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BOUND STATES AND SCATTERING LENGTHS OF THREE TWO-COMPONENT PARTICLES WITH ZERO-RANGE INTERACTIONS UNDER ONE-DIMENSIONAL CONFINEMENT

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The universal three-body dynamics in ultracold binary gases confined to one-dimensional motion is studied. The three-body binding energies and the $(2+1)$-scattering lengths are calculated for two identical particles of mass m and a different particle of mass m_1, whose interaction is described in the low-energy limit by zero-range potentials. The critical values of the mass ratio m/m_1 at which three-body states occur and the $(2+1)$-scattering length vanishes are determined for both zero and infinite interaction strength λ_1 of the identical particles. A number of exact results are listed and asymptotic dependences for both $m/m_1 \to \infty$ and $\lambda_1 \to -\infty$ are derived. Combining the numerical and analytic results, we deduce a schematic diagram showing the number of three-body bound states and the sign of the $(2+1)$-scattering length in the plane of the mass ratio and the interaction-strength ratio. The results provide a description of the homogeneous and mixed phases of atoms and molecules in dilute binary quantum gases.

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1. INTRODUCTION

Dynamics of few particles confined in low dimensions is of interest in connection with numerous investigations ranging from atoms in ultracold gases [1–7] to nanostructures [8–10]. Experiments with ultracold gases in the one-dimensional ($1D$) and quasi-$1D$ traps have recently been performed [1, 11–13], motivated by the rapidly growing interest in the investigation of mixtures of ultracold gases [14–20]. Different aspects of the three-body dynamics in one dimension have been analyzed in a number of recent papers, e. g., the bound-state spectrum of two-component compound in [21], low-energy three-body recombination in [22], application of the integral equations in [23], and variants of the hyperradial expansion in [24–26].

We emphasize that the exact solutions are known for an arbitrary number of identical particles with contact interaction in one dimension [27, 28]; in particular, it was found that the ground-state energy E_N of N attracting particles scales as $E_N/E_{N=2} = N(N^2-1)/6$. There is a vast literature in which the exact solution is used to analyze different properties of few- and many-body systems; several examples of this approach can be found in Refs. [29–32].

The main parameters characterizing the multicomponent ultracold gases, i. e., the masses and interaction strengths, can be easily tuned within wide ranges in the modern experiments, which deal with different compounds of ultracold atoms and adjust the two-body scattering lengths to arbitrary values by using the Feshbach-resonance and confinement-resonance technique [33]. Under properly chosen scales, all the properties of the system depend on two dimensionless parameters, i. e., the mass ratio and the interaction-strength ratio, the most important characteristics being the bound-state energies and the $(2+1)$-scattering lengths. In particular, knowledge of these cha-

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racteristics is essential for describing the concentration dependence and phase transitions in dilute two-component mixtures of ultracold gases.

In this paper, the two-component three-body system consisting of a particle of mass m_1 and two identical particles of mass m interacting via a contact (δ-function) inter-particle potential is studied. In the low-energy limit, the contact potential is a good approximation for any short-range interaction and its use provides a universal, i. e., independent of the potential form, description of the dynamics [23, 26, 34–37]. More specifically, it is assumed that one particle interacts with the other two via an attractive contact interaction of strength $\lambda < 0$, and the sign of the interaction strength λ_1 for the identical particles is arbitrary. This choice of the parameters is conditioned by the intention to consider a sufficiently rich three-body dynamics (three-body bound states exist only if $\lambda < 0$).

Most of the numerical and analytic results can be obtained by solving a system of hyperradial equations (HREs) [38]. It is important that all the terms in HREs are derived analytically; the derivation method and the analytic expressions are similar to those obtained in a number of problems with zero-range interactions [26, 36, 37]. To describe the dependence on the mass ratio and interaction-strength ratio for the three-body binding energies and the (2+1)-scattering length, the two limit cases $\lambda_1 = 0$ and $\lambda_1 \to \infty$ are considered and the precise critical values of m/m_1 for which the three-body bound states occur and the $(2 + 1)$-scattering length vanishes are determined. Combining the numerical calculations, exact analytic results, qualitative considerations, and the deduced asymptotic dependences, we produce a schematic phase diagram that shows the number of the three-body bound states and the sign of the $(2 + 1)$-scattering lengths in the plane of the parameters m/m_1 and $\lambda_1/|\lambda|$. This sign is important in studying the stability of mixtures containing both atoms and diatomic molecules.

This paper is organized as follows. In Sec. 2, the problem is formulated, the relevant notation is introduced, and the method of "surface" functions is described; the analytic solutions, numerical results, and asymptotic dependences are presented and discussed in Sec. 3; conclusions are given in Sec. 4.

