

Universal description of the rotational-vibrational spectrum of three particles with zero-range interactions

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Submitted 26 September 2007

A comprehensive universal description of the rotational-vibrational spectrum for two identical particles of mass m and the third particle of mass m_1 in the zero-range limit of the interaction between different particles is given for arbitrary values of the mass ratio m/m_1 and the total angular momentum L . It is found that the number of vibrational states is determined by the functions $L_c(m/m_1)$ and $L_b(m/m_1)$. Explicitly, if the two-body scattering length is positive, the number of states is finite for $L_c(m/m_1) \leq L \leq L_b(m/m_1)$, zero for $L > L_b(m/m_1)$, and infinite for $L < L_c(m/m_1)$. If the two-body scattering length is negative, the number of states is zero for $L \geq L_c(m/m_1)$ and infinite for $L < L_c(m/m_1)$. For the finite number of vibrational states, all the binding energies are described by the universal function $\varepsilon_{LN}(m/m_1) = \mathcal{E}(\xi, \eta)$, where $\xi = (N - 1/2)/\sqrt{L(L+1)}$, $\eta = \sqrt{m/m_1 L(L+1)}$, and N is the vibrational quantum number. This scaling dependence is in agreement with the numerical calculations for $L > 2$ and only slightly deviates from those for $L = 1, 2$. The universal description implies that the critical values $L_c(m/m_1)$ and $L_b(m/m_1)$ increase as $0.401\sqrt{m/m_1}$ and $0.563\sqrt{m/m_1}$, respectively, while the number of vibrational states for $L \geq L_c(m/m_1)$ is within the range $N \leq N_{\max} \approx 1.1\sqrt{L(L+1)} + 1/2$.

PACS: 03.65.Ge, 03.75.Ss, 21.45.+v, 36.90.+f

The universal low-energy few-body dynamics of two-species compounds is of much interest both for atomic and many-body physics. In this respect, the study of the three-body energy spectrum gives insight into the role of triatomic molecules and few-body scattering. The area of applications includes the investigation of multi-component ultra-cold quantum gases, e. g., binary Fermi-Bose [1, 2] and Fermi [3–5] mixtures and of impurities embedded in a quantum gas [6, 7], which are presently under thorough experimental and theoretical study. In addition, one should mention the reactions with negative atomic and molecular ions [8, 9].

The universal isotopic dependence of the three-body energy spectrum was multiply discussed [10–14], nevertheless, the main objective was the description of Efimov's spectrum. Recently, the infinite number of the 1^+ bound states was predicted [15] for three identical fermions with the resonant p -wave interaction. Concerning the low-energy scattering, one should mention a two-hump structure in the isotopic dependence of the three-body recombination rate of two-component fermions [16–18] and the two-component model for the three-body recombination near the Feshbach resonance [19].

The main aim of the paper is a comprehensive description of the finite three-body rotational-vibrational spectrum in the zero-range limit of the interaction between different particles. Both qualitative and numerical results are obtained by using the solution of hyper-

radial equations (HREs) [20–22]. The detailed study of the bound state and scattering problems for the total angular momentum $L = 1$ was presented in [18].

Particle 1 of mass m_1 and two identical particles 2 and 3 of mass m are described by using the scaled Jacobi variables $\mathbf{x} = \sqrt{2\mu}(\mathbf{r}_2 - \mathbf{r}_1)$, $\mathbf{y} = \sqrt{2\bar{\mu}}[\mathbf{r}_3 - (m_1\mathbf{r}_1 + m\mathbf{r}_2)/(m_1 + m)]$ and the corresponding hyper-spherical variables $x = \rho \cos \alpha$, $y = \rho \sin \alpha$, $\hat{\mathbf{x}} = \mathbf{x}/x$, and $\hat{\mathbf{y}} = \mathbf{y}/y$, where \mathbf{r}_i is the position vector of the i th particle and $\mu = mm_1/(m + m_1)$ and $\bar{\mu} = m(m + m_1)/(m_1 + 2m)$ are the reduced masses. In the universal low-energy limit, only the s-wave interaction between different particles will be taken into account provided the s-wave interaction is forbidden between two identical fermions and is strongly suppressed between two heavy bosons in the states of $L > 0$. The two-body interaction is defined by imposing the boundary condition at the zero inter-particle distance, which depends on a single parameter, e. g., the two-body scattering length a [18]. This type of interaction is known in the literature as the zero-range potential [23], the Fermi [24] or Fermi-Huang [25] pseudo-potential, and an equivalent approach is used in the momentum-space representation [26]. The units $\hbar = 2\mu = |a| = 1$ are used throughout; thus, the binding energy becomes the universal function depending on the mass ratio m/m_1 and the rotational-vibrational quantum numbers L and N . In view of the wave-function symmetry under permutation of identical particles, a sum of

