# Four-body system of <sup>4</sup>He atoms: Dimer-dimer scattering

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The strong short-range repulsion, characteristic to realistic interatomic potentials, complicates the description of weakly bound few-body systems such as those of <sup>4</sup>He atoms. The present work proposes an approach for solving this problem and applies it to a realistic system of four <sup>4</sup>He atoms. The potential is gradually softened such that rigorous four-body equations for bound and scattering states can be accurately solved in the momentum-space framework, and the results are extrapolated back to the limit of the original potential. Linear correlations between three- and four-body quantities. Results for the <sup>4</sup>He tetramer ground-state and excited-state binding energies and atom-trimer scattering agree well with at least some of earlier determinations and shed light on the existing disagreements. An additional case of the Phillips correlation line is established for the dimer-dimer scattering length. The trimer production rate via the ultracold two-dimer collisions is estimated; it exhibits significant finite-range effects despite the weak binding of the dimer.

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## I. INTRODUCTION

Cold <sup>4</sup>He atoms constitute one of the simplest quantum systems exhibiting the phenomenon of the Efimov physics [1,2] (see Refs. [3,4] for recent reviews). In contrast to atomic systems of alkali metals, no external fine-tuning is needed since the interatomic <sup>4</sup>He interaction supports a single shallow dimer bound state in the *S* wave. Consequently, the two-atom scattering length is large compared to the interaction or effective range, ensuring conditions for the realization of the Efimov physics. It manifests itself by the existence few-body states. In systems consisting of N = 3 (4) atoms of <sup>4</sup>He this leads to two bound trimer (tetramer) states, a more tightly bound ground state, and a shallow excited state located near the two-cluster breakup threshold.

The system of three <sup>4</sup>He atoms has been studied in a large number of works employing realistic interaction models, and a good agreement between different theoretical methods has been achieved, not only for binding energies but also for the atom-dimer scattering length [5-12]. Several existing calculations for the ground-state <sup>4</sup>He tetramer also agree well, but significant differences show up in the excited tetramer binding energy [5,7,10,11]. The latter is correlated with the atom-trimer scattering length, the few existing results being in sizable disagreement, thereby calling for further studies with alternative methods. Furthermore, all available four-atom calculations with realistic <sup>4</sup>He potentials are limited to energies very close to the atom-trimer threshold, with no predictions at higher energy where inelastic scattering channels become open, enabling rearrangement reactions such as the dimertrimer conversion.

The most important reason for the abovementioned disagreements and limitations is the form of the realistic interaction between two <sup>4</sup>He atoms, namely, the weakly attractive van der Waals tail and the very strong repulsion at short distance. For spatially extended weakly bound or scattering states the physical observables result from a very subtle interplay of those two features, rendering the numerical solution very sensitive to fine details and eventually leading to a significant accuracy loss. For example, to overcome these difficulties when solving the coordinate space Faddeev-Yakubovsky equations, Lazauskas and Carbonell [7] had to impose additional boundary conditions in the hard-core region and apply extrapolation in the grid size. The momentum-space method based on the Alt, Grassberger, and Sandhas (AGS) equations [13] for the four-particle transition operators, although very efficient in realistic four-nucleon reaction calculations [14], has not yet been successfully applied to the problem of four <sup>4</sup>He atoms with realistic potential models.

The aim of the present work is to develop the momentumspace method for the four-body calculation in the multichannel regime with a realistic interatomic <sup>4</sup>He potential, to show its reliability and evaluate the complex dimer-dimer scattering length. The idea is to reduce gradually the strength of the short-range repulsion, such that accurate solutions of the integral equations for transition operators or wave-function components can be obtained, and then perform extrapolation of the results back to the original potential.

Section II introduces the scheme for reducing the shortrange repulsion, whereas Sec. III demonstrates its validity in the three-body system. Section IV shortly recalls the equations for the four-body system together with the essential aspects of calculations. Section V presents results for tetramer binding energies and atom-trimer and dimer-dimer scattering. Summary and conclusions are collected in Sec. VI.