2. GENERAL OUTLINE AND THE METHOD

The Hamiltonian of three particles confined in one dimension and interacting through the pairwise contact potentials with strengths λ_i is given by

$$H = -\sum_i \frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial x_i^2} + \sum_i \lambda_i \delta(x_{jk}), \qquad (1)$$

where x_i and m_i are the coordinate and mass of the ith particle, $x_{jk} = x_j - x_k$, and $\{ijk\}$ is a permutation of $\{123\}$. To study the aforementioned two-component three-body systems, we assume that particle 1 interacts with two identical particles 2 and 3 through attractive potentials and set $m_2 = m_3 = m$ and $\lambda_2 = \lambda_3 \equiv \lambda < 0$ for simplicity. The corresponding solutions are classified by their parity and are symmetric or antisymmetric under the permutation of identical particles, depending on whether these particles are bosons or fermions. The even (odd) parity solutions are denoted by $P = 0$ ($P = 1$).

In what follows, the dependences of the three-body bound-state energies and the $(2+1)$-scattering lengths on two dimensionless parameters m/m_1 and $\lambda_1/|\lambda|$ are investigated. Hereafter, we set $\hbar = |\lambda| = m = 1$, and therefore $m\lambda^2/\hbar^2$ and $\hbar^2/m|\lambda|$ are the units of energy and length. Furthermore, we let A and A_1 denote the respective scattering lengths for the collision of the third particle with the bound pair of different and identical particles. The scattering length is considered at the lowest two-body threshold, which corresponds to determination of A if $\lambda_1/|\lambda| > -\sqrt{2/(1 + m/m_1)}$ and A_1 otherwise. With the chosen units, $E_{th} = -1/2(1 + m/m_1)$ and $E'_{th} = -\lambda_1^2/4$ are two-body thresholds, i. e., the respective bound-state energies of two different and two identical particles.

The binding energy and the scattering length are monotonic functions of the interaction strength, and therefore much attention is given to calculations in two limit cases of zero ($\lambda_1 = 0$) and infinite ($\lambda_1 \to \infty$) interaction between identical bosons. It is interesting to recall here that due to the one-to-one correspondence of the solutions [39], all the results derived for systems in which the identical particles are bosons and $\lambda_1 \to \infty$ are applicable to systems in which the identical particles are fermions and the s-wave interaction between them is zero ($\lambda_1 = 0$) by definition.

The numerical and analytic results are mostly obtained by solving a system of HREs [38] where the various terms are derived analytically [26, 36, 37]. The HREs are written using the center-of-mass coordinates ρ and α, which are expressed via the scaled Jacobi variables as $\rho \sin\alpha = x_2 - x_3$ and $\rho\cos\alpha = (2x_1 - x_2 - x_3)\operatorname{ctg}\omega$ given the kinematic rotation angle $\omega = \operatorname{arctg}\sqrt{1 + 2m/m_1}$, with $E_{th} = -\cos^2\omega$. The total wave function is expanded as in papers [24–26, 37],

$$\Psi = \frac{1}{\sqrt{\rho}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\alpha, \rho), \tag{2}$$

with respect to a set of functions $\Phi_n(\alpha, \rho)$ satisfying the equation

$$\left(\frac{\partial^2}{\partial \alpha^2} + \xi^2 \right) \Phi_n(\alpha, \rho) = 0 \tag{3}$$

at fixed ρ, supplemented by the condition

$$\left. \frac{\partial \Phi_n(\alpha, \rho)}{\partial \alpha} \right|_{\alpha=\omega-0}^{\alpha=\omega+0} + 2\rho \cos\omega \, \Phi_n(\omega, \rho) = 0, \tag{4}$$

which represents the contact interaction between different particles [26, 35, 37, 40]. Taking the symmetry requirements into account, we can consider the variable α in the range $0 \le \alpha \le \pi/2$ and impose the boundary conditions

$$\left[(1-P) \frac{\partial \Phi_n}{\partial \alpha} + P \Phi_n \right]_{\alpha=\pi/2} = 0\,, \tag{5}$$

$$\left[(1-T) \frac{\partial \Phi_n}{\partial \alpha} + T \Phi_n \right]_{\alpha=0} = 0\,, \tag{6}$$

where $P = 0$ ($P = 1$) for even (odd) parity and $T = 0$ ($T = 1$) for $\lambda_1 = 0$ ($\lambda_1 \to \infty$). These boundary conditions are imposed if two identical particles are bosons, but the case $T = 1$ is equally applicable if two identical particles are noninteracting ($\lambda_1 = 0$) fermions.

