

Search for Borromean states in the He-He-Rb triatomic system

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We search for the existence of weakly bound He-He-Rb molecules. The He-He-Rb molecule is treated as a three-body system. By using hyperspherical coordinates, the Schrödinger equation for the triatomic system is solved in the adiabatic approximation. A bound state is found for each of the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, ${}^3\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, and ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$ trimers, respectively. The bound state for the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ molecule is a Borromean state found in a realistic molecular systems because there are no bound states in both the ${}^3\text{He}-{}^3\text{He}$ and ${}^3\text{He}-{}^{85}\text{Rb}$ dimers.

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I. INTRODUCTION

The bound states of a three-body system when its two-body system does not have any bound state is called the Borromean (halo) states [1,2], after the Borromean rings, which are interlaced in a subtle topological way such that if any one of them is removed, the two other become unlocked. The adjective Borromean is nowadays broadly accepted in the field of quantum few-body systems [3,4].

Some Borromean systems have been known for several years in nuclear physics. For instance, if one neglects the internal structure of α particle, a fairly realistic approximation, ${}^6\text{He}$ is a bound (α - n - n) system, while neither (α - n) nor (n - n) is bound. Thus, ${}^6\text{He}$ is Borromean [5].

For three identical particles in real atomic and molecular systems, Lim *et al.* and Esry *et al.* have shown that the second bound state of the helium trimer appears to have properties similar to those of an Efimov state [6,7]. Blume *et al.* have predicted that the single vibrational bound state of the quartet tritium trimer is a Borromean state [8], and Kraemer *et al.* observed an Efimov resonance in an ultracold gas of cesium trimer [9], which confirms central theoretical predictions of Efimov physics and represent a starting point with which to explore the universal properties of resonantly interacting few-body systems. So far, ${}^3\text{He}_2-{}^{39}\text{K}$ is the only mixed molecular system for which the Borromean state has been predicted theoretically [10].

In this article we present the results of searching for weakly bound states of the He-He-Rb molecule. The He-He-Rb molecule is treated as a three-body system. By means of the best empirical interaction between each pair of particles, the Schrödinger equation for the triatomic system is solved using hyperspherical coordinates in the adiabatic approximation. The results show that there is a bound state for each of the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ molecules, respectively. The bound state for the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ molecule is the Borromean (halo) states found in the realistic molecular system because there are no bound states in both the ${}^3\text{He}-{}^3\text{He}$ and ${}^3\text{He}-{}^{85}\text{Rb}$ dimers. And this Borromean state is the ground state of the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ system.

II. METHODS AND RESULTS

Neglecting the internal structure of the atoms, we consider He-He-Rb molecule as consisting of three atoms, He, He, and Rb. The Schrödinger equation for three interacting atoms is expressed by the hyperspherical coordinates and we solve this Schrödinger equation within the adiabatic approximation [7,11,12]. Only the most favorable condition for the lowest states of the He-He-Rb molecules or the case of $J = 0$ is considered. Given the detailed description in Ref. [10] of the calculation procedure, we mention here only some key points of the method.

In the adiabatic hyperspherical approach, we treat R initially as a fixed parameter and solve the eigenvalue equation,

$$\left[\frac{\Lambda^2 - \frac{1}{4}}{2\mu R^2} + V(R, \phi, \theta) \right] \Phi_v(R, \phi, \theta) = U_v(R) \Phi_v(R, \phi, \theta) \quad (1)$$

with boundary conditions

$$\Phi_v(R, 0, \theta) = \Phi_v\left(R, \frac{\pi}{2}, \theta\right) = 0 \quad (2)$$

and

$$\frac{\partial \Phi_v(R, \phi, \theta)}{\partial \theta} \Big|_{\theta=0} = \frac{\partial \Phi_v(R, \phi, \theta)}{\partial \theta} \Big|_{\theta=\pi} = 0. \quad (3)$$

The full solution to the Schrödinger equation has the following form:

$$\psi(R, \phi, \theta) = \sum_v F_v(R) \Phi_v(R, \phi, \theta). \quad (4)$$

If the coupling terms between different channels are neglected, then we obtain the hyperradial equation in the adiabatic approximation,

$$\left[-\frac{1}{2\mu} \frac{d^2}{dR^2} + U_v(R) + W_{vv}(R) \right] F_{vn}(R) = E_{vn} F_{vn}(R), \quad (5)$$

where

$$W_{vv}(R) = -\frac{1}{2\mu} \langle \Phi_v(R) | \frac{\partial^2}{\partial R^2} | \Phi_v(R) \rangle. \quad (6)$$

It can be shown [13,14] that the ground-state energy obtained by solving Eq. (5) is an upper bound to the true ground-state

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energy. If we solve Eq. (5) without $W_{vv}(R)$, it also can be shown [13,14] that the ground-state energy obtained in this way is a lower bound to the ground-state energy. Thus, after Eq. (5) is solved with and without $W_{vv}(R)$, we can obtain the range of the ground-state energy.

