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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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Энергии связи и длины рассеяния в одномерной задаче трех частиц с контактным взаимодействием

Изучена универсальная трехчастичная динамика ультрахолодных двухкомпонентных газов в случае одномерного движения. Для двух тождественных частиц массой m и отличной от них частицы массой m_1, взаимодействие между которыми в низкоэнергетическом пределе описывается с помощью потенциалов нулевого радиуса, были вычислены трехчастичные энергии связи и длина рассеяния (2 + 1). Для нулевой и бесконечной силы взаимодействия тождественных частиц λ_1 определены критические значения отношения масс m/m_1, при которых возникают трехчастичные связанные состояния и длина рассеяния (2 + 1) становится равной нулю. Получен ряд аналитических результатов и асимптотических зависимостей для $m/m_1 \to \infty$ и $\lambda_1 \to -\infty$. На основе численных и аналитических результатов построена схематическая диаграмма, показывающая число трехчастичных связанных состояний и знак длины рассеяния (2 + 1) на плоскости параметров — отношения масс и отношения сил взаимодействий. Результаты позволяют описать атомные и молекулярные фазы различного состава двухкомпонентных квантовых газов.

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Kartavtsev O. I., Malykh A. V., Sofianos S. A. E4-2008-146
Bound States and Scattering Lengths of Three Two-Component Particles with Zero-Range Interactions under One-Dimensional Confinement

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 one of mass m_1, between which interactions are described in the low-energy limit by zero-range potentials. The critical values of the mass ratio m/m_1, at which the three-body states arise and the (2 + 1)-scattering length equals zero, are determined both for zero and infinite interaction strength λ_1 of the identical particles. A number of exact results are enlisted and asymptotic dependences both for $m/m_1 \to \infty$ and $\lambda_1 \to -\infty$ are derived. Combining the numerical and analytical results, a schematic diagram showing the number of the three-body bound states and the sign of the (2 + 1)-scattering length in the plane of the mass ratio and interaction-strength ratio is deduced. The results provide a description of the homogeneous and mixed phases of atoms and molecules in dilute binary quantum gases.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR and at the Physics Department, University of South Africa.

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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 nonostructures [8–10]. Experiments with ultracold gases in the one-dimensional (1D) and quasi-1D traps have been recently performed [1,11–13], amid the rapidly growing interest to the investigation of mixtures of ultracold gases [14–20]. Different aspects of the three-body dynamics in 1D 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].

It is necessary to emphasize that the exact solutions are known for an arbitrary number of identical particles in 1D with contact interactions [27,28]; in particular, it was found that the ground-state energy E_N of N attractive particles scales as $E_N/E_2 = N(N^2-1)/6$. There is a vast literature, in which the exact solution is used to analyze different properties of few- and many-body systems; few examples of this approach can be found in Ref. [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 handle with different compounds of ultracold atoms and adjust the two-body scattering lengths to an arbitrary values by using the Feshbach-resonance and confinement-resonance technique [33]. Under properly chosen scales, all the properties of the system depend on the two dimensionless parameters, viz., mass ratio and interaction strength ratio, the most important characteristics being the bound-state energies and the $(2+1)$-scattering lengths. In particular, knowledge of these characteristics is essential for description of the concentration dependence and phase transitions in dilute two-component mixtures of ultracold gases.

In the present paper, the two-component three-body system consisting of a particle of mass m_1 and two identical particles of mass m interacting via contact (δ function) interparticle potential is studied. In the low-energy limit, the contact potential is a good approximation for any short-range interaction and its usage 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 $\lambda < 0$ while the sign of the interaction strength λ_1 for the identical particles is arbitrary. This choice of the parameters is conditioned by an intention to consider a sufficiently rich three-body dynamics since the three-body bound states exist only if $\lambda < 0$.

Most of the numerical and analytical results can be obtained by solving a system of hyper-radial equations (HREs) [38]. It is of importance that all the terms in HREs are derived analytically; the method of derivation and the analytical expressions are similar to those obtained for 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 limiting 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 arise and the $(2 + 1)$-scattering length becomes zero are determined. Combining the numerical calculations, exact analytical results, qualitative considerations, and deduced asymptotic dependences, one produces a schematic «phase» diagram, which shows the number of the three-body bound states and a 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 two-atomic molecules.