The solution of Eq. (3) satisfying boundary conditions (5) and (6) can be written as

$$\Phi_n(\alpha, \rho) = B_n \times \\ \times \begin{cases} \cos\left[\xi_n \left(\omega - \frac{\pi}{2} \right) - \frac{P\pi}{2} \right] \cos\left(\xi_n \alpha - \frac{T\pi}{2} \right), \\ \qquad \alpha \le \omega, \\ \cos\left(\xi_n \omega - \frac{T\pi}{2} \right) \cos\left[\xi_n \left(\alpha - \frac{\pi}{2} \right) - \frac{P\pi}{2} \right], \\ \qquad \alpha \ge \omega, \end{cases} \tag{7}$$

where the normalization constant is given by

$$B_n^2 = -\left\{ 2\cos^2 \left[\xi_n \left(\omega - \frac{\pi}{2} \right) - \frac{P\pi}{2} \right] \times \right. \\ \left. \times \cos^2 \left[\xi_n \omega - \frac{T\pi}{2} \right] \cos\omega \right\}^{-1} \frac{d\xi_n^2}{d\rho}. \tag{8}$$

To meet condition (4), the eigenvalues $\xi_n(\rho)$ must satisfy the equation

$$2\rho \cos\omega \cos[\xi_n \omega - (\xi_n + P)\pi/2] \cos(\xi_n \omega - T\pi/2) + \\ + \xi_n \sin[(\xi_n + P - T)\pi/2] = 0. \tag{9}$$

We note that the case $P = 1$ and $T = 0$ is formally equivalent to the case $P = 0$ and $T = 1$ under the replacement of ω with $\pi/2 - \omega$.

The expansion of the total wave function (2) leads to an infinite set of coupled HREs for the radial functions $f_n(\rho)$,

$$\left[\frac{d^2}{d\rho^2} - \frac{\xi_n^2(\rho) - 1/4}{\rho^2} + E \right] f_n(\rho) - \\ - \sum_{m=1}^{\infty} \left[P_{mn}(\rho) - Q_{mn}(\rho) \frac{d}{d\rho} - \frac{d}{d\rho} Q_{mn}(\rho) \right] \times \\ \times f_m(\rho) = 0. \tag{10}$$

Using the method described in Refs. [26, 36, 37], we can derive analytic expressions for all the terms in Eq. (10),

$$Q_{nm}(\rho) \equiv \langle \Phi_n \mid \Phi'_m \rangle = \frac{\sqrt{\varepsilon'_n \varepsilon'_m}}{\varepsilon_m - \varepsilon_n}\,, \tag{11}$$

$$P_{nm}(\rho) \equiv \langle \Phi'_n \mid \Phi'_m \rangle = \\ = \begin{cases} Q_{nm} \left[\frac{\varepsilon'_n + \varepsilon'_m}{\varepsilon_m - \varepsilon_n} + \frac{1}{2} \left(\frac{\varepsilon''_n}{\varepsilon'_n} - \frac{\varepsilon''_m}{\varepsilon'_m} \right) \right], \\ \qquad n \ne m, \\ -\frac{1}{6} \frac{\varepsilon'''_n}{\varepsilon'_n} + \frac{1}{4} \left(\frac{\varepsilon''_n}{\varepsilon'_n} \right)^2, \quad n = m, \end{cases} \tag{12}$$

where $\varepsilon_n = \xi_n^2$ and the prime denotes derivative with respect to ρ.

The obvious boundary condition for HREs (10), $f_n(\rho) \to 0$ as $\rho \to 0$ and $\rho \to \infty$, was used in solving the eigenvalue problem. To calculate the scattering length A, we should impose the asymptotic boundary condition for the first-channel function

$$f_1(\rho) \sim \rho \sin\omega - A. \tag{13}$$

All other boundary conditions remain the same as for the eigenvalue problem. Condition (13) follows from the asymptotic form of the threshold-energy wave function as $\rho \to \infty$, which tends to the two-body bound-state wave function times a function describing the relative motion of the third particle and the bound pair. The linear dependence of the latter function at large distance between the third particle and the bound pair leads to asymptotic expression (13) for the first-channel function in expansion (2). On the other hand, expression (13) is consistent with the asymptotic solution of the first-channel equation in (10), in which the long-range terms $P_{11}(\rho)$ and $-1/4\rho^2$ cancel each other at large ρ.

3. RESULTS

3.1. Exact solutions

There are several examples where an analytic solution of the Schrödinger equation for the systems under consideration can be obtained. First, for a system containing one heavy and two light particles (in the limit $m/m_1 \to 0$), using the separation of variables, the solutions can be straightforwardly written for both zero and infinite interaction strength between the light particles. In particular, for $\lambda_1 = 0$, there is a single bound state with the binding energy $E_3 = -1$ and the (unnormalized) wave function is

$$\Psi_b = \exp\left(-|x_{12}| - |x_{13}|\right), \quad (14)$$

and the scattering wave function at the threshold energy $E_{th} = -1/2$ is

$$\Psi_{sc} = (|x_{12}| - 1)\exp(-|x_{13}|) + + (|x_{13}| - 1)\exp(-|x_{12}|), \quad (15)$$

which gives the $(2+1)$-scattering length $A = 1$. On the other hand, for $\lambda_1 \to \infty$, the three-body system is not bound, and the scattering wave function at the threshold energy $E_{th} = -1/2$ is

$$\Psi_{sc} = |x_{12}\exp(-|x_{13}|) - x_{13}\exp(-|x_{12}|)|, \quad (16)$$

which gives $A = 0$.