two interactions between different particles is expressed by a single boundary condition at the zero distance between particles 1 and 2,

$$\lim_{\alpha \rightarrow \pi/2} \left[\frac{\partial}{\partial \alpha} - \tan \alpha - \rho \frac{a}{|a|} \right] \Psi = 0. \quad (1)$$

The problem under study is conveniently treated by using the expansion of the properly symmetrized wave function,

$$\Psi = (1 + S\hat{P}) \frac{Y_{LM}(\hat{\mathbf{y}})}{\rho^{5/2} \sin 2\alpha} \sum_{n=1}^{\infty} f_n(\rho) \varphi_n^L(\alpha, \rho), \quad (2)$$

which leads to the hyper-radial equations for the functions $f_n(\rho)$ [18]. Here \hat{P} denotes permutation of the identical particles 2 and 3, $S = 1$ and $S = -1$ if these particles are bosons and fermions, respectively, $Y_{LM}(\hat{\mathbf{y}})$ is the spherical function. The action of \hat{P} on the angular variables in the limit $\alpha \rightarrow \pi/2$ is given by $\hat{P}Y_{LM}(\hat{\mathbf{y}}) \rightarrow (-1)^L Y_{LM}(\hat{\mathbf{y}})$ and $\hat{P}\alpha \rightarrow \omega$, where $\omega = \arcsin(1 + m_1/m)^{-1}$. The functions $\varphi_n^L(\alpha, \rho)$ in the expansion (2) are the solutions of the equation on a hypersphere (at fixed ρ),

$$\left[\frac{\partial^2}{\partial \alpha^2} - \frac{L(L+1)}{\sin^2 \alpha} + \gamma_n^2(\rho) \right] \varphi_n^L(\alpha, \rho) = 0, \quad (3)$$

complemented by the boundary conditions $\varphi_n^L(0, \rho) = 0$ and

$$\lim_{\alpha \rightarrow \pi/2} \left(\frac{\partial}{\partial \alpha} - \rho \frac{a}{|a|} \right) \varphi_n^L(\alpha, \rho) = \frac{2S(-)^L}{\sin 2\omega} \varphi_n^L(\omega, \rho), \quad (4)$$

where a set of discrete eigenvalues $\gamma_n^2(\rho)$ plays the role of the effective channel potentials in a system of the hyper-radial equations [18]. The functions satisfying Eq. (3) and the zero boundary condition are straightforwardly expressed [27] via the Legendre function

$$\varphi_n^L(\alpha, \rho) = \sqrt{\sin \alpha} Q_{\gamma_n(\rho)-1/2}^{L+1/2}(\cos \alpha) \equiv \phi_{L, \gamma_n(\rho)}(\alpha). \quad (5)$$

The functions $\phi_{L, \gamma}(\alpha)$ are odd functions on both variables γ and α satisfying the recurrent relations $\sin \alpha \phi_{L+1, \gamma}(\alpha) = (\gamma - L - 1) \cos \alpha \phi_{L, \gamma}(\alpha) - (\gamma + L) \phi_{L, \gamma-1}(\alpha)$, which follow from those for the Legendre functions. It is convenient to write $\phi_{L, \gamma}(\alpha) = A_{L, \gamma}(\cot \alpha) \sin \gamma \alpha + B_{L, \gamma}(\cot \alpha) \cos \gamma \alpha$, where $A_{L, \gamma}(x)$ and $B_{L, \gamma}(x)$ are simple polynomials on γ and x , which are explicitly given for few lowest L by $A_{0, \gamma}(x) = 1$, $B_{0, \gamma}(x) = 0$, $A_{1, \gamma}(x) = -x$, $B_{1, \gamma}(x) = \gamma$, $A_{2, \gamma}(x) = 1 - \gamma^2 + 3x^2$, $B_{2, \gamma}(x) = -3\gamma x$, $A_{3, \gamma}(x) = 3x(2\gamma^2 - 3 - 5x^2)$, and $B_{3, \gamma}(x) = \gamma(15x^2 + 4 - \gamma^2)$. Substituting (5) into

