state $\Psi$ can be expressed as

$$\phi = \sum_\ell \phi_\ell(\rho)e^{i\ell \theta},$$

where $\tan \theta = (z_1 - z_2)/(y_1 - y_2)$ is the polar angle of $A_1$-$A_2$ relative motion in the $y$-$z$ plane, and the radial wave function $\phi_\ell(\rho)$ satisfies the 2D Schrödinger equation

$$\left[-\frac{1}{2m_*} \left( \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{\ell^2}{\rho^2} \right) + V_{\text{eff}}(\rho) \right] \phi_\ell(\rho) = E_{\ell}\phi_\ell(\rho).$$

Here, the quantum number $\ell = 0, \pm 1, \pm 2, ...$ indicates the relative angular momentum of $A_1$-$A_2$ along the $x$-direction.

**IV. THREE-BODY UNIVERSAL BOUND STATES IN 2D-2D-3D SYSTEMS**

The discussion on 1D-1D-3D systems outlined in the previous section can be directly generalized to other mixed-dimensional configurations. In this section we consider a 2D-2D-3D system [Fig. 1(b)] where the two heavy atoms $A_{1,2}$ are trapped individually in two 2D confinements, localized in the planes of $x = \pm L/2$. The light atom $B$ is also assumed to move freely in the 3D space. we also adopt the natural units with $\hbar = m_B = L = 1$. To further investigate the relationship between the binding energy and the two-body scattering lengths, we focus on the case of $a_1 = a_2 = a$, and illustrate in Fig. 3 the binding energy in terms of $1/a$ with respect to different reduced masses $m_*$ of the two heavy atoms. One significant feature of this result is that the resonant behavior is present for all different reduced masses, i.e. the binding energy of the ground trimer state reaches its maximum in the region around $a = 1$. Besides, we also notice that for a given two-body scattering length, the binding energy increases with reduced mass $m_*$, and approaches to an asymptotic value in the limit $m_* \to \infty$. This tendency is also confirmed by Fig. 4 where the binding energies for $a_1 = a_2 = a = 1$ and $a_1 = a_2 = a = \infty$ are plotted as functions of the reduced mass $m_*$. The three-body bound states in the 1D-1D-3D systems with $a_1 = a_2$ are also discussed in Ref. [36] within an effective field theory or the exact solution of three-body Schrödinger equation. In Fig. 7 we compare our BOA results of the ground trimer state energy with the exact expression given by Ref. [36] for $m_* = 3.33$ and $a_1 = a_2 = a$. Notice that the BOA results are very close to the exact solution around the resonance point $a = 1$ for such a rather small mass ratio. This consistency suggests that the BOA approach is reliable provided that the three-body bound state energy is away from the threshold.
The pure ground state of the system occurs in the channel \( \ell = 0 \).

The radial equation \( \text{(24)} \) can be solved numerically as in the 1D-1D-3D case. For the ground zero-angular momentum channel \( \ell = 0 \), we also find three-body bound states with reduced mass \( m_\ast = 3.33 \) and \( 9.5 \). The binding energy of the ground trimer state is illustrated in Fig. 8 in terms of \( 1/a_1 \) and \( 1/a_2 \). Notice that the binding energy is significantly amplified in the parameter region \( a_1 \sim a_2 \), and reaches its maximum when the scattering lengths are resonant with the 2D surfaces spacing \( a_1 \sim a_2 \sim 1 \). Besides, the binding energy also increases with reduced mass \( m_\ast \) of the two heavy atoms. In Fig. 9 we also compare the BOA results with the exact expression \( \text{(25)} \) for the case of \( m_\ast = 3.33 \) and \( a_1 = a_2 = a \), and find good agreement when the trimer binding energy is away from the threshold. All these features are analogous with the case of 1D-1D-3D geometry.

From the discussion in the previous sections, we notice that the BOA works well throughout a wide range of scattering length for a fairly small mass ratio of about 6, provided that the binding energy of the bound trimer state is away from the threshold. This observation suggests that this approach can be directly applied to mixed dimensional systems with more than three atoms, and to give reliable results for few-body bound state energy when it is sizable. In this section, we consider as an example the 1D-1D-1D-3D system with three heavy atoms \( A_1, A_2, \) and \( A_3 \) trapped individually in parallel 1D tubes and a single light atom \( B \) moving freely in 3D.