The hyperradial equation Eq. (5) is solved by numerical integration method and Eq. (1) is solved by using B -spline expansion.

Given a knot sequence on the x axis [15]

$$\{x_1 \leq x_2 \leq \dots \leq x_N \leq \dots \leq x_{N+k}\}, \quad (7)$$

B -spline functions of order k are defined as

$$B_{i,1} = \begin{cases} 1, & x_i \leq x < x_{i+1} \\ 0, & \text{otherwise} \end{cases}$$

$$B_{i,k}(x) = \frac{x - x_i}{x_{i+k-1} - x_i} B_{i,k+1}(x) + \frac{x_{i+k} - x}{x_{i+k} - x_{i+1}} B_{i+1,k-1}(x). \quad (8)$$

It is immediately seen that $B_{i,k}(x)$ ($i = 1, 2, \dots$) are piecewise polynomials of order $k - 1$ localized within $[x_i, x_{N+k}]$, while $B_{i,k}(x)$ is nonvanishing only within $[x_i, x_{i+k}]$. The behavior of B -spline functions can be readily adjusted with the knot sequence, viz., the choice of knot point x_i , order k , and number of B splines N , which offers a means to optimize the B splines as a basis set to expand the wave functions of one or several states concerned.

In our case for Eq. (1), there are two variables (ϕ, θ), for a fixed R , and the channel function $\Phi(R, \phi, \theta)$ in Eq. (1) can be constructed with the B splines as a basis set,

$$\Phi(R, \phi, \theta) = \sum_{i,j=1}^{M,N} C_{ij} B_{i,k}(\phi) B_{j,k}(\theta) \quad (9)$$

Substituting $\Phi(R, \phi, \theta)$ into Eq. (1), we obtain

$$\tilde{H}\tilde{C} = E\tilde{S}\tilde{C}, \quad (10)$$

where \tilde{H} is the Hamiltonian matrix and \tilde{S} is the overlap matrix of B splines. E and \tilde{C} are eigenvalues and eigenvectors, respectively. Solving this generalized eigenvalue equation, we obtain the channel function $\Phi(R, \phi, \theta)$ and the adiabatic potential $U_v(R)$ at a fixed R .

We treat the He-He-Rb molecule as a three-body system. The three-body interaction is expected to be small and in the case of the He-He-He system it has been shown to affect less than 1% of the ground-state energy [16,17]. Therefore, we do not consider any possible three-body interaction in our calculations and the interactions of the system are the two-body interactions between each atom.

For the He-He dimer, the potential from Aziz and Slaman [18] is used, and the potential proposed by Kleinekathofer [19] is used for the He-Rb system. These potentials are considered to be among the best available and they are obtained from quantum chemistry calculations and then fitted and adjusted so that the low-energy atom-atom scattering data are reproduced. In Fig. 1, we show the pairwise interaction potentials for the He-He and He-Rb dimers.

To determine the dissociation limit of the lowest channel potential for He-He-Rb molecule, we search for the bound

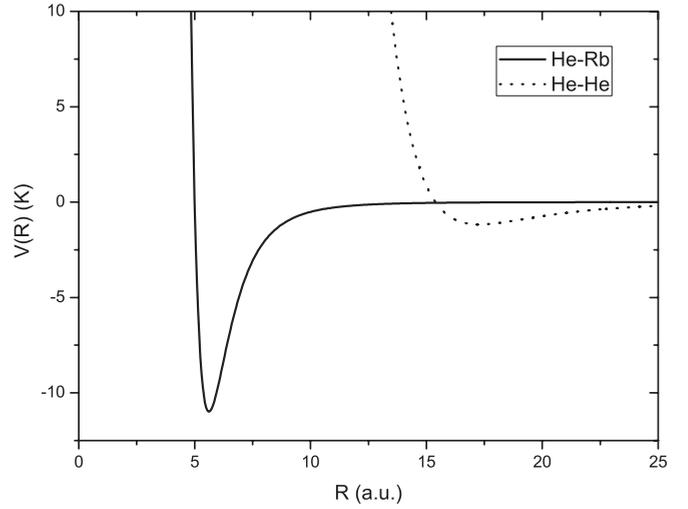


FIG. 1. Interatomic potentials for He-He and He-Rb systems.