# **II. TRANSFORMATION OF THE POTENTIAL**

All realistic interatomic <sup>4</sup>He potentials have in common the weakly attractive van der Waals tail and strong repulsion at short distances r < 2.5 Å [15,16]. Though the potential [16] is considered to be one of the most sophisticated, the

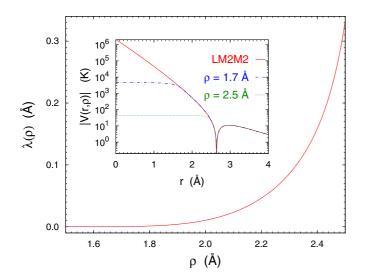


FIG. 1. The function  $\lambda(\rho)$  controlling the momentum-dependent reduction in the potential (3). The inset compares the original LM2M2 potential (solid curve) and the auxiliary potential (1) at  $\rho = 1.7$  and 2.5 Å, given by the dashed-dotted curve and the dotted curve, respectively.

older parametrization LM2M2 by Aziz and Slaman [15] better reproduces the experimental <sup>4</sup>He binding energy and the bond length [17]. LM2M2 is probably the most widely used parametrization, especially for benchmarks; it is adopted also in the present work with the  $\hbar^2/m = 12.11928$  K Å<sup>2</sup> value recommended in Ref. [9], slightly different from the approximation  $\hbar^2/m = 12.12$  K Å<sup>2</sup> used in Ref. [7] and many other works, where *m* is the mass of the <sup>4</sup>He atom. Anyway, as Refs. [9,11] demonstrated, the changes in three- and fourbody results due to different  $\hbar^2/m$  are small and can be accounted for by a simple perturbative correction.

In nuclear physics, the short-range repulsion in the two-nucleon potentials can be softened by the similarity renormalization group (SRG) method [18], which is a unitary transformation decoupling low- and high-momentum components while preserving the deuteron binding and two-nucleon phase shifts. However, in the interatomic <sup>4</sup>He force the relative impact of the short-range repulsion is considerably stronger than in the nuclear force, precluding the application of the SRG or similar method; no successful attempt has been reported so far.

The present work will, therefore, use a different strategy. Following Ref. [12], an auxiliary potential  $V(r, \rho)$  with the strength of the short-range repulsion reduced at distances  $r < \rho$  is defined as

$$V(r,\rho) = \Theta(\rho-r)V(\rho)[2 - e^{(\rho-r)\kappa(\rho)}] + \Theta(r-\rho)V(r).$$
(1)

Here V(r) is the original potential,  $\Theta(x)$  is the step function equal to 1 (0) for the positive (negative) argument *x*, while  $\kappa(\rho) = V'(r)/V(r)|_{r=\rho}$  ensures the smoothness of the auxiliary potential by the continuity of itself and its first derivative. The comparison of the original LM2M2 potential with  $V(r, \rho)$ is shown in the inset of Fig. 1. While the LM2M2 potential rapidly increases towards r = 0,  $V(r, \rho)$  remains quite flat for  $r < \rho$ . For momentum-space partial-wave calculations the potential has to be transformed into the corresponding representation, i.e.,

$$\langle p'|V_L(\rho)|p\rangle = \frac{2}{\pi} \int_0^\infty j_L(p'r)V(r,\rho)j_L(pr)r^2dr, \quad (2)$$

