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Nonuniversal bound states of two identical heavy fermions and one light particle

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We study the behavior of the bound-state energy of a system consisting of two identical heavy fermions of mass $M$ and a light particle of mass $m$. The heavy fermions interact with the light particle through a short-range two-body potential with positive $s$-wave scattering length $a_s$. We impose a short-range boundary condition on the $s$-wave scattering length $a_s$. We impose a short-range boundary condition on the logarithmic derivative of the hyperradial wave function and show that, in the regime where Efimov states are absent, a nonuniversal three-body state cuts through the universal three-body states previously described by Kartavtsev and Malykh [O. I. Kartavtsev and A. V. Malykh, J. Phys. B 40, 1429 (2007)]. The presence of the nonuniversal state alters the behavior of the universal states in certain regions of the parameter space. We show that the existence of the nonuniversal state is predicted accurately by a simple quantum defect theory model that utilizes hyperspherical coordinates. An empirical two-state model is employed to quantify the coupling of the nonuniversal state to the universal states.

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I. INTRODUCTION

The unprecedented control over ultracold atomic Fermi gases in optical lattices has made them prime candidates for studying and engineering novel quantum phases as well as probing fundamental theories such as the Bose-Einstein condensation (BEC) to BCS crossover [1–6]. This progress has been facilitated by the tunability of the two-body interactions using Feshbach resonances or by changing the lattice confinement. If the interspecies two-body $s$-wave scattering length $a_s$ is much larger than the range $r_0$ of the underlying two-body potential, the few- and many-body behaviors of equal-mass two-component Fermi gases is universal, i.e., completely determined by $a_s$.

Presently significant efforts are directed at creating ultracold atomic Fermi gas mixtures composed of two chemically distinct species [7–9]. This introduces a new parameter, the mass ratio $\kappa$ between the two species. This new parameter affects the many-body physics of the system, allowing one to realize novel quantum phases such as the interior gap superfluid [10]. Here we show that at the few-body level this additional degree of freedom leads to new three-body resonances that may destabilize the system, making it harder for experiments to explore novel quantum phases with unequal-mass mixtures. In particular, we study a system of two identical heavy fermions with mass $M$, which interact with a light particle through a short-range potential with positive $s$-wave scattering length $a_s$.

Previous studies revealed two intriguing properties. First, Kartavtsev and Malykh [11] predicted the existence of a universal trimer state with energy $E_{u,1}$ for $\kappa_1 < \kappa < \kappa_2$ and the existence of two universal states with energies $E_{u,1}$ and $E_{u,2}$ for $\kappa_2 < \kappa < 13.606$; $\kappa_1$ and $\kappa_2$ were found to be 8.173 and 12.917, respectively. Second, Endo et al. [12] investigated how the universal trimer states, which are completely determined by the $s$-wave scattering length and the mass ratio $\kappa$, are connected to Efimov trimers, which have been predicted to exist for $\kappa \gtrsim 13.606$. By analyzing the trimer system within the framework of the Skorniakov–Ter-Martirosian equation with a momentum cutoff $\Lambda_c$, Endo et al. predicted the existence of a third class of trimer states, termed crossover trimers, which were shown to continuously connect the universal trimers described by Kartavtsev and Malykh and Efimov trimers.

Our study employs, as in Ref. [11], the hyperspherical coordinates. However, while Ref. [11] enforced that the $s$-wave wave function vanishes at hyperradius $R = 0$, we explore the entirety of physically allowed boundary conditions by introducing a short-range three-body or hyperradial phase $\delta(R_0)$. We determine the eigenspectrum as a function of the value of the three-body phase $\delta$, the hyperradius $R_0$ at which the hyperradial boundary condition is imposed, and the mass ratio $\kappa$. The universal states of Kartavtsev and Malykh are recovered for $R_0 \rightarrow 0$ and $\delta(R_0) = \pi/2$. However, for other boundary conditions we find deviations from universality, which are linked to the existence of a nonuniversal three-body state. Analogous nonuniversal three-body states have previously been shown to exist [13,14] (see also Refs. [15–17]) in the $a_s \rightarrow \infty$ limit. The existence of the nonuniversal state for positive $a_s$ is described accurately within a quantum defect theory (QDT) framework. Moreover, within a two-state model, deviations from universality are explained as being due to the coupling between the nonuniversal state and the universal states. Our work provides a simple intuitive Schrödinger-equation-based description of the energy spectra of heavy-light trimers and an alternative means to understanding the connection between universal trimers and Efimov trimers.