states for the $^4\text{He}-^{85}\text{Rb}$ and $^3\text{He}-^{85}\text{Rb}$ molecules. The related two-body radial Schrödinger equation is solved numerically with the He-Rb potential from Fig. 1. The results for the bound states are shown in Table I together with the results for the helium dimers. We can see that there is a bound state for $^4\text{He}-^{85}\text{Rb}$ dimer with binding energy -10.3 mK, and no bound state for the $^3\text{He}-^{85}\text{Rb}$ diatom. It is well known that there is a bound state for the $^4\text{He}-^4\text{He}$ dimer with the binding energy -1.31 mK, but there are no bound states for both the $^4\text{He}-^3\text{He}$ and $^3\text{He}-^3\text{He}$ diatoms. Therefore, if there are bound states for the $^3\text{He}-^3\text{He}-^{85}\text{Rb}$ molecule, they would be the Borromean states in realistic molecular systems. And the dissociation limit of the lowest channel potential is -10.3 mK for both $^4\text{He}-^3\text{He}-^{85}\text{Rb}$ and $^4\text{He}-^4\text{He}-^{85}\text{Rb}$ molecules, and the dissociation limit of the lowest channel potential is 0 K for the $^3\text{He}-^3\text{He}-^{85}\text{Rb}$ molecule.

As mentioned, to search for the bound states for the He-He-Rb system, we solve the Schrödinger equation for the triatomic system using hyperspherical coordinates in the adiabatic approximation. The hyperspherical method with adiabatic approximation is one of the most powerful theoretical techniques for searching for stable bound states. In this approach, the adiabatic hyperspherical potential is first calculated. If the potential curve is repulsive, there is no possibility for the existence of any bound states. If the potential curve is both attractive and deep enough, stable bound states are expected. This technique has been successfully applied to many three-body systems. The previous results show that the stability and the binding energies of these systems depend sensitively on the interaction potentials and the masses of the

TABLE I. The calculated binding energies of the ground states for the He-Rb dimers together with the results for helium dimers. The interatomic potential between Rb and He is taken from Ref. [19]. Missing entries indicate that no bound is found.

^3He	^4He	^{85}Rb
^3He		
^4He	-1.31 mK	-10.3 mK

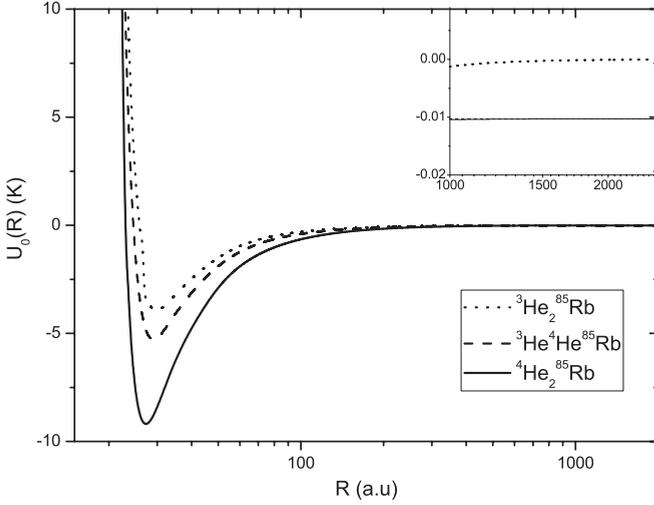


FIG. 2. The lowest hyperspherical potential curves for each of the triatomic systems, ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers. The curves of both the ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ and ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$ trimers converge to the bound state of the ${}^4\text{He}-{}^{85}\text{Rb}$ dimer with binding energy of -10.3 mK . The curve of ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimer converges to zero, the three-body breakup threshold, at large R .

particles. Quantum symmetry is also known to play an essential role [20] in determining the stability of systems and the binding energies.