Furthermore, as mentioned in the Introduction, the exact solution is known for an arbitrary number N of identical particles with contact interactions in one dimension [27, 28], and if the interaction is attractive, then there is a single bound state, whose energy equals $E_N = -N(N^2-1)/24$. In particular, for three identical particles ($m = m_1$ and $\lambda_1 = \lambda$), there is only one bound state with the energy $E_3 = -1$, and the (unnormalized) wave function is

$$\Psi_b = \exp\left(-\frac{1}{2}\sum_{i<j}|x_{ij}|\right), \quad (17)$$

and the exact scattering wave function at the two-body threshold $E_{th} = E'_{th} = -1/4$ is

$$\Psi_{sc} = \sum_{i<j}\exp\left(-\frac{1}{2}|x_{ij}|\right) - - 4\exp\left(-\frac{1}{4}\sum_{i<j}|x_{ij}|\right), \quad (18)$$

which implies that the $(2+1)$-scattering length is infinite, $|A| \to \infty$, i.e., there is a virtual state at the two-body threshold [24].

Further exact results can be obtained by using the above correspondence of the three-body solutions for the infinite interaction strength ($\lambda_1 \to \infty$) between two identical bosons and for two noninteracting fermions ($\lambda_1 \to 0$). For example, for three equal-mass particles ($m = m_1$), the exact wave function at the two-body threshold ($E_{th} = -1/4$) is given by

$$\Psi_{sc} = \begin{cases} \exp\left(-\frac{x_{13}}{2}\right) + \exp\left(\frac{x_{12}}{2}\right) - -2\exp\left(-\frac{x_{23}}{2}\right), & x_{13} \ge 0, \\ \left|\exp\left(\frac{x_{13}}{2}\right) - \exp\left(\frac{x_{12}}{2}\right)\right|, & x_{13} \le 0. \end{cases} \quad (19)$$

As follows from (19), the $(2+1)$-scattering length is infinite; as a matter of fact, this implies a rigorous proof of the conjecture in [21] that $m = m_1$ is the exact critical value for the emergence of a three-body bound state in the case of infinite repulsion ($\lambda_1 \to \infty$) between two identical bosons.

It is worthwhile to recall the exact solution for three equal-mass particles ($m = m_1$) if the interaction between two of them is turned off ($\lambda_1 = 0$) [41]. A transcendental equation was derived for the ground-state energy, whose approximate solution gives the ratio of three-body and two-body energies $E_3/E_{th} \approx 2.08754$.

3.2. Numerical calculations

For even-parity states ($P = 0$) and the two limit values of the interaction strength between identical bosons, $\lambda_1 = 0$ and $\lambda_1 \to \infty$, HREs (10) are solved to determine the mass-ratio dependence of three-body binding energies and the $(2+1)$-scattering length A. The calculations show a sufficiently fast convergence as the number of channels increases; 15-channel results are presented in Fig. 1. The precise critical values of the mass ratio value at which the three-body bound states arise ($|A| \to \infty$) and the $(2+1)$-scattering length $A = 0$ are presented in the Table and are marked by crosses in Figs. 1 and 3. The condition that the ground-state energy is twice the threshold energy is important because it determines whether production of the triatomic molecules is possible in a gas of diatomic molecules. The mass ratio value at which $E_3/E_{th} = 2$ is determined to be $m/m_1 \approx 49.8335$ as $\lambda_1 \to \infty$; for the excited states, the condition $E_3/E_{th} = 2$ is satisfied for