The paper is organized in the following way. In Sec. 2 the problem is formulated, the relevant notations are introduced, and the method of surface function is described; the analytical solutions, numerical results and asymptotic dependences are presented and discussed in Sec. 3; the conclusions are summarized in Sec. 4.

2. GENERAL OUTLINE AND METHOD

The Hamiltonian of three particles confined in 1D, interacting through the pairwise contact potentials with strengths λ_i, reads

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

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 $\{123\}$. In order to study the aforementioned two-component three-body systems, one assumes that particle 1 interacts with two identical particles 2 and 3 through attractive potentials and denotes for simplicity $m_2 = m_3 = m$ and $\lambda_2 = \lambda_3 \equiv \lambda < 0$. The corresponding solutions are classified by their parity and are symmetrical or antisymmetrical under the permutation of identical particles, depending on whether these particles are bosons or fermions. The even (odd) parity solutions will be denoted by $P = 0 (P = 1)$.

In the following, the dependence of the three-body bound state energies and the (2 + 1)-scattering lengths on two dimensionless parameters m/m_1 and $\lambda_1/|\lambda|$ will be investigated. Hereafter, one lets $\hbar = |\lambda| = m = 1$ and thus $m\lambda^2/\hbar^2$ and $\hbar^2/(m|\lambda|)$ are the units of energy and length. Furthermore, one denotes by A and A_1 the scattering lengths for the collision of the third particle off the bound pair of different and identical particles, respectively. 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, $E_{\rm th} = -1/[2(1+m/m_1)]$ and $E'_{\rm th} = -\lambda_1^2/4$ are two-body thresholds, i. e., the bound-state energies of two different and two identical particles, respectively.

The binding energy and the scattering length are monotonic functions of the interaction's strength and for this reason much attention is paid to calculations for two limiting cases of zero ($\lambda_1 = 0$) and infinite ($\lambda_1 \to \infty$) interaction between the identical bosons. It is of interest to recall here that due to 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 those in which the identical particles are fermions and the s-wave interaction between them is zero ($\lambda_1 = 0$) by definition.

The numerical and analytical results will be obtained mostly by solving a system of HREs [38] where the various terms are derived analytically [26, 36, 37]. The HREs are written by 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 $\rho\cos\alpha = \cot\omega\,(2x_1 - x_2 - x_3)$ given the kinematic-rotation angle $\omega = \arctan\sqrt{1+2m/m_1}$ so that $E_{\rm th} = -\cos^2\omega$. The total wave function is expanded as in papers [24–26, 37],

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

in a set of functions $\Phi_n(\alpha,\rho)$ satisfying the equation at fixed ρ

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

complemented 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 into account the symmetry requirements, one can consider the variable α within the range $0 \leqslant \alpha \leqslant \pi/2$ 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 posed if two identical particles are bosons, however, the case $T = 1$ is equally applicable if two identical particles are noninteracting ($\lambda_1 = 0$) fermions.

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

$$\Phi_n(\alpha,\rho) = B_n \begin{cases} \cos[\xi_n(\omega-\pi/2) - P\pi/2)]\cos(\xi_n\alpha - T\pi/2), & \alpha \leqslant \omega, \\ \cos(\xi_n\omega - T\pi/2)\cos[\xi_n(\alpha-\pi/2) - P\pi/2], & \alpha \geqslant \omega, \end{cases} \tag{7}$$

where the normalization constant is given by

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

In order to meet the condition (4), the eigenvalues $\xi_n(\rho)$ should satisfy the equation

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

Notice that the case $P = 1$ and $T = 0$ is formally equivalent to the case $P = 0$ and $T = 1$ under the substitution of ω for $\pi/2 - \omega$.