We consider the configuration of three 1D tubes arranged along the \( z \) direction, and intersect with the \( x-y \) plane at \((x = \pm L/2, y = 0)\) and \((x = x_0, y = y_0)\), as shown schematically in Fig. 10. The three intersection points form a triangle in the \( x-y \) plane. Since the system properties are invariant under different length scales, we assume that \( L \) is the shortest side of the triangle, and use it as the length unit \( L = 1 \) in the following discussion.

The quantum states of such a system can be described by the wave function \( \Psi(\bar{r}_B; z_1, z_2, z_3) \), where \( z_i \) is the \( z \)-coordinate of the heavy atom \( A_i \), and \( \bar{r}_B \) is the coordinate of the light atom \( B \). Within the BOA, the wave function \( \Psi \) can be separated as

\[
\Psi(\bar{r}_B; z_1, z_2, z_3) = \phi(z_1, z_2, z_3)\psi(\bar{r}_B; z_1, z_2, z_3). \tag{27}
\]

Here, \( \psi \) is the wave function of the instantaneous bound state of the light atom, which is given by the Schrödinger
where \( U(a; X, Y) \) is the regularized part.

We first consider the special geometry where the three 1D tubes are arranged equidistantly to form an equilateral triangle in the \( x-y \) plane (i.e., \( x_0 = 0 \) and \( y_0 = \sqrt{3}/2 \)). In Fig. 11 we show the regularized effective potential \( U(a; X, Y) \) for scattering length \( a = 1 \). Notice that the effective potential acquires its global minimum at \( (X = 0, Y = 0) \) or \( z_1 = z_2 = z_3 \), that is the three atoms are staying in a surface perpendicular to the 1D tubes and forming an equilateral triangle. Besides, we also observe three energy potential valleys, which correspond to the cases where the distance between two of the three atoms equals to 1.

The same phenomenon can also be observed for other values of scattering length \( a \neq 1 \). In fact, the effective potential \( U(a; X, Y) \) always reaches its minimum at \( (X = 0, Y = 0) \). However, the potential is deepest only when the scattering length \( a = 1 \). In Fig. 12 we show the depth of the effective potential well as a function of \( a \), which reaches its maximum at \( a = 1 \). This result suggests that the resonance we observed in three-body problems as discussed above also occurs in the four-body system.

With the knowledge of the effective potential, we can numerically solve the Schrödinger equation (32) to obtain the eigenenergies of four-body bound states. In the new set of variables \( X \) and \( Y \), this equation can be rewritten as

\[
- \frac{1}{m} \frac{\partial^2}{\partial X^2} - \frac{3}{4m} \frac{\partial^2}{\partial Y^2} + V_{\text{eff}}(X, Y) \phi(X, Y) = E \phi(X, Y),
\]

where \( \phi(X, Y) \) is the wave function of the heavy atoms. As in the three-body calculation, the binding energy of the tetramer states is defined as the difference between the eigenenergy \( E \) and the effective potential energy for \( X \rightarrow \infty \) and \( Y \rightarrow \infty \),

\[
E_{4b} = V_{\text{eff}}(\infty, \infty) - E.
\]
we consider two mass ratios as in the previous discussion. Notice that the binding energy reaches its maximum near $a = 1$, as we expected from the effective potential. This result confirms the appearance of the resonance phenomenon in the four-body system.

Up to now, we consider only a special configuration of 1D±1D-1D±3D geometry where the three 1D tubes form an equilateral triangle, and observe a resonance phenomenon for tetramer binding energy as the scattering length gets close to the mutual distance between 1D tubes. An intuitive expectation is that this most symmetric configuration should be the case of maximal resonance, for the scattering length can be resonant with any two of the three atoms. In order to demonstrate this idea, we consider general configurations of the three 1D tubes, such that they form a triangle of arbitrary shape with three sides $L = 1$, $L_1$ and $L_2$ (see Fig. 10). For the system properties are invariant as scaled with length, we assume $L = 1$ to be the shortest side of the triangle. We further take the scattering lengths $a_1 = a_2 = a_3 = 1$.

In Fig. 13, we show the depth of the effective potential $U(a; X, Y)$ for arbitrary arrangement of the three 1D tubes. It is clearly shown that, the depth of the effective potential takes its maximum value when $L_1 = L_2 = 1$ or the 1D tubes have the configuration of equilateral triangle. This is consistent with our expectation that maximal resonance appears in this most symmetric configuration.