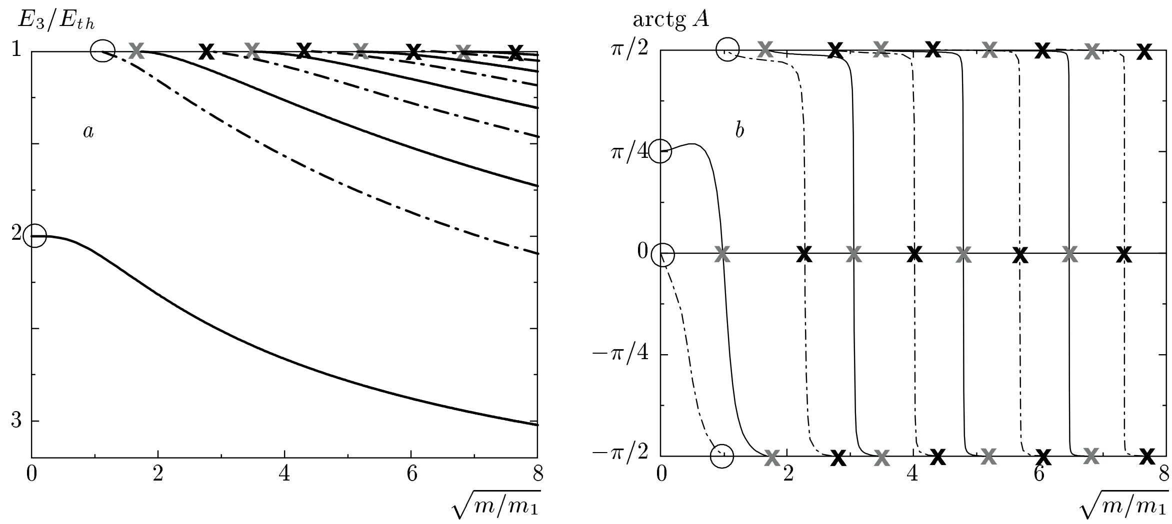

Fig. 1. Mass-ratio dependences for the even-parity states; shown are the ratio of the three-body bound-state energies to the two-body threshold energy (a) and the $(2+1)$-scattering length A (b). Presented are the calculations for a system containing two identical bosons with zero (solid lines) and infinite (dash-dotted lines) interaction strength λ_1. The dash-dotted lines also represent the results for a system containing two identical noninteracting ($\lambda_1 = 0$) fermions. Encircled are the points at which the exact analytic solution is known

Table. The even-parity critical values of the mass ratio m/m_1 at which the $(2+1)$-scattering length becomes zero (marked by $A = 0$) and the nth three-body bound state arises (marked by $|A| \to \infty$). Calculations are done for two values of the interaction strength between the identical particles, $\lambda_1 = 0$ and $\lambda_1 \to \infty$

	$\lambda_1 = 0$		$\lambda_1 \to \infty$	
n	$m/m_1(A=0)$	$m/m_1(\|A\| \to \infty)$	$m/m_1(A=0)$	$m/m_1(\|A\| \to \infty)$
1	–	–	0*	1*
2	0.971	2.86954	5.2107	7.3791
3	9.365	11.9510	16.1197	19.0289
4	22.951	26.218	32.298	35.879
5	41.762	45.673	53.709	57.923
6	65.791	70.317	80.339	85.159
7	95.032	100.151	112.179	117.583
8	129.477	135.170	149.222	155.193
9	169.120	175.374	191.463	197.989
10	213.964	220.765	238.904	245.973

* Exact.

$m/m_1 \approx 130.4516$ if $\lambda_1 = 0$ and $m/m_1 \approx 266.1805$ if $\lambda_1 \to \infty$.

As is shown in Fig. 1, the binding energies increase with increasing the mass ratio, whereas the scattering length A has a general trend to decrease with increasing the mass ratio on each interval between two consecutive critical mass ratios at which the bound states appear. Nevertheless, the calculations for $\lambda_1 = 0$ show that $A(m/m_1)$ becomes a nonmonotonic function at small m/m_1. More precisely, the scattering length takes a maximum value $A \approx 1.124$ at $m/m_1 \approx 0.246$. We note again that the mass-ratio dependence of the energy and scattering length (plotted in Fig. 1) and the critical values of the mass ratio (presented in the Table) are the same both for the three-body system containing two identical bosons as $\lambda_1 \to \infty$ and for the three-body system containing two identical noninteracting ($\lambda_1 = 0$) fermions.

It is interesting to note that the calculated binding energy $E_3/E_{th} \approx 2.087719$ for three equal-mass particles ($m = m_1$) if two identical ones do not interact with each other ($\lambda_1 = 0$) is very close to the result $E_3/E_{th} \approx 2.08754$ obtained in [41] from an analytic transcendental equation (see Sec. 3.1). A small discrepancy most probably stems from the approximations made in numerical solution of the transcendental equation in [41]. The (2+1)-scattering length turns out to be small and negative, $A \approx -0.09567$, for $m = m_1$ and $\lambda_1 = 0$ and takes a zero value at a slightly smaller mass ratio $m/m_1 \approx 0.971$ (see Table).

Analogously, the odd-parity ($P = 1$) solutions for the three-body system containing two identical noninteracting bosons ($\lambda_1 = 0$) were obtained. As follows from Eq. (9), the eigenvalues $\xi_n(\rho)$ entering HREs (10) are nonnegative, which implies that there are no three-body bound states. The calculated dependence of the scattering length A is shown in Fig. 2; A increases monotonically with increasing the mass ratio following the asymptotic dependence discussed in Sec. 3.3.