The remainder of this paper is organized as follows. Section II describes the hyperspherical framework. Section III determines the three-body energies as functions of $\delta(R_0)$ and $\kappa$ by solving the hyperradial Schrödinger equation numerically. Section IV develops an analytical description, which accounts for the universal and nonuniversal states of the energy spectrum. Finally, Sec. V summarizes.

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II. SYSTEM HAMILTONIAN

We model the interactions between the heavy and light particles by a zero-range two-body pseudopotential with s-wave scattering length \( a_s \). If we denote the heavy fermions of mass \( M \) as 1 and 2 and the light particle of mass \( m \) as 3, the Hamiltonian is given by

\[
H_{\text{tot}} = -\frac{\hbar^2}{2M} \left( \nabla_i^2 + \nabla_j^2 \right) - \frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{int}},
\]

where \( \vec{r}_i \) is the position vector of the \( i \)th particle, \( \nabla_i^2 \) is the Laplacian of the \( i \)th particle, and \( V_{\text{int}} = V_p(\vec{r}_{13}) + V_p(\vec{r}_{23}) \) with

\[
V_p(r_{ij}) = \frac{2\pi\hbar^2 a_s}{\mu_{2b}} \delta(\vec{r}_{ij}) - \frac{\partial \mu_{2b}}{\partial r_{ij}}.
\]

Here \( \mu_{2b} \) is the reduced mass of the heavy-light pair, \( \mu_{2b} = m \frac{\kappa}{\kappa^2 + 1} \), and \( r_{ij} = |\vec{r}_{ij}| = |\vec{r}_i - \vec{r}_j| \). The pseudopotential \( V_p \) imposes the Bethe-Peierls boundary condition on the three-body wave function in the limit \( r_{ij} \to 0 \).

To solve the Schrödinger equation for the Hamiltonian \( H_{\text{tot}} \), we separate the center-of-mass motion and write the relative wave function \( \Psi \) in terms of the hyperradius \( R \) and five hyperangles, collectively denoted by \( \Omega \) [11,18]. The hyperradius \( R \), which provides a measure of the overall size of the system, is defined by \( \mu R^2 = M(\vec{r}_i - \vec{R}_{\text{cm}})^2 + (\vec{r}_j - \vec{R}_{\text{cm}})^2 \), where \( \mu \) is the three-body reduced mass associated with the hyperradius, \( \mu = mk/\sqrt{2k + 1} \), and \( \vec{R}_{\text{cm}} \) denotes the center-of-mass vector. We expand the relative wave function \( \Psi \) in terms of a set of weight functions \( F_n(R, \Omega) \) and adiabatic channel functions \( \Phi_n(R; \Omega) \), which depend parametrically on the hyperradius \( R \) [19].

\[
\Psi(R, \Omega) = \sum_n R^{-5/2} F_n(R) \Phi_n(R; \Omega).
\]

The adiabatic channel functions \( \Phi_n(R; \Omega) \) satisfy the hyperangular Schrödinger equation at fixed \( R \),

\[
\left[ \frac{\Lambda^2}{4} + \frac{2\mu R^2}{\hbar^2} V_{\text{int}}(R, \Omega) \right] \Phi_n(R; \Omega) = \left[ s_0^2(R) - 4 \right] \Phi_n(R; \Omega).
\]

In Eq. (4), \( \Lambda \) denotes the grand angular momentum operator, which accounts for the kinetic energy associated with the hyperangles \( \Omega \) [18]. Inserting Eq. (3) into the relative Schrödinger equation yields a set of coupled equations for the weight functions \( F_n(R) \).