After Eq. (1) is solved by using B -spline expansion, we obtain the lowest adiabatic hyperspherical potentials for the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ molecules. The calculated hyperspherical potentials are presented in Fig. 2. In the large- R limit, each potential curve converges to the related dissociation limit. The dissociation limits for both the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$ and ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers are the bound state of the ${}^4\text{He}-{}^{85}\text{Rb}$ dimer with the binding energy of -10.3 mK . For the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ molecule, both the ${}^3\text{He}-{}^3\text{He}$ and ${}^3\text{He}-{}^{85}\text{Rb}$ dimers have no bound states, so the potential curve approaches zero, the three-body breakup threshold, at large R .

Once the adiabatic hyperspherical potentials are obtained, we can search for the bound states supported by each curve by shoveling the hyperradial equation. The results show that each curve can support only one bound state. The binding energies are listed in Table II. We can see from Table II that the upper bounds of the binding energies are -152 , -65.9 , and -38.6 mK for the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers, respectively, and the lower bounds of the binding energies are -155 , -69.0 , and -40.8 mK for the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers,

TABLE II. The calculated binding energies of the ground states for ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers together with the results for ${}^4\text{He}-{}^4\text{He}-{}^{39}\text{K}$, ${}^4\text{He}-{}^3\text{He}-{}^{39}\text{K}$, and ${}^3\text{He}-{}^3\text{He}-{}^{39}\text{K}$ trimers.

	${}^3\text{He}-{}^3\text{He}$		${}^3\text{He}-{}^4\text{He}$		${}^4\text{He}-{}^4\text{He}$	
	Low bound	Up bound	Low bound	Up bound	Low bound	Up bound
${}^{39}\text{K}$	-9.01 mK	-0.728 mK	-42.2 mK	-11.0 mK	-115 mK	-66.6 mK
${}^{85}\text{Rb}$	-40.8 mK	-38.6 mK	-69.0 mK	-65.9 mK	-155 mK	-152 mK

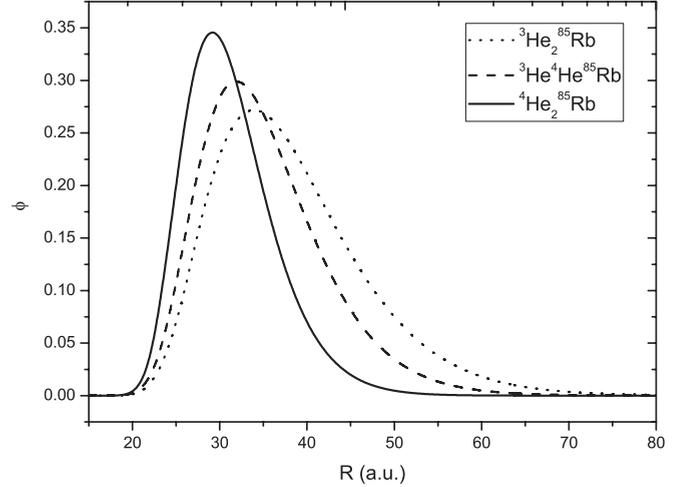


FIG. 3. The wave functions for the bound states of the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers. The Borromean state of the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimer has an larger spatial extent.

respectively. The bound state for the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimer is a predicted Borromean state in the ground of the trimer since there are no bound states in both the ${}^3\text{He}-{}^3\text{He}$ and ${}^3\text{He}-{}^{85}\text{Rb}$ dimers. The wave functions with $W_{\nu\nu}(R)$ for the bound states of the ${}^4\text{He}-{}^4\text{He}-{}^{85}\text{Rb}$, ${}^4\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$, and ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimers are shown in Fig. 3, which shows that the Borromean state of the ${}^3\text{He}-{}^3\text{He}-{}^{85}\text{Rb}$ trimer has an larger spatial extent.

For the purpose of comparison, Table II also includes the results from Li *et al.* for the He-He- ${}^{39}\text{K}$ trimer [10]. The results in Table II show that the binding energies of the triatomic molecules depend sensitively on the mass of each of the particles in the system, and the binding energies for He-He- ${}^{85}\text{Rb}$ are deeper than those for He-He- ${}^{39}\text{K}$ system since the mass of ${}^{85}\text{Rb}$ is heavier than that of ${}^{39}\text{K}$. Note that the relative gap between the lower and upper bounds for He-He- ${}^{85}\text{Rb}$ is about 20 times smaller than for the similar He-He- ${}^{39}\text{K}$ molecules. This can be understood in the following way. The He-He- ${}^{85}\text{Rb}$ and He-He- ${}^{39}\text{K}$ molecules are similar and they have the similar diagonal coupling term $W_{\nu\nu}(R)$. The adiabatic hyperspherical potentials for He-He- ${}^{39}\text{K}$ system are shallower than those for He-He- ${}^{85}\text{Rb}$ system. Therefore, the diagonal coupling term has a larger influence on the He-He- ${}^{39}\text{K}$ system in Eq. (5). This leads to the bigger relative gap between the lower and upper bounds for the He-He- ${}^{39}\text{K}$ trimer.