3.3. Asymptotic dependences

3.3.1. Large attractive interaction of two identical particles

In the limit of large attractive interaction between the identical particles, $\lambda_1 \to -\infty$, the even-parity wave function takes, with a good accuracy, the factored form $\Psi = \phi_0(x_{23})u(y)$, $y = (2x_1 - x_2 - x_3)\,\mathrm{ctg}\,\omega$, where $\phi_0(x) = \sqrt{|\lambda_1|/2}\exp(-|\lambda_1 x|/2)$ is the wave function of the tightly bound pair of identical particles with the energy $E'_{th} = -\lambda_1^2/4$, and $u(y)$ describes the relative motion of a different particle 1 with respect to this pair. Within this approximation, $u(y)$ is a solution of the equation

$$\left[\frac{d^2}{dy^2}+2|\lambda_1|\exp\left(-\sqrt{1+\frac{2m}{m_1}}|\lambda_1 y|\right)+\frac{\lambda_1^2}{4}+E\right]\times u(y) = 0, \quad (20)$$

which gives the λ_1-independent leading-order terms in the asymptotic expansion of the three-body binding energy $\varepsilon \approx 4/(1 + 2m/m_1)$ and the $(2 + 1)$-scattering length

$$A_1 \approx \frac{1}{4}\left(1+\frac{2m}{m_1}\right). \quad (21)$$

3.3.2. One light and two heavy particles

For a large mass ratio m/m_1, we can use the adiabatic and semiclassical approximations, which provide a universal description of the energy spectrum [40]. To describe the three-body properties in the limit of large $m/m_1 \to \infty$ ($\omega \to \pi/2 - \sqrt{m_1/2m}$), we consider the first eigenvalue $\xi_1(\rho) \equiv i\kappa(\rho)$, whose large-$\rho$ asymptotic dependence is approximately given by

$$\rho\cos\omega = \frac{\kappa}{1+(-1)^P e^{-\kappa(\pi-2\omega)}}, \quad (22)$$

as follows from Eq. (9) for the system containing two identical bosons for both $\lambda_1 = 0$ and $\lambda_1 = \infty$ and, equivalently, for the system containing two identical noninteracting fermions.

The number n of the three-body even-parity ($P = 0$) bound states can be determined for large m/m_1 using the one-channel approximation in (10) and the effective potential $-\kappa^2(\rho)/\rho^2$ obtained from Eq. (22). In the framework of the semiclassical approximation, taking the large-ρ asymptotic dependence (22) into account, we obtain the relation $m/m_1 \approx C(n+\delta)^2$ in the limit of large n and m/m_1. The constant C can be found as

$$C = \frac{\pi^2}{2}\left[\int_0^1 \sqrt{2t+t^2}\,\frac{1+(1-\ln t)t}{2t(1+t)^2}dt\right]^{-2} \approx \approx 2.59, \quad (23)$$

where the integral is expressed by setting $t = \exp[-\kappa(\pi - 2\omega)]$ in the leading term of the semiclassical estimate,

$$\cos\omega\int_0^\infty d\rho\left\{\left[(1+e^{\kappa(\rho)(\pi-2\omega)}\right]^2-1\right\}^{1/2} = \pi n. \quad (24)$$

Fitting the calculated mass-ratio dependence of the critical values at which the bound states appear to the n-dependence $C(n+\delta)^2$ (up to $n = 20$, see the Table for 10 lowest values), we obtain $C \approx 2.60$ for both $\lambda_1 \to \infty$ and $\lambda_1 = 0$, in good agreement with semiclassical estimate (23). Simultaneously, we obtain $\delta = 0.73$ if $\lambda_1 \to \infty$ and $\delta = 0.22$ if $\lambda_1 = 0$ for the parameter that determines the next-to-leading-order term of the large-n expansion.

The asymptotic dependence of the effective potential $-\kappa^2(\rho)/\rho^2$ obtained from Eq. (22) allows finding the leading-order mass-ratio dependence of the odd-parity ($P = 1$) scattering length:

$$A = \frac{m}{m_1}\sqrt{1+\frac{m_1}{2m}}\left(\ln\frac{m}{m_1}+2\gamma\right), \quad (25)$$