In the following we employ the adiabatic approximation, which neglects the coupling between the different channels [18,20,21]. This approximation has been shown to provide a qualitatively correct description for a number of three-body systems [11,22–24]. In this approximation, the hyperradial Schrödinger equation for the lowest adiabatic channel reads

\[
\frac{\hbar^2}{2\mu} \left[ \frac{d^2}{dR^2} - \frac{s_0^2(R) - 1/4}{R^2} + Q_{00}(R) \right] F_0(R) = EF_0(R),
\]

where \( Q_{00}(R) \) is the diagonal correction to the adiabatic energies,

\[
Q_{00}(R) = \left\{ \Phi_0(R; \Omega) \right\} \frac{\partial^2}{\partial R^2} \Phi_0(R; \Omega).
\]

We determine the three-body energies \( E \) using a two-step process. First we find the hyperangular eigenvalues \( s_0(R) \) and coupling elements \( Q_{00}(R) \). Then we solve the radial Schrödinger equation (5). For states with \( L^2 = 1^− \) symmetry and zero-range interactions, the scaled hyperangular eigenvalues \( s_0(R) \) can be obtained semianalytically by solving the transcendental equation [11,18]

\[
\frac{R}{a_s} = \sqrt{(s_0^2 - 1)(1 + 2\kappa)}^{1/4} \sec \left( \frac{s_0 \kappa}{2} \right) \frac{1}{2} \left( \frac{3}{2} - s_0 \right) \left( \frac{1}{2} + \frac{1}{2} \right) \left( \frac{3}{2} - s_0 \right) \left( \frac{5}{2} + 2\kappa \right) - 3(1 + \kappa) \sin \left( \frac{s_0 \kappa}{2} \right).
\]

For \( s_0(R) \geq 1 \) and \( R_0/a_s \to 0 \), the irregular solution is not normalizable and thus does not contribute, implying that \( F_0(R) \) goes to zero as \( R \to 0 \) [15–17]. In contrast, in the regime \( 0 < s_0 < 1 \) both solutions are well behaved and must be included when constructing the general solution [15–17]. We parametrize the short-range boundary condition of the wave function \( F_0(R) \) at \( R_0 \) using the logarithmic derivative \( L(F_0(R_0)) \),

\[
R_0 L(F_0(R_0)) = \frac{R_0 \frac{d}{dR} F_0(R)}{F_0(R)} \bigg|_{R_0} = \tan(\delta(R_0)),
\]

where \(-\pi/2 \leq \delta(R_0) \leq \pi/2\). We refer to \( \delta(R_0) \) as the short-range three-body or hyperradial phase. Using the parametrization given in Eq. (8), we cover all possible short-range
occur if the next section we discuss deviations from universality that
\(\kappa\) ratio \(\kappa\) with increasing bound states with \(\kappa\) for \(R_0/a_s = 0.0001\). The dashed lines labeled I and II mark the mass ratios \(\kappa_1\) and \(\kappa_2\), at which the universal states with energies \(E_{u,1}\) and \(E_{u,2}\) first become bound.

phases. In the special case of \(\delta(R_0) = \pi/2\) and \(R/a_s \to 0\), this boundary condition and the resulting three-body energies agree with those of Ref. [11]. We refer to this boundary condition as a universal boundary condition since the three-body states are completely determined by the regular solution. We refer to the corresponding states as universal states with energies \(E_{u,1}\) for \(\kappa_1 \leq \kappa \leq \kappa_2\) and \(E_{u,1}\) and \(E_{u,2}\) for \(\kappa_2 \leq \kappa \leq 13.606\). In the next section we discuss deviations from universality that occur if \(\delta(R_0)\) is not equal to \(\pi/2\). These deviations increase with increasing \(\kappa\) (for a fixed \(R_0\)) and increasing \(R_0\) (for a fixed \(\kappa\)).