VI. BOA FOR MANY-BODY PROBLEMS IN MIXED-DIMENSIONAL SYSTEMS

In the previous sections, we study the three-body and four-body bound states in mixed-dimensional systems within the BOA. Now we generalize this approach to mixed-dimensional problems with arbitrary $N$ heavy atoms trapped individually in 1D or 2D confinements, while a single light atom moving freely in the 3D space. In such a configuration, the wave function of the possible few-body bound states takes the form

$$\Psi(\vec{r}; \vec{s}) = \phi(\vec{s})\psi(\vec{r}; \vec{s}),$$

where $\vec{s} = (\vec{s}_1, \vec{s}_2, ..., \vec{s}_N)$ are the 1D or 2D coordinates of the heavy atoms $A_1, A_2, ..., A_N$, and $\vec{r_B}$ is the coordinate of the light atom $B$. As in the previous sections, $\psi(\vec{r_B}; \vec{s})$ is the wave function of the instantaneous bound state of the light atom, which is determined by the Schrödinger equation

$$-\frac{1}{2}\nabla^2_B \psi(\vec{r_B}; \vec{s}) = V_{\text{eff}}(\vec{s})\psi(\vec{r_B}; \vec{s}),$$

with Bethe-Peierls boundary conditions

$$\psi(r_{iB} \to 0) \propto \left(1 - \frac{a_i}{r_{iB}}\right) + O(r_{iB}).$$

Here, $r_{iB}$ is the distance between the atoms $A_i$ and $B$. 

FIG. 12: (color online) The depth $D(a)$ of the regularized part $U(a; X, Y)$ of the effective interaction. In this plot, we consider the case of $a_1 = a_2 = a_3 = a$ in the 1D-1D-1D-3D system with equilateral triangle configuration. Notice that $D(a)$ takes maximum value at the resonance point of $a = 1$.

FIG. 13: (color online) The binding energy $E_{4b}$ of the ground four-body bound state in the 1D-1D-1D-3D system with equilateral triangle configuration. For different values of $a$ with reduced mass $m_s = 9.5$ (blue solid line with circles) and 3.33 (green solid line with triangle).

FIG. 14: (color online) The depth of the effective potential $U(a; X, Y)$ in the 1D-1D-1D-3D system with $a_1 = a_2 = a_3 = 1$ and the inter-tube distances $L_1 = 1$ and $L_{1,2}$ defined in Fig. 10.
By solving Eq. [33], we obtain the general form of the instantaneous bound state

$$\psi(\vec{r}_B; \vec{s}) = e^{-\kappa_{1B}r} + \sum_{i=2}^{N} c_i e^{-\kappa_{iB}r}$$

(40)

where the value of $\kappa$ and the coefficients $c_i$ are given by the equations

$$\frac{1}{a_1} = -\kappa - \sum_{j=2}^{N} c_j e^{-\kappa_{jB}r}$$ \hspace{1cm} (41)

$$\frac{c_i}{a_i} = \kappa c_i - \sum_{l \neq i}^{N} c_l e^{-\kappa_{lB}r}$$ \hspace{1cm} (42)

From the equations above, we can solve for the value of $\kappa$ in terms of the coordinate $\vec{s}$ of the heavy atoms, and then obtain the instantaneous wave function of $\psi(\vec{r}_B; \vec{s})$ and the effective interaction among the heavy atoms

$$V_{\text{eff}}(\vec{s}) = -\frac{\kappa^2}{2}.$$ \hspace{1cm} (43)

Finally, the heavy-atoms wave function $\phi(\vec{s})$ of the few-body bound state is given by

$$\left[-\sum_{i=1}^{N} \frac{1}{2m_i} \nabla_i^2 + V_{\text{eff}}(\vec{s})\right] \phi(\vec{s}) = E\phi(\vec{s})$$ \hspace{1cm} (44)

with $m_i$ the mass of the heavy atom $A_i$.