the boundary condition (4) and using the identity $\phi_{L+1, \gamma}(\pi/2) = \left. \frac{\partial \phi_{L, \gamma}(\alpha)}{\partial \alpha} \right|_{\alpha=\pi/2}$ one comes to the transcendental equation for $\gamma_n^2(\rho)$,

$$\rho \frac{a}{|a|} \phi_{L, \gamma}(\pi/2) = \phi_{L+1, \gamma}(\pi/2) - \frac{2S(-)^L}{\sin 2\omega} \phi_{L, \gamma}(\omega). \quad (6)$$

The attractive lowest effective potential determined by $\gamma_1^2(\rho)$ plays the dominant role for the binding-energy and low-energy-scattering calculations, while the effective potentials in the upper channels for $n \geq 2$ contain the repulsive term $\gamma_n^2(\rho)/\rho^2$ and are of minor importance. Thus, a fairly good description will be obtained by using the one-channel approximation for the total wave function (2) where the first-channel radial function satisfies the equation [18]

$$\left[\frac{d^2}{d\rho^2} - \frac{\gamma_1^2(\rho) - 1/4}{\rho^2} + E \right] f_1(\rho) = 0. \quad (7)$$

Note that the diagonal coupling term is omitted in Eq. (7), which does not affect the final conclusions and leads to the calculation of a lower bound for the exact three-body energy. Our calculations [18] shows that the one-channel approximation provides better than few percent overall accuracy of the binding energy.

The most discussed feature [10–13] of the three-body system under consideration is the infinite number of the bound states for small L and large m/m_1 (more precisely, for the finite interaction radius r_0 the number of states unrestrictedly increases with increasing $|a|/r_0$). As the effective potential in (7) is approximately given by $(\gamma_1^2(0) - 1/4)/\rho^2$ at small ρ , the number of vibrational states is finite (infinite) if $\gamma_1^2(0) > 0$ ($\gamma_1^2(0) < 0$). According to Eq. (6), $\gamma_1^2(0)$ decreases with increasing m/m_1 and becomes zero at the critical value $(m/m_1)_{cL}$. Thus, one can define the step-like function $L_c(m/m_1)$, which increases by unity at the points $(m/m_1)_{cL}$, so that the number of vibrational states is infinite for $L < L_c(m/m_1)$ and finite for $L \geq L_c(m/m_1)$. Solving Eq. (6) at $\gamma_1 \rightarrow 0$ and $\rho \rightarrow 0$, one obtains the exact values $(m/m_1)_{cL}$, which approximately equal 13.6069657, 38.6301583, 75.9944943, 125.764635, and 187.958355 for $L = 1 - 5$. Originally, the dependence $L_c(m/m_1)$ was discussed in [10].

Analyzing the eigenvalue equation (6) one concludes that for $a > 0$ and $S(-)^L = -1$ the effective potential exceeds the threshold energy $E = -1$, $\gamma_1^2(\rho)/\rho^2 > -1$, therefore, the bound states only exist if either two identical particles are bosons and L is even or two identical particles are fermions and L is odd. Furthermore, one obtains the trivial answer if $a < 0$ and $L \geq L_c(m/m_1)$, for which $\gamma_1^2(\rho) > 0$ and there are no three-body bound states.

The mass-ratio dependence of the binding energies $\varepsilon_{LN}(m/m_1)$ for $L \geq L_c(m/m_1)$ and $a > 0$ is determined numerically by seeking the square-integrable solutions to Eq. (7). Mostly, the properties of the energy spectrum are similar to those for $L = 1$, which were carefully discussed in [18]. For given L , there is the critical value of m/m_1 at which the first bound state arise, in other words, there are no three-body bound states for $L \geq L_b(m/m_1)$, where the step-like function $L_b(m/m_1)$ undergoes unity jumps at those critical values. Furthermore, all the bound states arise at some values of m/m_1 being the narrow resonances just below them. For the mass ratio near these values, the binding energies and resonance positions depend linearly and the resonance widths depend quadratically on the mass-ratio excess. Exactly at these values one obtains the threshold bound states, whose wave functions are square-integrable with a power fall-off at large distances. A set of these values of m/m_1 (more precisely, the lower bounds for them) is obtained numerically and presented in Table. With increasing m/m_1 , the binding energies monotonically increase reaching the finite values (shown in Table) at $(m/m_1)_{cL}$; just below $(m/m_1)_{cL}$ they follow the square-root dependence on the difference $m/m_1 - (m/m_1)_{cL}$. Correspondingly, the number of the vibrational states increases with increasing m/m_1 taking the finite number N_{\max} at $(m/m_1)_{cL}$ and jumping to infinity beyond $(m/m_1)_{cL}$; in the present calculations $N_{\max} = L + 1$ for $L < 9$ and $N_{\max} = L + 2$ for $10 \leq L \leq 12$.