III. NUMERICAL TREATMENT

In this section we examine the behavior of the three-body bound states with \(L^{11} = 1^−\) symmetry, obtained numerically using the shooting algorithm, as a function of the logarithmic derivative boundary condition for selected mass ratios. The three-body energies \(E\) for \(\kappa = 8.6\) and 10 are shown in Figs. 2(a) and 2(b), respectively. Dotted, dashed, and dash-dotted lines show \(E\) as a function of the three-body phase \(\delta\) for \(R_0/a_s = 0.0001, 0.0003,\) and 0.001, respectively. In Fig. 2 the three-body energies have been scaled by the zero-range two-body binding energy \(E_{2b}\). The three-body state becomes unbound with respect to the breakup into a dimer and an atom for \(E/E_{2b} > -1\). For \(\kappa = 8.6\) and \(\delta = \pi/2\), the system supports one three-body bound state. For \(R_0/a_s = 0.0001\) and \(\kappa = 8.6, E/E_{2b}\) is nearly constant for \(\delta \gtrless -0.5\). At \(\delta \approx -0.5\), referred to as the critical angle \(\delta_c(R_0)\), the energy rapidly goes to a large negative value and a second bound state, whose energy is approximately equal to \(E_{u,1}\), is supported for \(\delta < \delta_c(R_0)\). Here \(\delta_c\) is the phase at which the nonuniversal three-body state first becomes bound with respect to the dimer threshold, i.e., for which the numerically obtained three-body energy is equal to \(-E_{2b}\). We refer to the feature in the vicinity of \(\delta_c\) as three-body resonance. As \(R_0/a_s\) increases [see dashed and dash-dotted lines in Fig. 2(a)] the width of the three-body resonance increases. Note, however, that the deviations from \(E_{u,1}\) are small for all \(R_0/a_s\) considered, except for three-body phases very close to \(\delta_c(R_0)\). As \(\kappa\) increases [see Fig. 2(b)], the overall behavior of the energy spectrum is unchanged. The key trends with increasing \(\kappa\) are that, at a fixed \(R_0\), the energy away from \(\delta_c(R_0)\) becomes more negative and both \(\delta_c(R_0)\) and the width of the three-body resonance increase (see also symbols in Figs. 3 and 7).

For \(\kappa \gtrsim \kappa_2\), the three-body system supports a second bound state. As an example, Fig. 3 shows the three-body bound state energy for \(\kappa = 13\) and \(R_0/a_s = 0.0001\) as a function of \(\delta\). Away from \(\delta_c(R_0) \approx 0.15\), there exist two bound states whose energies depend weakly on \(\delta\). For \(\delta > \delta_c\), the corresponding hyperradial functions \(\Phi_0(R)\) possess 0 nodes and 1 node, respectively. For \(\delta < \delta_c\), the corresponding hyperradial functions \(\Phi_0(R)\) possess 1 node and 2 nodes.

FIG. 1. Hyperangular eigenvalue \(s_0(R_0)\) as a function of the mass ratio \(\kappa\) for \(R_0/a_s = 0.0001\). The dashed lines labeled I and II mark the mass ratios \(\kappa_1\) and \(\kappa_2\), at which the universal states with energies \(E_{u,1}\) and \(E_{u,2}\) first become bound.

FIG. 2. (Color online) Dotted, dashed, and dash-dotted lines show the scaled three-body energy \(E/E_{2b}\) as a function of \(\delta\) using \(R_0/a_s = 0.0001, 0.0003,\) and 0.001, respectively, for (a) \(\kappa = 8.6\) and (b) \(\kappa = 10\). The solid horizontal lines show the energy \(E_{u,1}\) of the universal state and the solid vertical lines show the energy \(E_{nu}\) of the nonuniversal state in the two-state model (see Sec. IV) for \(R_0/a_s = 0.001\).

FIG. 3. Solid lines show the scaled three-body energies \(E/E_{2b}\) as a function of \(\delta\) for \(\kappa = 13\) and \(R_0/a_s = 0.0001\). The three-body resonance is located at \(\delta_c \approx 0.15\).
respectively. This reflects the fact that a new bound state is being pulled in at $\delta = \delta_c(R_0)$.