VII. CONCLUSION

In this manuscript we show our BOA-based results on the stable three-body or four-body bound states in mixed dimensional systems with $N \geq 2$ heavy atoms individually trapped in different 1D or 2D confinements, while a single light atom moving freely in the 3D space. The BOA approach can provide a clear physical picture with a well-defined effective interaction among the heavy atoms. We show that in mixed dimensions, the three-body or four-body bound states can occur within a broad range of two-body scattering lengths, as the Efimov states in 3D. Nevertheless, the binding energy of the ground bound state reaches its maximum value when the two-body scattering length gets close to the distance between the low-dimensional traps. This is due to a new resonance phenomenon in mixed dimensions, where the effective interaction among the heavy atoms acquires a deepest potential well under the resonant condition. The feasibility of this BOA approach is then confirmed by a direct comparison with exact results in 1D-1D-3D and 2D-2D-3D configurations, hence suggests a possible extension in the problems with more than three atoms in mixed dimensions.

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Appendix A: The Bethe-Peierls Boundary Condition for BOA in Mixed-Dimensional Systems

In this appendix, we derive the Bethe-Peierls boundary condition [e.g., Eqs. (4), (5), (29) and (39)] used in the Born-Oppenheimer approach for the mixed dimensional systems. For simplicity, here we consider the system with one heavy atom $A$ confined in a 1D trap which is arranged along the $z$-axis, plus a light atom $B$ moving freely in 3D. The generalization to other cases is straightforward.

The expression of Bethe-Peierls boundary condition should be derived from the asymptotic behavior of the two-body wave functions. As a first-principle discussion, we first take into account the 3D motions of both atoms $A$ and $B$, and then reduce our result in the mixed-dimensional model where only the motion along the $z$-direction is considered for atom $A$. The total Hamiltonian of the two atoms is given by

$$H_{AB} = T_{Az} + T_{A\perp} + V_{A\perp} + T_B + V_{AB}(|\vec{r}_{AB}|).$$ \hspace{1cm} (A1)

Here, the kinetic energy of atom $A$ along the $z$ direction is given by

$$T_{Az} = \frac{1}{2m_A} \frac{\partial^2}{\partial z_A^2}$$ \hspace{1cm} (A2)

with $m_A$ the mass of atom $A$, and $\vec{r}_i = (x_i, y_i, z_i)$ the coordinate of the corresponding atoms. The transverse kinetic energy $T_{A\perp}$ of atom $A$ and the total kinetic energy $T_B$ of atom $B$ are defined as

$$T_{A\perp} = -\frac{1}{2m_A} \left( \frac{\partial^2}{\partial x_A^2} + \frac{\partial^2}{\partial y_A^2} \right);$$ \hspace{1cm} (A3)

$$T_B = -\frac{1}{2} \nabla_B^2.$$ \hspace{1cm} (A4)

Here we use the natural unit $\hbar = m_B = 1$. In the Hamiltonian (A1) we also have the transverse harmonic potential

$$V_{A\perp} = \frac{m_A \omega_A^2}{2} (x_A^2 + y_A^2)$$ \hspace{1cm} (A5)

with frequency $\omega_A$, and the atom-atom interaction potential $V_{AB}(|\vec{r}_{AB}|)$ which is a function of the distance between the two particles $r_{AB} = |\vec{r}_A - \vec{r}_B|$. We further denote the effective range of the interaction potential as
\( r_\ast \), such that we have \( V_{AB}(r_{AB}) \approx 0 \) in the region of \( r_{AB} \gg r_\ast \).

When the confinement of the heavy atom \( A \) is strong, the transverse motion of atom \( A \) in the \( x\text{-}y \) plane is much more rapid than its motion along the \( z \) direction. Therefore, we need to consider both the position \( \vec{r}_B \) of the light atom \( B \) and the transverse coordinates \((x_A, y_A)\) of the heavy atom \( A \) as fast degrees of freedom. Only the longitudinal coordinate \( z_A \) of atom \( A \) is treated as the slow variable.

Within the BOA, the total wave function of the system takes the form

\[
\Psi(\vec{r}_A, \vec{r}_B) = \phi(z_A) \psi(\vec{r}_B, x_A, y_A; z_A), \tag{A6}
\]

where \( \psi(\vec{r}_B, x_A, y_A; z_A) \) is given by the eigen-equation

\[
H_F(z_A) \psi(\vec{r}_B, x_A, y_A; z_A) = E(z_A) \psi(\vec{r}_B, x_A, y_A; z_A) \tag{A7}
\]

of the Hamiltonian

\[
H_F(z_A) = T_{A\perp} + V_{A\perp} + T_B + V_{AB}(r_{AB}) \tag{A8}
\]

with fixed values of \( z_A \). To solve Eq. (A7), we expand the solution \( \psi \) with eigen-states of the transverse Hamiltonian \( T_{A\perp} + V_{A\perp} \) of atom \( A \)

\[
\psi(\vec{r}_B, x_A, y_A; z_A) = \sum_{n=0}^{\infty} \phi_n(x_A, y_A) \psi_n(\vec{r}_B; z_A). \tag{A9}
\]