N	$L = 1$	$L = 2$	$L = 3$	$L = 4$	$L = 5$
1	7.9300	22.342	42.981	69.885	103.06
2	12.789	31.285	55.766	86.420	123.31
3	-	37.657	67.012	101.92	142.82
4	-	-	74.670	115.08	160.64
5	-	-	-	123.94	175.48
6	-	-	-	-	185.51
1	5.906	12.68	22.59	35.59	52.16
2	1.147	1.850	2.942	4.392	6.216
3	-	1.076	1.417	1.920	2.566
4	-	-	1.057	1.273	1.584
5	-	-	-	1.049	1.206
6	-	-	-	-	1.045

Upper part: Mass ratios for which the N -th bound state of the total angular momentum L arises. Lower part: Binding energies ε_{LN} for the mass ratio fixed at $(m/m_1)_{cL}$

A comprehensive description of the spectrum is obtained by using the large- L (correspondingly, large- m/m_1) asymptotic expression for the binding energies $\varepsilon_{LN}(m/m_1)$. Taking the quasi-classical solution of Eq. (3) satisfying the zero boundary condition,

$$\phi_{L,i\kappa}(\alpha) = \exp\left(\kappa \arccos \frac{x \cos \alpha}{\sqrt{1+x^2}}\right) \times \left(\frac{\sqrt{1+x^2 \sin^2 \alpha} - \cos \alpha}{\sqrt{1+x^2 \sin^2 \alpha} + \cos \alpha}\right)^{L/2+1/4}, \quad (8)$$

where $\gamma_1 = i\kappa$ and $x = \kappa/(L + 1/2)$, one writes the eigenvalue equation (6) in the form,

$$\frac{\rho}{L + 1/2} = \sqrt{1+x^2} - \frac{2 \exp\left(\kappa \arcsin \frac{x \cos \omega}{\sqrt{1+x^2}}\right)}{(L + 1/2) \sin 2\omega} \times \left(\frac{\sqrt{1+x^2 \sin^2 \omega} - \cos \omega}{\sqrt{1+x^2 \sin^2 \omega} + \cos \omega}\right)^{L/2+1/4}. \quad (9)$$

In the limit of large L and m/m_1 the eigenvalue equation (9) reduces to

$$\rho \cos \omega = u - e^{-u}, \quad (10)$$

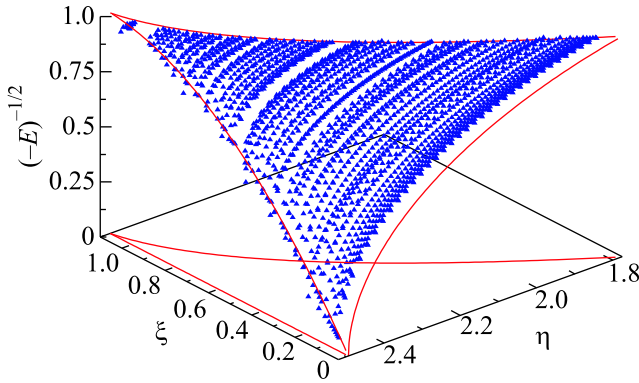
where $u = \cos \omega \sqrt{\kappa^2 + (L + 1/2)^2}$. Notice that taking the limit $\kappa \rightarrow 0$ and $\rho \rightarrow 0$ in (10) one immediately obtains the relation $\cos \omega_{cL} = u_0/(L + 1/2)$, where $\sin \omega_{cL} = (m/m_1)_{cL}/[1 + (m/m_1)_{cL}]$ and $u_0 \approx 0.567143$ is the root of the equation $u = e^{-u}$; as a result, one finds the asymptotic dependence $(m/m_1)_{cL} \approx 6.2179(L + 1/2)^2$ and the inverse relation $L_c(m/m_1) \approx (u_0 \sqrt{2m/m_1} - 1)/2 \approx 0.40103 \sqrt{m/m_1} - 1/2$. Now the asymptotic dependence $\varepsilon_{LN}(m/m_1)$ for large L and m/m_1 can be obtained by the quasi-classical solution of (7) with $\gamma_1^2(\rho) = (L + 1/2)^2 - [u(\rho)/\cos \omega]^2$ and $u(\rho)$ determined by (10),