In general, we find that $\delta_c(R_0)$ depends relatively weakly on $R_0$ as long as $R_0/\alpha_s < 1$. Moreover, the three-body energy depends relatively strongly on $R_0$ in the vicinity of $\delta_c$ but comparatively weakly on $R_0$ away from $\delta_c$. This suggests that the states near $\delta_c$ and away from $\delta_c$ can be classified as nonuniversal and universal, respectively. This interpretation is corroborated by our analysis of the hyperradial wave function $F_0(R)$ for $\kappa = 10$, $R_0/\alpha_s = 0.0001$, and $\delta \approx \delta_c$. The main part of Fig. 4 shows that the wave function has an appreciable amplitude in the small-$R/\alpha_s$ region, signaling nonuniversal behavior.

Away from $\delta_c$, in contrast, $F_0(R)$ has a vanishingly small amplitude in the small-$R/\alpha_s$ region (see the inset of Fig. 4). We find that $F_0(R)$ depends fairly weakly on $R_0$ when $\delta$ is away from $\delta_c$, lending further support to our assertion that the three-body system behaves universally in this region. For larger $R_0/\alpha_s$ we observe deviations from universality for a larger range of three-body phases. Similar nonuniversal behavior has been previously reported for the three-body system at unitarity [13,14] and for the four-body system with positive $s$-wave scattering length [25].

IV. ANALYTICAL TREATMENT

Section IV A applies a QDT framework to predict the short-range phase $\delta_c(R_0)$ at which the nonuniversal state first becomes bound. Section IV B develops a two-state model to describe the behavior of the universal and nonuniversal states as a function of $\delta(R_0)$.

A. The QDT treatment

To predict the short-range phase $\delta_c(R_0)$ at which the nonuniversal state first becomes bound with respect to the breakup into a dimer and an atom we apply QDT [13,14,26,27]. In the short-range limit, i.e., for $R \ll \alpha_s$, where $s_0(R)$ approaches a constant, the wave function $F_0(R)$ can be approximated by [13,14]

$$F_{SR}(R) = \sqrt{R} J_{\delta_c(R)} \left( \frac{2\mu E}{\hbar^2} R \right) - \tan(\pi \alpha) Y_{\delta_c(R)} \left( \frac{2\mu E}{\hbar^2} R \right),$$

where $J_{\delta_c(R)}$ and $Y_{\delta_c(R)}$ denote the Bessel functions of the first and second kinds, respectively. The quantum defect $\alpha$ controls the relative contribution of the regular solution $J_{\delta_c(R)}$ and the irregular solution $Y_{\delta_c(R)}$. A new three-body state is expected to be pulled in when the hyperradial solution is dominated by the irregular solution, i.e., for $\alpha = 1/2$. The critical angle $\delta_c(R_0)$ is then given by

$$\tan \delta_c(R_0) = \Re \{ R_0 L(F_{SR}(R_0)) \},$$

where $\Re$ denotes the real part and $F_{SR}(R_0)$ is evaluated for $E = -E_{2b}$ and $\alpha = 1/2$. In Eq. (10), we take the real part since we restricted ourselves to real-valued logarithmic derivatives in Sec. III.

The solid, dotted, and dashed lines in Fig. 5 show $\delta_c(R_0)$ determined using the QDT framework for $R_0/\alpha_s = 0.0001$, 0.0003 and 0.001, respectively. It is interesting to note that $\delta_c(R_0)$ is very weakly dependent on $R_0$ for small $\kappa$. The symbols in Fig. 5 show the critical angle $\delta_c(R_0)$ obtained by analyzing the numerical solutions of the hyperradial Schrödinger equation (5) for $R_0/\alpha_s = 0.0001$. The numerical results are in excellent agreement with the QDT prediction. For $\kappa \geq 13$ (see the inset of Fig. 5), the dependence of $\delta_c$ on $R_0$ becomes more pronounced. Figure 5 shows that the three-body system supports a nonuniversal bound state not only for $\kappa \gtrsim 8.619$, but also for $\kappa \lesssim 8.619$ [for $\kappa = 8.619$ one has $s_0(0) = 1$]. Thus it may be surprising at first sight that the system supports a nonuniversal state for $\kappa \gtrsim 8.619$ since the irregular solution cannot be normalized if $s_0 > 1$ for $R_0/\alpha_s \to 0$. However, since we impose the boundary condition at a finite $R_0/\alpha_s$ and not at $R_0/\alpha_s = 0$, the resulting wave function can, even though it contains an admixture of the irregular solution, be normalized. Correspondingly, nonuniversal states can exist for $\kappa < 8.619$. In fact, we find that the system supports a nonuniversal bound state even for
\[ \kappa < \kappa_1, \text{i.e., for mass ratios where universal states are not supported. The nonuniversal states for } \kappa < \kappa_1 \text{ are similar to those for } \kappa > \kappa_1, \text{ with appreciable amplitude in the small-} R/\alpha_c \text{ region.} \]