where p(p') is the initial (final) relative two-particle momentum, L is the orbital angular momentum, and  $j_L(x)$  is the spherical Bessel function. The upper integration limit is formally infinite, but Ref. [12] showed that at least five-digit accuracy for observables is achieved with a finite upper limit of 75 Å; the present work uses 100 Å, which is fully sufficient, since the integral equation formulation of the scattering theory in momentum space includes the asymptotic boundary conditions implicitly. Reference [12] investigated also the  $\rho$ dependence of the three-body binding energy and atom-dimer phase shifts and demonstrated that within the five-digit accuracy the results remain unchanged for  $\rho$  ranging from 0 to 1.7 Å. This means that practically there is no penetration into the  $\rho \leq 1.7$  Å region even if the potential is reduced by more than two orders of magnitude at r = 0, as the inset of Fig. 1 indicates. On the other hand, it is quite obvious that the proposed approach will fail beyond  $\rho \approx 2.5$  Å, where the barrier height and the minimum depth become of comparable size. However, already beyond  $\rho = 1.7$  Å, a further increase of  $\rho$  reduces the short-range repulsion to the extent that it becomes insufficient to preserve the fine-tuned balance with the longer-range attraction. As a consequence, the binding energies of few-body bound states start to increase with  $\rho$  for  $\rho > 1.7$  Å. To keep the same energy scale for all considered  $\rho$ , I choose to fix the dimer binding energy  $B_2 = 1.3094$  mK. For this, a further modification of the potential is needed that removes the overbinding. In effective field theories this is achieved by a repulsive short-range counterterm, but such a solution is unwanted in the present context as it would increase again the short-range repulsion. Therefore I propose a different approach, rendering the potential (2) weaker. There are many ways to achieve this goal, e.g., to rescale the potential (2) by a constant or a momentum-dependent factor, or even by a combination of them. My primary choice is the modified potential

$$\langle p'|v_L(\rho)|p\rangle = e^{-[\lambda(\rho)p']^2} \langle p'|V_L(\rho)|p\rangle e^{-[\lambda(\rho)p]^2}, \quad (3)$$

where the function  $\lambda(\rho)$  controls the momentum-dependent reduction. It is determined by fitting the dimer binding energy  $B_2 = 1.3094$  mK in the L = 0 partial wave, but the same  $\lambda(\rho)$  is used for all partial waves. Thus, none of the phase shifts are explicitly fitted, and therefore, they may deviate from their original values. Nevertheless, this deviation is not really important as long as no new bound or resonant states appear. Since  $\lambda(\rho)$  smoothly approaches zero with decreasing  $\rho$  and vanishes for  $\rho < 1.7$  Å as shown in Fig. 1, the potential (3) smoothly converges towards the original potential and all observables should do so as well. Further important advantage of the potential (3) is the suppression of high-momentum components that is favorable for the stability of numerical calculations. Low-momentum components corresponding to the long-range tail are barely affected. Though the potential

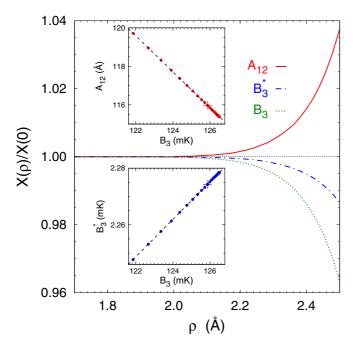


FIG. 2. Atom-dimer scattering length and trimer ground- and excited-state binding energies, all normalized by the respective predictions obtained with the original LM2M2 potential, are shown as functions of the softening parameter. Insets display correlations between trimer binding energies and atom-dimer scattering length. Crosses label data points with  $\rho = 2.3$  Å, and the lines result from linear fits to data points at 2.3 Å  $\leq \rho \leq 2.5$  Å.

(3) becomes nonlocal in the coordinate space, this presents no additional difficulty for momentum-space calculations.

In summary, few-body equations have to be solved for a series of potentials (3) with different values of the softening parameter  $\rho$ , large enough for a numerically stable solution, and the obtained results are extrapolated towards smaller  $\rho$  values until the independence of  $\rho$  is achieved. For brevity, the method is referred to as "softening and extrapolation" (SE).

## **III. TEST CASE: THREE-BODY SYSTEM**

The bound state and scattering problem of three <sup>4</sup>He atoms with realistic interaction in the momentum-space framework was solved using the original potential or the one of Eq. (2) with  $\rho \leq 1.7$  Å [12]. Thus, the SE is not needed to obtain physical results, but it is a good test case to demonstrate its validity.