$$\int_{u_-}^{u_+} \frac{du(1+e^u)}{ue^u-1} \sqrt{\frac{u^2 - \varepsilon_{LN}(u - e^{-u})^2}{L(L+1) \cos^2 \omega}} - 1 = \pi \frac{N - 1/2}{\sqrt{L(L+1)}}, \quad (11)$$

where u_- and u_+ are zeros of the integrand.

Following Eq. (11), one expects to express the binding energies via the universal function $\varepsilon_{LN}(m/m_1) = \mathcal{E}(\xi, \eta)$ of two scaled variables $\xi = (N - 1/2)/\sqrt{L(L+1)}$ and $\eta = \sqrt{m/m_1 L(L+1)}$. This two-parameter dependence is confirmed by the numerical calculations (up to $m/m_1 \sim 700$), which reveal that the calculated energies for $L > 2$ lie on a smooth surface as shown in Figure. Even for the smallest $L = 1, 2$ the calculated energies are in good agreement with the two-parameter dependence showing only a slight deviation from the surface.

The variables ξ and η take values within the area limited by the line $\xi = 0$, the line $\eta = \eta_{\max} \approx \sqrt{2}/u_0 \approx 2.493574$ stemming from the condition of finiteness of



Universal dependence of the bound-state energy E on the scaled variables $\xi = (N - 1/2)/\sqrt{L(L + 1)}$ and $\eta = \sqrt{m/m_1}L(L + 1)$. The calculated values for $L = 3, 12$ are plotted by symbols. The surface boundary and its projection on the $\xi - \eta$ plane are shown by solid lines

bound states $L \geq L_c(m/m_1)$, and the line $\mathcal{E}(\xi, \eta) = 1$ expressing the condition of arising of the bound states at the two-body threshold. As shown in Figure, the smallest value $\eta = \eta_{\min}$ is at $\xi = 0$, which corresponds to the condition of arising of the first bound state in the large- L limit. To find it one requires that $u_+ = u_- \equiv u_b$ at $\varepsilon_{LN} = 1$ in Eq. (10), which leads to $\eta_{\min} \approx \sqrt{2/(u_b^2 - 1)} \approx 1.775452$, where $u_b \approx 1.278465$ is the root of the equation $u = 1 + e^{-u}$. This gives the asymptotic dependence for arising of the first bound state, $L_b \approx \eta_{\min}^{-1} \sqrt{m/m_1} - 1/2 \approx 0.563237 \sqrt{m/m_1} - 1/2$. At the line $\eta = \eta_{\max}$ the variable ξ takes its largest value ξ_{\max} , which determines the large- L dependence of the number of the vibrational states N_{\max} for a given L . The calculation of the quasi-classical integral (11) gives $u_- = u_0$, $u_+ \approx 2.872849$,

$$\xi_{\max} = \frac{1}{\pi u_0} \int_{u_-}^{u_+} \frac{1 + e^{-u}}{u e^u - 1} \sqrt{e^u (2u - u_0^2 e^u) - 1} du \approx 1.099839,$$

and the large- L estimate $N_{\max} = \xi_{\max} \sqrt{L(L + 1)} + 1/2$. Taking the entire part of this expression, one can predict that the dependence $N_{\max} = L + 1$ for $L < 10$ changes to $N_{\max} = L + 2$ at $L = 10$, which is in agreement with the numerical result.