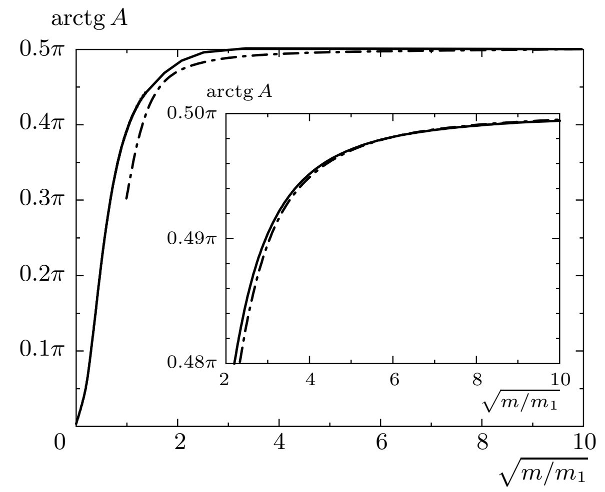

Fig. 2. Mass-ratio dependence of the $(2+1)$-scattering length A for odd-parity states ($P = 1$) of a system containing two identical noninteracting bosons ($\lambda_1 = 0$). The numerical calculation (solid lines) is compared with the large-mass-ratio asymptotic behavior given by Eq. (25) (dash-dotted lines). The dependence corresponding to large $A > 15$ is shown in the inset

where $\gamma \approx 0.5772$ is the Euler constant. The convergence of the calculated dependence $A(m/m_1)$ to asymptotic dependence (25) is shown in Fig. 2 in the case of two identical noninteracting bosons ($\lambda_1 = 0$).

3.4. Mass-ratio and interaction-strength ratio dependences

Collecting the numerical and the exact analytic results, the asymptotic expressions, and qualitative arguments, we obtain a schematic phase diagram that depicts the number of three-body bound states and the sign of the $(2+1)$-scattering lengths in the m/m_1–$\lambda_1/|\lambda|$ plane (Fig. 3).

The plane of parameters is divided into two parts by a dotted line, $\lambda_1/|\lambda| = -\sqrt{2/(1+m/m_1)}$, with the low-energy three-body properties being essentially different in the upper and lower parts, where the respective two-body threshold is determined by the bound-state energy of two different and identical particles. The lines representing the condition $|A| = \infty$ or $|A_1| = \infty$ (arising for the three-body bound state) separate areas with different numbers of bound states, and the condition $A = 0$ or $A_1 = 0$ splits each area into two parts of different signs of the scattering lengths.

It can be proved rigorously that in the upper part of the diagram (above the dotted line), the number n of three-body bound states increases and the $(2+1)$-scattering length A decreases as the interaction strength λ_1 decreases, while in the lower part (below the dotted line), n increases and A_1 decreases as the mass ratio m/m_1 decreases. The proof is based on the representation in which the lowest two-body threshold is respectively independent of λ_1 and m_1 in the former and latter case. The required conclusion follows from the monotonic dependence of the Hamiltonian on λ_1 and m_1. A schematic phase diagram demonstrated in Fig. 3 is drawn by using a stricter assumption on the positive slope of the lines that show where the three-body bound states arise ($|A| \to \infty$) and where the $(2+1)$-scattering lengths vanish ($A = 0$ and $A_1 = 0$ in the upper and lower parts of the $\lambda_1/|\lambda|$–m/m_1 plane, respectively). Tentatively, this assumption seems to correctly reflect the general trend; nevertheless, we note that the slope of the isolines of constant scattering length is not positive in general. In particular, A is not a monotonic function of the mass ratio for $\lambda_1 = 0$, as shown in Fig. 2; this implies a nonmonotonic dependence of the constant-A isolines in the vicinity of the point ($m/m_1 = 0$, $\lambda_1/|\lambda| = 0$).

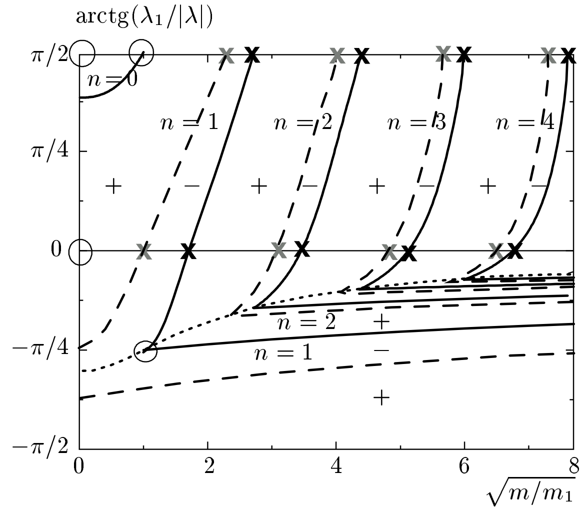

Fig. 3. Schematic phase diagram for the even-parity states of two identical bosons and a different third particle. The dotted line marks the border between two areas where the lowest two-body threshold is set by the energy of two different and two identical particles. The number of three-body bound states is marked by n in the corresponding areas separated by solid lines. The sign of the $(2+1)$-scattering lengths A and A_1 is marked by $\pm$ and the corresponding areas are separated by dashed lines. The crosses show the calculated critical values of the mass ratio (listed in the Table). Encircled are the points at which the exact analytic solution is known