The considered three-body observables are the atom-dimer scattering length  $A_{12}$  and binding energies for the trimer ground and excited states,  $B_3$  and  $B_3^*$ , respectively. More details of calculations can be found in Ref. [12], the only difference here being the updated  $\hbar^2/m$  value and the modified potential (3). At  $\rho \leq 1.7$  Å the predictions  $A_{12} = 115.39$  Å,  $B_3 = 126.50$  mK, and  $B_3^* = 2.2784$  mK agree perfectly with the benchmark calculation [9].

Figure 2 presents the dependence of the atom-dimer scattering length and trimer binding energies on the softening parameter  $\rho$ . The quantities are normalized by their original values taken at  $\rho = 0$  and listed above, in order to keep a single scale. The ratios start deviating from the unity above  $\rho = 2.0$  Åand reach nearly 4% difference at  $\rho = 2.5$  Å. As functions of  $\rho$ , the deviations grow with increasing rate, which makes the extrapolation in  $\rho$  problematic if data points near the plateau regime are not available. However, a closer inspection reveals that for all three quantities in Fig. 2 the shapes of the deviations are very similar. The consequence of this feature are linear correlations between trimer binding energies and atom-dimer scattering length; two pairs,  $A_{12}(B_3)$ and  $B_3^*(B_3)$ , are shown in the insets of Fig. 2, and the third pair  $A_{12}(B_3^*)$  correlates equally well. These correlations are expected in the context of Efimov physics; they are known as Tjon and Phillips lines also in nuclear physics [3,4].

The observed correlations suggest an alternative way of extrapolation by changing the extrapolation variable, instead of  $\rho$  considering one of the three-body quantities, for example,  $B_3(\rho)$ , given that it can be reliably calculated for small  $\rho$ , reproducing the original limit  $B_3 = B_3(0)$ . Other three-body quantities like  $A_{12}(\rho)$  and  $B_3^*(\rho)$  show (nearly) linear dependence on  $B_3(\rho)$  and, therefore, even if calculated only at  $\rho$  values beyond the plateau region, as functions of  $B_3(\rho)$  can be reliably extrapolated to the point  $B_3(0)$ , thereby yielding  $A_{12}(0)$  and  $B_3^*(0)$  estimations. The lines in the insets of Fig. 2 are linear fits to data in the regime 2.3 Å  $\leq \rho \leq 2.5$  Å. The extrapolation towards the  $B_3(0)$  value reproduces the  $A_{12}(0)$  and  $B_3^*(0)$  within 0.01% accuracy, confirming the reliability of the proposed extrapolation approach.

At a first glance it may appear that shapes of observable deviation in Fig. 2 and of  $\lambda(\rho)$  in Fig. 1 are similar, suggesting  $\lambda(\rho)$  as a suitable extrapolation variable. However, this is not true since in the regime 1.7 Å  $< \rho < 2.0$  Å there are small but visible changes in  $\lambda(\rho)$ , in contrast to  $A_{12}(\rho)$ ,  $B_3(\rho)$ , and  $B_3^*(\rho)$ . Consequently, their dependence on  $\lambda(\rho)$  is nearly linear at  $\rho > 2.3$  Å, but bends for smaller  $\rho$ , preventing reliable extrapolation. One could find perhaps a better behaving function of  $\rho$  like  $(\rho - \rho_0)^n$  or  $[\lambda(\rho)]^n$  that could be more suitable as an extrapolation variable, but it is not trivial to achieve the linearity as good as with  $B_3(\rho)$ .

## **IV. FOUR-BODY EQUATIONS**

The momentum-space integral-equation approach to the four-body problem starts with the two-body transition operator

$$t = v + vG_0t \tag{4}$$

that sums up the respective pair interaction v to all orders. The dependence on the available energy E arises via the free resolvent  $G_0 = (E + i0 - H_0)^{-1}$  with the kinetic energy operator  $H_0$ . The bound-state energy in the system of four identical bosons can be obtained from symmetrized Faddeev-Yakubovsky equations [19] for wave-function components

$$|\psi_1\rangle = G_0 t P_1[(1+P_{34})|\psi_1\rangle + |\psi_2\rangle],$$
 (5a)

$$|\psi_2\rangle = G_0 t P_2[(1+P_{34})|\psi_1\rangle + |\psi_2\rangle],$$
 (5b)

where *t* acts within pair (12) and  $P_{ab}$  interchanges particles *a* and *b*, while  $P_1 = P_{12}P_{23} + P_{13}P_{23}$  and  $P_2 = P_{13}P_{24}$ .