The universal surface $\mathcal{E}(\xi, \eta)$ is bound by three lines, which are described by fitting the calculated energies for $L \geq 3$ to simple dependencies plotted in Figure. As a result, the line defined by $\mathcal{E}(\xi, \eta) = 1$ is fairly well fitted to $\eta = (\eta_{\min} + a\xi)[1 - c\xi(\xi - \xi_{\max})]$, where $a = (\eta_{\max} - \eta_{\min})/\xi_{\max} \approx 0.652933$ is fixed by the evident condition $\mathcal{E}(\xi_{\max}, \eta_{\max}) = 1$ and the only fitted parameter is $c = 0.1865$. Furthermore, the analysis shows that the next boundary line defined by $\eta = \eta_{\max}$ is described

by $\mathcal{E}^{-1/2}(\xi, \eta_{\max}) = a_1 \xi (1 - a_2 \xi) [1 - c_1 \xi (\xi - \xi_{\max})]$, where $a_1 = 1 + u_0 \approx 1.56714$ is fixed by the asymptotic behaviour of the integral (11) at $L \rightarrow \infty$ and $\eta = \eta_{\max}$, $a_2 \approx 0.38171$ is fixed by the condition $a_1 \xi_{\max} (1 - a_2 \xi_{\max}) = 1$, and the only fitted parameter is $c_1 = 0.1881$. In particular, at the critical mass ratio the binding energy of the deep states in the limit of large L is described by $\mathcal{E}(\xi, \eta_{\max}) \rightarrow (a_1 \xi)^{-2}$, i. e., $\varepsilon_{NL}[(m/m_1)_{cL}] = L(L + 1)/(N - 1/2)^2 (1 + u_0)^2$. The third boundary line at $\xi \rightarrow 0$ is described by the dependence $\mathcal{E}^{-1/2}(0, \eta) = a_3 \sqrt{\eta_{\max} - \eta} [1 + c_2 (\eta - \eta_{\min})]$, where $a_3 = 1/\sqrt{\eta_{\max} - \eta_{\min}} \approx 1.18$ is fixed by $\mathcal{E}(0, \eta_{\min}) = 1$ and the only fitted parameter is $c_2 = 0.3992$.

The presented results complemented by the accurate calculations for $L = 1$ [18] provide in the universal low-energy limit a comprehensive description of the rotational-vibrational spectrum of three two-species particles with the short-range interactions. Essentially, all the binding energies are described by means of the universal function $\mathcal{E}(\xi, \eta)$ for those $L_c(m/m_1) \leq L \leq L_b(m/m_1)$ which correspond to the finite number of vibrational states. One expects that the universal picture should be observed in the limit $|a| \rightarrow \infty$, e. g., if the potential is tuned to produce the loosely bound two-body state as discussed in [28, 22].

It is of interest to discuss briefly the effect of the finite, though small enough interaction radius $r_0 \ll a$. For $L < L_c(m/m_1)$ Efimov's infinite energy spectrum is extremely sensitive to the interaction radius r_0 and to the interaction in the vicinity of the triple-collision point, whereas for $L \geq L_c(m/m_1)$ the binding energies depend smoothly on the interaction parameters provided $r_0 \ll a$. For this reason, one expects not an abrupt transition from the finite to infinite number of bound states for $L = L_c(m/m_1)$ but a smeared off dependence for any finite value of r_0/a .

It is worthwhile to mention that arising of the three-body bound states with increasing mass ratio is intrinsically connected with the oscillating behaviour of the $2 + 1$ elastic-scattering cross section and the three-body recombination rate. In particular, for $L = 1$ it was shown in [18] that two interference maxima of the scattering amplitudes are related to the arising of two three-body bound states. Analogously, the dependence of the scattering amplitudes on the mass ratio for higher L would exhibit the number of interference maxima which are related to arising of up to $N_{\max} = 1.099839 \sqrt{L(L + 1)} + 1/2$ bound states.

Concerning possible observations of the molecules containing two heavy and one light particles in the higher rotational states, one should mention the ultra-cold mixtures of ^{87}Sr with lithium isotopes [18] and mixtures of

cesium with either lithium or helium. In particular, for ^{133}Cs and ^6Li the mass ratio $m/m_1 \approx 22.17$ is just below the value $m/m_1 = 22.34$ at which the $L = 2$ bound state arises and $m/m_1 \approx 33.25$ for ^{133}Cs and ^4He is above the value $m/m_1 = 31.29$, which corresponds to arising of the second $L = 2$ bound state. Also, a complicated rotational-vibrational spectrum and significant interference effects are expected for the negatively charged atomic and molecular ions for which the typical total angular momentum up to $L \sim 100$ becomes important due to the large mass ratio.

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