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

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

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

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

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

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

The obvious boundary conditions for the HREs (10) $f_n(\rho) \to 0$ as $\rho \to 0$ and $\rho \to \infty$ were used for the solution of the eigenvalue problem. For the calculation of the scattering length A, one should impose the asymptotic boundary condition for the first-channel function

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

while all other boundary conditions remain the same as for the eigenvalue problem. The condition (13) follows from asymptotic form of the threshold-energy wave function at $\rho \to \infty$, which tends to a product of the two-body bound-state wave function and the 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 the 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 the analytical solution of the Schrödinger equation for the systems under consideration can be obtained. Firstly, 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 both for zero and infinite interaction strength between the light particles. In particular, for $\lambda_1 = 0$, there is a single bound state with binding energy $E_3 = -1$ and the (unnormalized) wave function is

$$\Psi_{\rm b} = {\rm e}^{-|x_{12}|-|x_{13}|}, \tag{14}$$

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

$$\Psi_{\rm sc} = (|x_{12}| - 1)\,{\rm e}^{-|x_{13}|} + (|x_{13}| - 1)\,{\rm e}^{-|x_{12}|}, \tag{15}$$

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 $E_{\rm th} = -1/2$ is

$$\Psi_{\rm sc} = |x_{12}\, {\rm e}^{-|x_{13}|} - x_{13}\, {\rm e}^{-|x_{12}|}|, \tag{16}$$

which gives $A = 0$.

Furthermore, as mentioned in Introduction, the exact solution is known for an arbitrary number N of identical particles with a contact interactions in 1D [27,28] and if the interaction is attractive there is a single bound state, which 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 energy $E_3 = -1$ and the (unnormalized) wave function is

$$\Psi_{\rm b} = \exp\left(-\frac{1}{2}\sum_{i<j}|x_{ij}|\right), \tag{17}$$

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

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

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-mentioned 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 ($E_{\rm th} = -1/4$) reads

$$\Psi_{\rm sc} = \begin{cases} {\rm e}^{-x_{13}/2} + {\rm e}^{x_{12}/2} - 2{\rm e}^{-x_{23}/2}, & x_{13} \geqslant 0 \\ |{\rm e}^{x_{13}/2} - {\rm e}^{x_{12}/2}|, & x_{13} \leqslant 0. \end{cases} \tag{19}$$

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

It is worthwhile to recall here 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, which approximate solution gives the ratio of three-body and two-body energies $E_3/E_{\rm th} \approx 2.08754$.

3.2. Numerical Calculations. For the even-parity states ($P = 0$) and the two limiting values of the interaction strength between identical bosons, $\lambda_1 = 0$ and $\lambda_1 \to \infty$, the 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 sufficiently fast convergence with increasing the number of channels; 15-channel results are presented in Fig. 1.

The precise critical values of the mass ratio, for 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 Fig. 1 and Fig. 3.

The condition that the ground state energy is twice the threshold energy is important as it determines whether production of the triatomic molecules is possible in a gas of diatomic molecules. The mass ratio, at which $E_3/E_{\rm th} = 2$ is determined to be $m/m_1 \approx 49.8335$ for $\lambda_1 \to \infty$, while for the excited states the condition $E_3/E_{\rm th} = 2$ is satisfied for $m/m_1 \approx 130.4516$ if $\lambda_1 = 0$ and $m/m_1 \approx 266.1805$ if $\lambda_1 \to \infty$.

As 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 nonmonotonic function at small m/m_1. More precisely, the scattering length takes a maximum value $A \approx 1.124$ at $m/m_1 \approx 0.246$. Again

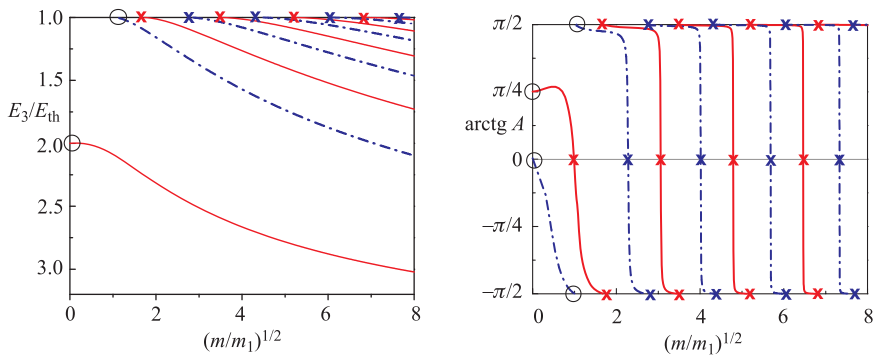

Fig. 1. Mass-ratio dependences for the even-parity states; shown are the ratio of the three-body bound-state energies to the two-body threshold energy (left) and the $(2+1)$-scattering length A (right). Presented are the calculations for a system containing two identical bosons with zero (solid lines)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

Table. The even-parity critical values of the mass ratio m/m_1 for which the $(2+1)$-scattering length becomes zero (marked by $A = 0$) and an nth three-body bound state arises (marked by $|A| \to \infty$). Calculations 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	$m/m_1(A=0)$	$m/m_1(\lvert A\rvert \to \infty)$	$m/m_1(A=0)$	$m/m_1(\lvert A\rvert \to \infty)$
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.

one has to note that the mass-ratio dependence of 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 if $\lambda_1 \to \infty$ and for the three-body system containing two identical noninteracting ($\lambda_1 = 0$) fermions.