Here, \( \phi_n(x_A, y_A) \) is the \( n \)th eigen-state of \( T_{A\perp} + V_{A\perp} \). Considering the translational symmetry along the \( z \)-axis, we take \( z_A = 0 \), and the relevant wave function \( \psi_n(\vec{r}_B; 0) \) of the light atom \( B \) is given by

\[
[T_B + (n + 1) \omega_{\perp}] \psi_n + \sum_m V_{nm}(\vec{r}_B) \psi_m = E(0) \psi_n. \tag{A10}
\]

Here, the matrix element of the interaction potential takes the form

\[
V_{nm}(\vec{r}_B) = \int dx_A dy_A \phi_n^*(x_A, y_A) V_{AB}(r_{AB}) \phi_m(x_A, y_A). \tag{A11}
\]

Therefore, the eigen-equation (A7) or (A10) can be solved via a multi-channel scattering theory of atom \( B \), with the transverse states \( \phi_n(\vec{r}_B; z_A) \) of atom \( A \) serving as the scattering channels. In the low-energy case with \( \omega_{\perp} < E < 2\omega_{\perp} \), the ground channel with the transverse state \( \phi_0(x_A, y_A) \) assumes the only open channel.

Now we consider the asymptotic behavior of the wave function in the long-distance limit with \( |\vec{r}_B| \gg (r_\ast, l_{\perp}) \), where \( l_{\perp} = \sqrt{1/(m_A \omega_{\perp})} \) denotes the characteristic length of the transverse confinement. In this region, the mutual distance \( r_{AB} \) between the two atoms would be much larger than the effective range \( r_\ast \) of the interaction, such that we can neglect the term \( V_{AB} \) in Eq. (A8). According to the scattering theory, in such a region the wave function \( \psi_n(\vec{r}_B; 0) \) in the close channels with \( n > 0 \) decays exponentially with \( |\vec{r}_B| \), and can be safely neglected. The wave function \( \psi_0(\vec{r}_B; 0) \) in the open channel takes the form

\[
\psi_0(\vec{r}_B; 0) \sim \sum_{n=0}^{\infty} \sum_{l=-l}^{l} C_{l,m} \frac{Y_{lm}(\theta_B, \phi_B)}{k|\vec{r}_B|} \times \left[ \hat{j}_l(k|\vec{r}_B|) + k f_l(m(k) \hat{h}_l^+(k|\vec{r}_B|) \right], \tag{A12}
\]

where \( k = \sqrt{2(E - \omega_{\perp})} \), \( Y_{lm}(\theta, \phi) \) are the spherical harmonic functions of the azimuth angles \( (\theta_B, \phi_B) \) of \( \vec{r}_B \), \( \hat{j}_l(z) \) is the Riccati-Bessel function, and \( \hat{h}_l^+(z) \) is the Riccati-Hankel function. The coefficients \( C_{l,m} \) are given by the boundary condition, while the scattering amplitudes \( f_l,m(k) \) are determined by the effective potential \( V_{nm}(\vec{r}_B) \) defined in (A11). In the low-energy case with small \( k \), we can neglect all the high-partial wave scattering amplitudes \( f_l,m(k) \) with \( l \geq 1 \), and approximate the \( s \)-wave scattering amplitude \( f_{0,0}(k) \) with \( f_{0,0}(k = 0) \).