For a sufficiently large repulsion λ_1 and a small mass ratio m/m_1, the three-body bound states do not exist. The limit $m/m_1 \to 0$ (a $1D$ analogue of the helium atom with contact interactions between particles) was discussed in [42], where the binding energy as a function of the repulsion strength between light particles was calculated and the critical value of the repulsion strength for which the three particles become unbound was determined. Recently, a very precise critical value $\lambda_1/|\lambda| \approx 2.66735$ was found in [21]. The boundary of the $n = 0$ area (shown in the upper left corner in Fig. 3) extends from the point ($m/m_1 = 0$, $\lambda_1/|\lambda| \approx 2.66735$) to the point ($m/m_1 = 1$, $\lambda_1 \to \infty$), as was conjectured in [21] and proved in Sec. 3.1 by using the exact solution at the second of these points. Taking this result, the above-discussed monotonic dependence on λ_1, and the exact solution for three identical particles into account, we come to an interesting conclusion that there is exactly one bound state ($n = 1$) of three equal-mass particles, irrespective of the interaction strength λ_1. There is exactly one bound state ($n = 1$) also for a sufficiently large attraction between identical particles, whereas a second bound state appears for $m > m_1$ and $|\lambda_1| < 1$ (as shown in Fig. 3). Therefore, the scattering length A_1 changes from the positive value given by (21) at $\lambda_1 \to -\infty$ to the negative one as λ_1 increases. The strip areas corresponding to $n > 1$ are located at higher values of the mass ratio with the large-n asymptotic dependence $n \propto \sqrt{m/m_1}$. In each parameter area corresponding to n bound states, the scattering lengths take all the real values, tending to infinity at the boundary with the $n-1$ area and to minus infinity at the boundary with the $n+1$ area.

4. CONCLUSION

The three-body dynamics of ultracold binary gases confined to $1D$ motion is studied. In the low-energy limit, the description is universal, i. e., independent of the details of the short-range two-body interactions, which can be taken as a sum of contact δ-function potentials. Thus, the three-body energies and the $(2 + 1)$-scattering lengths are expressed as universal functions of two parameters, the mass ratio m/m_1 and the interaction-strength ratio $\lambda_1/|\lambda|$. The mass-ratio dependences of the binding energies and the scattering length are numerically calculated for even and odd parity and the accurate critical values of the mass ratio at which the bound states arise and the scattering length vanishes are determined. It is rigorously proved that $m/m_1 = 1$ is the exact boundary above which at least one bound state exists (as conjectured in [21]); the related conclusion is the existence of exactly one bound state for three equal-mass particles independently of the interaction strength between the identical particles. Asymptotic dependences of the bound-state number and the scattering length A in the limit $m/m_1 \to \infty$ and of the binding energy and the scattering length A_1 in the limit $\lambda_1 \to -\infty$ are determined. Based on the numerical calculations, analytic results, and qualitative considerations, a schematic diagram is drawn that shows the number of the three-body bound states and the sign of the $(2+1)$-scattering length as a function of the mass ratio and the interaction-strength ratio.

The obtained qualitative and quantitative results on the three-body properties provide a firm base for the description of the equation of state and phase separation in dilute binary mixtures of ultracold gases. In particular, the sign of the $(2+1)$-scattering lengths essentially controls the transition between the homogeneous and mixed phases of atoms and diatomic molecules. The condition $E_3/E_{th} > 2$ defines the parameter area where the production of the triatomic molecules is energetically favorable in a gas of diatomic molecules.

The analysis of the phase diagram in Fig. 3 implies that there remain interesting problems deserving further elucidation. These include the problem of the nonmonotonic dependence of the constant-A isolines in the $\lambda_1/|\lambda| - m/m_1$ plane, the behavior of the lines separating the positive and negative scattering lengths within the $n = 1$ area, and the description of the beak formed by the lines separating the $n = 1$ and $n = 2$ areas in the vicinity of the exact solution for three identical particles ($\lambda_1 = \lambda$ and $m = m_1$).

One should discuss the connection of the present results with those that take the finite interaction radius R_e and (quasi)-$1D$ geometry into account. Finding the corrections due to a finite interaction radius is not a trivial task, but one expects that the corrections should be small for all calculated values if R_e/a and R_e/a_1 are small, where a and a_1 are the two-body scattering lengths. On the other hand, for sufficiently tight transverse confinement, one expects that the main ingredient is the relation between the $3D$ and quasi-$1D$ two-body scattering lengths established in [33]. Moreover, the role of the transverse confinement does not simply reduce to renormalization of the scattering lengths; the full-scale three-body calculations are needed to determine the energy spectrum and the scattering data in the (quasi)-$1D$ geometry.

It is worthwhile to mention that more few-body problems are of interest in binary mixtures. In particular, the low-energy three-body recombination plays an important role in the kinetic processes, and the elastic and inelastic cross sections for collisions of either diatomic molecules or atoms on triatomic molecules are needed to describe the properties of molecular compounds.

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