III. SUMMARY

We have searched for the existence of the weakly bound He-He- ${}^{85}\text{Rb}$ molecule. The He-He- ${}^{85}\text{Rb}$ molecule is treated as

a three-body system. By using hyperspherical coordinates, the Schrödinger equation for the triatomic system is solved in the adiabatic approximation. A bound state is found for each of the ^3He - ^3He - ^{85}Rb , ^3He - ^4He - ^{85}Rb , and ^4He - ^4He - ^{85}Rb trimers, respectively. The bound state for the ^3He - ^3He - ^{85}Rb molecule is the Borromean state found in the realistic molecular system because there are no bound states in both the ^3He - ^3He and ^3He - ^{85}Rb dimers. Since they have binding energies of the order of less than 1 K, these weakly bound molecules can exist only in a cold environment. Using laser cooling and

other cooling methods for atoms and molecules [21–23], it may be possible to make direct observations of these molecules.

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- [1] J. M. Richard and S. Fleck, *Phys. Rev. Lett.* **73**, 1464 (1994).
[2] D. V. Fedorov, A. S. Jensen, and K. Riisager, *Phys. Rev. Lett.* **73**, 2817 (1994).
[3] J. M. Richard, *Few-Body Syst.* **38**, 79 (2006).
[4] M. V. Zhukov, B. V. Danilin, D. V. Fedorov, J. M. Bang, I. S. Thompson, and J. S. Vaagen, *Phys. Rep.* **231**, 151 (1993).
[5] J. Goy, J.-M. Richard, and S. Fleck, *Phys. Rev. A* **52**, 3511 (1995).
[6] T. K. Lim, S. K. Duffy, and W. C. Damer, *Phys. Rev. Lett.* **38**, 341 (1977).
[7] B. D. Esry, C. D. Lin, and C. H. Greene, *Phys. Rev. A* **54**, 394 (1996).
[8] D. Blume, B. D. Esry, C. H. Greene, N. N. Klausen, and G. J. Hanna, *Phys. Rev. Lett.* **89**, 163402 (2002).
[9] T. Kraemer *et al.*, *Nature (London)* **440**, 315 (2006).
[10] Y. Li, Q. Gou, and T. Shi, *Phys. Rev. A* **74**, 032502 (2006).
[11] J. H. Macek, *J. Phys. B* **1**, 831 (1968).
[12] C. D. Lin, *Phys. Rep.* **257**, 1 (1995).
[13] I. Aronson, C. J. Kleinman, and L. Spruch, *Phys. Rev. A* **4**, 841 (1971).
[14] A. F. Starace and G. L. Webster, *Phys. Rev. A* **19**, 1629 (1979).
[15] C. de Boor, *A Practical Guide to Splines* (Springer, New York, 1978).
[16] C. A. Parish and C. E. Dykstra, *J. Chem. Phys.* **101**, 7618 (1994).
[17] I. Roeggen and J. Almlöf, *J. Chem. Phys.* **102**, 7095 (1995).
[18] R. A. Aziz and M. J. Slaman, *J. Chem. Phys.* **94**, 8047 (1991).
[19] U. Kleinekathofer, K. T. Tang, J. P. Toennies, and C. L. Yiu, *Chem. Phys. Lett.* **249**, 257 (1996).
[20] C. G. Bao, X. Z. Yang, and C. D. Lin, *Phys. Rev. A* **55**, 4168 (1997).
[21] B. Friedrich *et al.*, *J. Chem. Soc., Faraday Trans.* **94**, 1783 (1998).
[22] J. D. Weinstein *et al.*, *Nature (London)* **395**, 148 (1998).
[23] J. M. Doyle, B. Friedrich, J. Kim, and D. Patterson, *Phys. Rev. A* **52**, R2515 (1995).