The scattering processes are described using AGS equations [13] for four-particle transition operators  $U_{\beta\alpha}$ . In the symmetrized form they read as follows:

$$\mathcal{U}_{11} = P_{34}(G_0 t G_0)^{-1} + P_{34} U_1 G_0 t G_0 \mathcal{U}_{11} + U_2 G_0 t G_0 \mathcal{U}_{21},$$
(6a)

$$\mathcal{U}_{21} = (1 + P_{34})(G_0 t G_0)^{-1} + (1 + P_{34})U_1 G_0 t G_0 \mathcal{U}_{11}, \quad (6b)$$

$$\mathcal{U}_{12} = (G_0 t G_0)^{-1} + P_{34} U_1 G_0 t G_0 \mathcal{U}_{12} + U_2 G_0 t G_0 \mathcal{U}_{22}, \quad (6c)$$

$$\mathcal{U}_{22} = (1 + P_{34})U_1 G_0 t G_0 \mathcal{U}_{12}. \tag{6d}$$

Here the subscripts  $\alpha$ ,  $\beta = 1$  (2) label the 3 + 1 (2 + 2) clustering, while

$$U_{\alpha} = P_{\alpha}G_0^{-1} + P_{\alpha}tG_0U_{\alpha} \tag{7}$$

are the 3 + 1 or 2 + 2 subsystem transition operators.

Physical transition amplitudes for two-cluster collisions are calculated as special on-shell matrix elements of transition operators  $\mathcal{U}_{\beta\alpha}$  between the channel states  $|\phi_{\alpha}(\mathbf{p}_{\alpha})\rangle$  with the relative two-cluster momenta  $\mathbf{p}_{\alpha}$ . The primary interest of the present work is the atom-trimer and dimer-dimer scattering lengths

$$A_{13} = 3\pi (3m/4) \langle \phi_1(0) | \mathcal{U}_{11} | \phi_1(0) \rangle |_{\mathcal{J}=0}, \qquad (8a)$$

$$A_{22} = 2\pi m \langle \phi_2(0) | \mathcal{U}_{22} | \phi_2(0) \rangle |_{\mathcal{J}=0}, \tag{8b}$$

where the matrix elements are taken between states with vanishing relative two-cluster momentum and total four-body angular momentum  $\mathcal{J} = 0$  at energies  $E = -B_3$  (atom-trimer) and  $-2B_2$  (dimer-dimer).

The momentum-space partial-wave basis  $|k_x k_y k_z[(l_x l_y) J l_z] \mathcal{JM} \rangle_{\alpha}$  is used to solve AGS equations (6) where they build a system of coupled integral equations with three continuous variables  $k_x$ ,  $k_y$ , and  $k_z$ , the magnitudes of Jacobi momenta [20]. The associated orbital angular momenta  $l_x$ ,  $l_y$ , and  $l_z$  via J are coupled to  $\mathcal{J}$  with the projection  $\mathcal{M}$ . Discretization of three Jacobi momenta results in a large system of linear algebraic equations. More details on the solution methods are given in Ref. [20].

#### V. RESULTS FOR THE FOUR-ATOM SYSTEM

# A. Tetramer ground-state energy

To validate the proposed SE method in the four-atom system I start with the calculation of the tetramer ground-state binding energy  $B_4$  where several well-established results are available [5,7,10,11]. The Faddeev-Yakubovsky equations (5) are solved including partial waves with orbital angular momenta  $l_x$ ,  $l_y$ ,  $l_z \leq 8$  and about 70 to 100 grid points for the discretization of Jacobi momenta; the trimer binding energy is calculated using the same model space. The results are obtained for 2.2 Å  $\leq \rho \leq 2.5$  Å; for brevity the dependence of binding energies on  $\rho$  is suppressed in the notation. Figure 3 shows the dependence of the tetramer ground-state binding energy on  $\rho$ , indicating that the extrapolation in  $\rho$  is problematic. Some particular function of  $\rho$  could be more suitable. As the inset of Fig. 3 demonstrates, extrapolation in  $B_3$  works very well since  $B_4(B_3)$  in the considered regime is nearly a linear function, as should be expected in the context of Efimov physics [3,4] and was shown for <sup>4</sup>He atoms in Ref. [21].