It is of interest to note that the calculated binding energy $E_3/E_{\rm th} \approx 2.087719$ 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 [41] $E_3/E_{\rm th} \approx 2.08754$ obtained from the analytical transcendental equation (see Subsec. 3.1). A small discrepancy most probably stems from the approximations of [41] made in numerical solution of the transcendental equation. 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 slightly smaller mass ratio $m/m_1 \approx 0.971$ (see the Table).

Analogously, the odd-parity ($P = 1$) solutions for three-body system containing two identical noninteracting bosons ($\lambda_1 = 0$) were obtained. As follows from Eq. (9), the eigenvalues $\xi_n(\rho)$ entering in 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 mass ratio following the asymptotic dependence discussed in Subsec. 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 factorized form

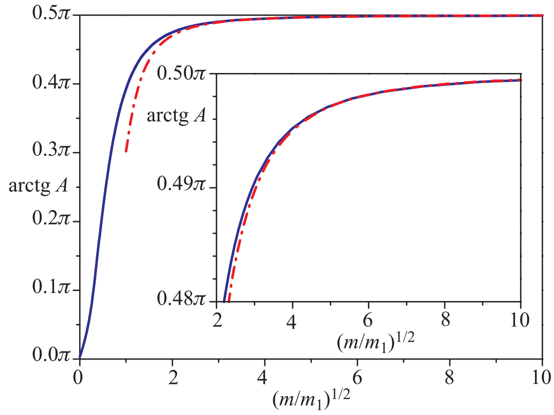

Fig. 2. Mass-ratio dependence of the $(2+1)$-scattering length A for odd-parity states ($P = 1$) of a system containing two identical noninteracting bosons ($\lambda_1 = 0$). The numerical calculation (solid lines) is compared with the large-mass-ratio asymptotic behaviour given by Eq. (25) (dash-dotted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

$\Psi \simeq \phi_0(x_{23})u(y)$ $[y = \cot\omega\,(2x_1 - x_2 - x_3)]$, 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 energy $E'_{\rm th} = -\lambda_1^2/4$ 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

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

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

$$A_1 \approx (1 + 2m/m_1)/4. \tag{21}$$

3.3.2. Two heavy and one light particles. For large mass ratio m/m_1, one can use the adiabatic and quasi-classical approximations which provide, e.g., a universal description for the energy spectrum [40]. To describe the three-body properties in the limit of large $m/m_1 \to \infty[\omega \to \pi/2 - \sqrt{m_1/(2m)}]$, one considers the first eigenvalue $\xi_1(\rho) \equiv i\kappa(\rho)$, which large-$\rho$ asymptotic dependence is approximately given by

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

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

The number of the three-body even-parity ($P = 0$) bound states n can be determined for large m/m_1, using the one-channel approximation in (10) and the effective potential $-\kappa^2(\rho)/\rho^2$, from (22). Within the framework of the quasi-classical approximations and taking into account the large-ρ asymptotic dependence (22), one obtains 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

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

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

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

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), one obtains in good agreement with the quasi-classical estimate (23) $C \approx 2.60$ both for $\lambda_1 \to \infty$ and $\lambda_1 = 0$. Simultaneously, one obtains $\delta = 0.73$ if $\lambda_1 \to \infty$ and $\delta = 0.22$ if $\lambda_1 = 0$ for the parameter, which 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 one to find the leading order mass-ratio dependence of the odd-parity ($P = 1$) scattering length,

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

where $\gamma \approx 0.5772$ is the Euler constant. The convergence of the calculated dependence $A(m/m_1)$ to the asymptotic dependence (25) is shown in Fig. 2 for 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 analytical results, the asymptotic expressions, and qualitative arguments, one obtains a schematic «phase» diagram, which 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 (shown in 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 two-body threshold is determined