### B. Two-state model

In this section we develop a two-state model that describes the behavior of the universal and nonuniversal states as a function of \( \delta(R_0) \). In our model the three-body resonance is an avoided crossing at \( \delta_c(R_0) \) between the universal state with energy \( E_u \) and a nonuniversal state with energy \( E_{nu} \). The energy of the universal state is the bound-state energy \( E \) calculated using the universal boundary condition \( \delta = \pi/2 \) and \( R/\alpha_i \to 0 \). In Fig. 6 we plot the quantity \( (E - E_u)/E_{2b} \) as a function of \( \delta - \delta_c \). The thick solid, dotted, and dashed lines correspond to \( \kappa = 10, 12.4, \text{ and } 13, \) respectively, with \( R_0/\alpha_i = 0.0001 \) and \( E_{nu} = E_{nu,1} \). The circles correspond to \( \kappa = 13, R_0/\alpha_i = 0.0001, \text{ and } E_{nu} = E_{nu,2} \).

Motivated by Fig. 6, we write the energy of the nonuniversal state as \( E_{nu} = E_u + \mathcal{A} [\delta - \delta_c(R_0)] \), where \( \mathcal{A} \) is a dimensionless scaling constant; in our analysis we use \( \mathcal{A} = 0.00007 \). This model provides a quantitatively correct description of the three-body spectra. Moreover, it provides an intuitive physical picture in which deviations from universality arise due to the coupling of the universal states to the nonuniversal state.

The circles, diamonds, and squares in Fig. 7 show \( \beta \) for \( E_u = E_{nu,1} \) and \( R_0/\alpha_i = 0.0001, 0.0003, \text{ and } 0.001, \) respectively, as a function of \( \kappa \). The value of \( \beta/E_{2b} \) increases with increasing \( \kappa \) for fixed \( R_0 \). Moreover, the dependence of \( \beta/E_{2b} \) on the value of \( R_0 \) increases with increasing \( \kappa \). Since \( \beta \) determines the coupling between the universal state and the nonuniversal state, it can be used to quantify the deviations from universality. For mass ratios larger than those considered in this work, the heavy-light trimer system supports three-body bound states with Efimov character [28–30]. Within the zero-range framework employed here, the exact number and energy of the Efimov trimers supported depends on the short-range hyperradial boundary condition. If the hyperradial boundary condition is fixed and \( \kappa \) is varied, the energy spectrum changes smoothly from (i) deviating from the universal spectrum only in a small region around \( \delta_c \) to (ii) deviating from the universal spectrum for a fairly large range of \( \delta \) to (iii) supporting three-body states with Efimov character for \( \kappa \gtrsim 13.606 \). Thus the deviations from universality discussed in this paper can be interpreted as connecting the universal states predicted by Kartavtsev and Malych and the Efimov trimers.