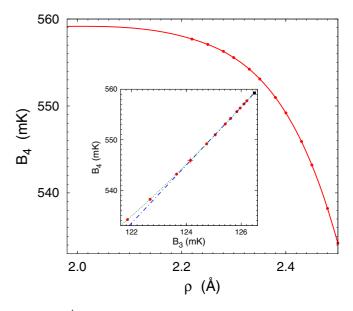


FIG. 3. <sup>4</sup>He tetramer ground-state binding energy  $B_4$  as a function of the softening parameter  $\rho$ . The curve is obtained by the extrapolation in the variable  $B_3$ . The inset shows the  $B_4$  dependence on the trimer ground-state binding energy  $B_3$ . The dashed-dotted line represents the linear fit to data points 2.2 Å  $\leq \rho \leq 2.43$  Å, while the dotted curve represents the quadratic fit to all data points up to  $\rho = 2.5$  Å. The cross labels the data point  $\rho = 2.43$  Å. Extrapolation to the  $B_3$  prediction of the original LM2M2 potential is given by the black square.

However, a slight deviation from the linearity is seen for  $\rho \ge 2.45$  Å. A probable reason is that a tetramer, being more compact and therefore more sensitive to the short-range force than a trimer, starts to "feel" the softening of the barrier at lower  $\rho$  values. Nevertheless, a high-quality fit is obtained by the inclusion of the quadratic term, as shown by the dotted curve. Alternatively, a linear fit (dashed-dotted curve) in the reduced region 2.2 Å  $\leq \rho \leq 2.43$  Å also works well. In both cases the extrapolation to the limit of the original LM2M2 potential yields the tetramer ground-state binding energy value  $B_4 = 559.3(1)$  mK. This result is in good agreement with the most accurate available prediction  $B_4 = 559.22$  mK obtained using the variational Gaussian expansion method [11]. The results obtained with other methods [7], perturbatively corrected for the updated  $\hbar^2/m$  value as in Ref. [11], range from 557.2 to 559.3 mK. The observed agreement confirms the reliability of the proposed SE method.

#### **B.** Dimer-dimer scattering length

In contrast to  $A_{12}$ , the presence of a lower-lying threshold, atom plus trimer, renders the dimer-dimer scattering length  $A_{22}$  complex. It is obtained by solving the AGS equations (6c) and (6d) at the energy  $E = -2B_2$ . Since the solution proceeds via the double Padé method [20], its convergence and accuracy are limited by a bad divergence of the Neumann series for four-body transition operators. This difficulty is characteristic to Efimovian systems owing to a rich spectrum of states, corresponding to transition operator poles, that spoil down the convergence [22]. The results therefore are shown with their

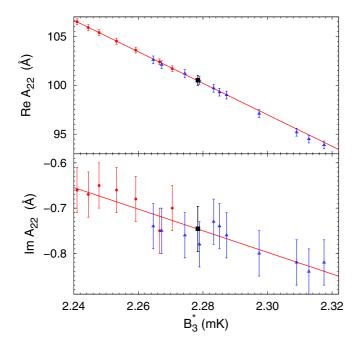


FIG. 4. Real and imaginary parts of the dimer-dimer scattering length as functions of the binding energy  $B_3^*$  of the excited trimer state. Results obtained using the potential (3) are shown as full circles, and the lines are linear fits to those results. Extrapolations to the  $B_3^*$  prediction of the original LM2M2 potential are given by full squares. The points shown by open triangles are obtained using potentials of type (10) and are not included in the fit.