Then the long-distance behavior of wave function \( \psi \) becomes

\[
\psi(\vec{r}_B, x_A, y_A; 0) \sim \phi_0(x_A, y_A) \psi_0(\vec{r}_B; 0) \sim \phi_0(x_A, y_A) \left[ \frac{1}{k|\vec{r}_B|} \left( \sin (k|\vec{r}_B|) - k \theta_{AB} e^{i k|\vec{r}_B|} \right) \right] + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} C_{l,m} \frac{Y_{lm}(\theta_B, \phi_B)}{k|\vec{r}_B|} \hat{j}_l(k|\vec{r}_B|) \tag{A13}
\]

with the scattering length \( a_{AB} \) defined as

\[
a_{AB} = -f_{0,0}(k = 0). \tag{A14}
\]

The expression (A13) implies that in the “intermediate” region of

\[
[r_\ast, l_{\perp}] \ll |\vec{r}_B| \ll \frac{1}{k}, \tag{A15}
\]

the behavior of \( \psi \) takes the form of

\[
\psi(\vec{r}_B, x_A, y_A; 0) \sim \phi_0(x_A, y_A) \left( 1 - \frac{a_{AB}}{|\vec{r}_B|} \right). \tag{A16}
\]

Therefore, we can replace the real interaction potential \( V_{AB}(r_{AB}) \) in (A11) with a Bethe-Peierls-type boundary condition

\[
\lim_{|\vec{r}_{AB}| \to 0} \psi(\vec{r}_B, x_A, y_A; 0) \propto \phi_0(x_A, y_A) \left( 1 - \frac{a_{AB}}{|\vec{r}_B|} \right) \tag{A17}
\]

Under this boundary condition, the solution of the eigen-equation

\[
[T_{A\perp} + V_{A\perp} + T_B] \psi(\vec{r}_B, x_A, y_A; 0) = E \psi(\vec{r}_B, x_A, y_A; 0) \tag{A18}
\]
takes the form of Eq. (A13) for all $|\vec{r}_B| \neq 0$, and becomes a reasonable approximation for the solution of (A7).

In this reduced mixed-dimensional model, the transverse coordinates $(x_A, y_A)$ of the heavy atom $A$ is taken to be fixed values of $(0, 0)$. Together with the assumption $z_A = 0$, we have

$$|\vec{r}_B| = r_{AB}, \quad (A19)$$

and then the boundary condition (A17) can be expressed as

$$\lim_{r_{AB} \to 0} \psi (\vec{r}_B; 0) \propto \left( 1 - \frac{a_{AB}}{r_{AB}} \right). \quad (A20)$$

Here, $\psi (\vec{r}_B; 0)$ is the wave function of the light atom $B$ with the position of atom $A$ fixed at $z_A = 0$. For non-zero $z_A$, the condition (A20) can be generalized to

$$\lim_{r_{AB} \to 0} \psi (\vec{r}_B; z_A) \propto \left( 1 - \frac{a_{AB}}{r_{AB}} \right). \quad (A21)$$

That is the Bethe-Peierls boundary condition used in the BOA discussed in the main text of this manuscript.

We notice that there is another type of Bethe-Peierls boundary condition as discussed in Ref. [31,32], where the total wave function $\Psi$ of the reduced mixed-dimensional two-body problem is assumed to satisfy the condition

$$\lim_{D_{AB} \to 0} \psi \propto \left( 1 - \frac{a_{\text{eff}}}{D_{AB}} \right) \quad (A22)$$

with

$$D_{AB} = \sqrt{x_B^2 + y_B^2 + \frac{m_B + 1}{m_A} (z_A - z_B)^2}. \quad (A23)$$

This condition is slightly different from our result of Eq. (A21). The difference can be understood by noticing that when solving for the wave function of atom $B$ under BOA, we fix the position of the heavy atom $A$, such that the relevant Bethe-Peierls boundary condition (A22) becomes isotropic. It is pointed out that, in the limit of $m_A \gg 1$, the condition (A22) approaches to (A21) and we have $a_{AB} = a_{\text{eff}}$. Therefore, we approximate $a_{AB}$ as $a_{\text{eff}}$ when comparing the BOA results with the effective field theory [30].

It is straightforward to generalize the discussion above to more general cases with $N$ heavy atoms $A_1, \ldots, A_N$ individually confined in $N$ low-dimensional traps, and one light atom $B$ moving freely in 3D. In that case, we can fix the positions of the heavy atoms under BOA, and use the Bethe-Peierls boundary condition

$$\lim_{r_{iB} \to 0} \psi (\vec{r}_A, \vec{r}_B) \propto \left( 1 - \frac{a_{iB}}{r_{iB}} \right) \quad (A24)$$

to solve the Schrödinger equation of the light atom. Here, $r_{iB}$ is the distance between the heavy atom $A_i$ and the light atom $B$. That is the approach we used in our main text.

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