In Ref. [12] the authors imposed a momentum cutoff \( \Lambda_c \) in the Skorniakov–Ter-Martirosian equation and used the quantity \( \frac{E - E_{nu}}{E_{nu}}(i = 1 \text{ or } 2) \) to determine the boundary of the universal states predicted by Kartavtsev and Malych and the crossover trimers in the \( \kappa\Lambda_c(a_i)^{-1} \) parameter space. The momentum cutoff was introduced in two ways, using a sharp and a Gaussian cutoff. We speculate that in our formulation a change in the three-body phase and/or hyperradius \( R_0 \) corresponds to a change in \( \Lambda_c \). A crossover trimer, in turn, corresponds to a trimer whose energy deviates appreciably from \( E_{nu,i} \). While the deviations from \( E_{nu,i} \) are, in our formulation, linked to the coupling of the universal state to a nonuniversal state, the treatment by Endo et al. does not seem to yield an analogous physical picture. Additionally we speculate that while Ref. [12] employs two different models predicted by the two-state Hamiltonian to the numerically determined energies. Thin dashed lines in Fig. 6 show the results for the two-state model. It can be seen that the two-state model provides a quantitatively correct description of the three-body spectra. Moreover, it provides an intuitive physical picture in which deviations from universality arise due to the coupling of the universal states to the nonuniversal state.

![Fig. 6](image1.png)

**Fig. 6.** (Color online) Thick solid, dotted, and dashed lines show the quantity \( (E - E_u)/E_{2b} \) as a function of \( \delta - \delta_c \) for \( R_0/\alpha_i = 0.0001 \) and \( \kappa = 10, 12.4, \text{ and } 13, \) respectively. The circles show the quantity \( (E - E_{nu,2})/E_{2b} \) for \( R_0/\alpha_i = 0.0001 \) and \( \kappa = 13. \) The thin dashed lines show the results of the two-state model.

![Fig. 7](image2.png)

**Fig. 7.** (Color online) Circles, diamonds, and squares show the off-diagonal coupling \( \beta/E_{2b} \) used in the two-state model (11) as a function of \( \kappa \) for \( R_0/\alpha_i = 0.0001, 0.0003, \text{ and } 0.001, \) respectively, on a logarithmic scale. We used \( E_u = E_{nu,1} \) in the two-state model. The dependence of \( \beta/E_{2b} \) on the value of \( R_0 \) increases with increasing \( \kappa \).
for the momentum cutoff $\Lambda_{\nu}$, it does not explore the entirety of the $(R_0, \delta(R_0))$ parameter space. In the future it will be interesting to investigate the precise connection between the formulations in the coordinate and momentum spaces by, e.g., comparing the wave functions. Such a comparison is needed to check if the above correspondences are correct.

V. CONCLUSION

In this paper we studied a system of two identical heavy fermions of mass $M$ and a light particle of mass $m$ with zero-range two-body interspecies interactions. In particular, we looked at deviations of the three-body bound-state energies from the universal energies $E_{u,1}$ for $\kappa > \kappa_1$ and $E_{u,1}$ and $E_{u,2}$ for $\kappa_2 < \kappa \lesssim 13.606$ as a function of the hyperradial short-range boundary condition. We imposed a short-range phase $\delta(R_0)$ using a logarithmic derivative boundary condition at various hyperradii $R_0$. This parametrization allowed us to explore the full range of possible short-range boundary conditions.

We found that (i) for $\delta(R_0) = \pi/2$ the universal states with energies $E_{u,1}$ and $E_{u,2}$, predicted by Kartavtsev and Malykh [11], are recovered; (ii) the three-body states deviate from universality in the vicinity of a three-body resonance located at the short-range phase $\delta_0(R_0)$, at which the nonuniversal state is first bound; (iii) the deviations from universality increase with increasing mass ratio $\kappa$ (at fixed $R_0$) and with increasing $R_0$ (at fixed $\kappa$); (iv) QDFT accurately predicts the values of $\delta_0(R_0)$; (v) a two-state model quantitatively describes the behavior of the universal and nonuniversal states as a function of $\delta(R_0)$; and, finally, (vi) the nonuniversal bound state exists for $\kappa < \kappa_1$ even though universal bound states are not supported in this regime. For well-behaved finite-range model interactions, the three-body short-range phase is set by the Hamiltonian and is not a free parameter. Thus the realization of three-body resonances does, in general, require some fine-tuning. This interpretation is consistent with the fact that three-body resonances have been predicted for heavy-light mixtures at unitarity interacting through a Gaussian model potential for just one specific mass ratio [13,14].

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