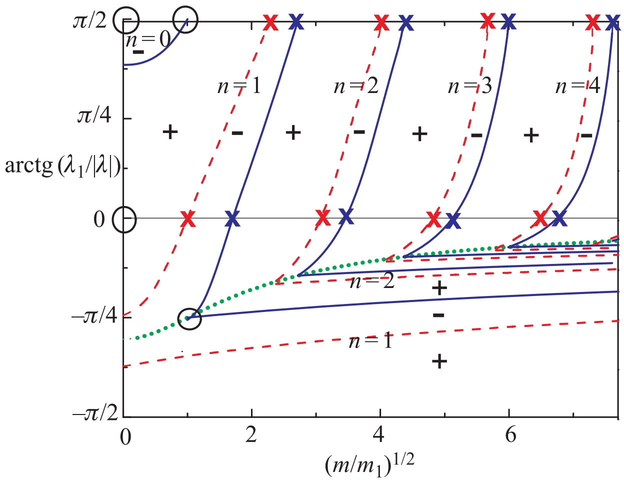

Fig. 3. Schematic «phase» diagram for the even-parity states of two identical bosons and the third different particle. The dotted line marks the border between two areas where the lowest two-body threshold is set by the energy of two different and two identical particles. The number of the three-body 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 (enlisted in the Table). Encircled are those points, in which the exact analytical solution is known

by the bound-state energy of two different and identical particles, respectively. The lines which represent the condition $|A| = \infty$ or $|A_1| = \infty$ (arising of the three-body bound state) separate areas with different number of the bound states, whereas the conditions $A = 0$ or $A_1 = 0$ split each area into two parts of different signs of the scattering lengths.

It can be proven rigorously that in the upper part of the diagram (above the dotted line), the number of the three-body bound states n increases and the $(2+1)$-scattering length A decreases with decreasing the interaction strength λ_1, while in the lower part (below the dotted line) n increases and A_1 decreases with decreasing the mass ratio m/m_1. The proof is based on the representation for which the lowest two-body threshold is independent of λ_1 and m_1 in the former and latter case, respectively. 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 more strict assumption on the positive slope of the lines, which show where the three-body bound states arise ($|A| \to \infty$) and where the $(2+1)$-scattering lengths ($A = 0$ and $A_1 = 0$ in the upper and lower parts of the $\lambda_1/|\lambda| - m/m_1$ plane, respectively) become zero. Tentatively, this assumption seems to reflect correctly the general trend; nevertheless, one should note that the slope of the isolines of constant scattering length is not generally positive. 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 a region near the point ($m/m_1 = 0$, $\lambda_1/|\lambda| = 0$).

For sufficiently large repulsion λ_1 and small mass ratio m/m_1 the three-body bound states are lacking. The limit $m/m_1 \to 0$ (1D analogue of the helium atom with contact interactions between particles) was discussed in paper [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) goes 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 proven in Subsec. 3.1 by using the exact solution at the latter point. Taking into account this result, the above-discussed monotonic dependence on λ_1, and the exact solution for three identical particles, one comes to an interesting conclusion that there is exactly one bound state ($n = 1$) of three equal-mass particles independently of the interaction strength λ_1. There is exactly one bound state ($n = 1$) also for a sufficiently large attraction between identical particles whereas the 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 run 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 one-dimensional 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, for which the bound states arise and the scattering length became zero, are determined. It is rigorously proven that $m/m_1 = 1$ is the exact boundary, above which at least one bound state exists (as conjectured by [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. Combining the numerical calculations, analytical results, and qualitative considerations, a schematic diagram is drawn, which 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 interaction-strength ratio.

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

From the analysis of the «phase» diagram in Fig. 3 it follows that still there are interesting problems deserving further elucidation. These include the problem of non-monotone dependence of the constant-A isolines in the $\lambda_1/|\lambda| - m/m_1$ plane, the behaviour 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, which take into account the finite interaction radius R_e and (quasi)-1D geometry. The determination of the corrections due to finite interaction radius is not a trivial task, however, one expects that the corrections should be small for all calculated values provided 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, a 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, while the elastic and inelastic cross sections for collisions either of diatomic molecules or of atoms off triatomic molecules are needed to describe the properties of the molecular compounds.

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