numerical error bars, typically below 0.5% for the real part, but above 5% for the much smaller imaginary part. Within those error bars, the real and imaginary parts of  $A_{22}$  are consistent with the typical  $\rho$  dependence, already seen in the case of three-body observables and tetramer binding energy; it is therefore not presented here again. Instead, Figure 4 displays Re  $A_{22}$  and Im  $A_{22}$  as functions of the binding energy  $B_3^*$  of the excited trimer state. The calculated data points are shown as full circles, and the lines are linear fits to those results. Extrapolation to the limit of the LM2M2 potential yields

$$A_{22} = [100.5(5) - i0.75(5)] \text{ Å.}$$
(9)

Thus, Fig. 4 suggests the existence of the Phillips line also for the dimer-dimer scattering. To strengthen this conclusion additional calculations are performed using a slightly different scheme for the softening of the potential, namely,

$$\langle p'|\bar{v}_L(\rho)|p\rangle = e^{-[\bar{\lambda}(\rho)p']^2} [1 - v\bar{\lambda}(\rho)] (\langle p'|V_L(\rho)|p\rangle e^{-[\bar{\lambda}(\rho)p]^2}.$$
(10)

 $\lambda(\rho)$  for each value of the parameter  $\nu$  is again determined by fitting the dimer binding energy  $B_2$ . Introducing  $\nu$  offers the flexibility to explore a broader range of  $A_{22}$  and  $B_3^*$ , both above and below the LM2M2 value. The additional data points in Fig. 4 represented by open triangles are obtained with  $\nu$ ranging from 0.1 to 0.5 Å<sup>-1</sup> and  $\rho$  between 2.45 and 2.52 Å. Within the error bars the additional data points obtained using softened potentials of type (10) are consistent with the linear correlation determined using the potential (3). In the above study the extrapolation was performed in the binding energy of the excited trimer state, the state closest to the two-dimer threshold. On the other hand, given that the linear correlations demonstrated in Sec. III are accurate to the level of 0.01%, one could chose  $B_3$  or  $A_{12}$  equally well without affecting numerical results within that accuracy, that is, without any changes of the numerical values presented in this work for all considered four-body observables, including those of next subsections. The associated inaccuracy is entirely irrelevant compared to other sources of numerical solution errors.

It is also interesting to compare the dimer-dimer scattering length (9), obtained for the realistic potential, with the universal zero-range prediction. From Fig. 2 of Ref. [22], at the physical  $B_3^*/B_2$  ratio one gets  $A_{22}/a \approx 0.945 - i0.004$ . Thus, with the LM2M2 two-atom scattering length a = 100.0 Å, the zero-range limit  $A_{22} \approx (94.5 - i0.4)$  Å reproduces reasonably the real part but fails significantly for the imaginary part. This is not very surprising since Im  $A_{22}$  is determined by the transition to the ground-state trimer that is more affected by finite-range corrections.

The collision of two dimers has an inelastic channel, i.e., rearrangement leading to the atom plus trimer state. In the gas consisting of dimers of the density  $n_2$ , this reaction would lead to the trimer density  $n_3$  increase in time as

$$\frac{dn_3}{dt} = \beta_{22 \to 31} \frac{n_2^2}{2!}.$$
(11)

In the ultracold limit corresponding to the vanishing relative dimer-dimer momentum  $p_2 \rightarrow 0$ , the inelastic cross section  $\sigma_{22\rightarrow31}^0 \sim |\langle \phi_1(\mathbf{p}_1) | \mathcal{U}_{12} | \phi_2(0) \rangle|^2 p_1 / p_2$  is formally infinite, but the reaction rate  $\beta_{22\rightarrow31}^0 \sim p_2 \sigma_{22\rightarrow31}^0$  is finite. Using the optical theorem it can be expressed via the imaginary part of the dimer-dimer scattering length as

$$\beta_{22 \to 31}^0 = -\frac{8\pi\hbar}{m} \operatorname{Im}(A_{22}). \tag{12}$$

The numerical value is  $\beta_{22\rightarrow 31}^0 = 3.0(2) \times 10^{-11} \text{ cm}^3/\text{s}$ ; the zero-range limit would underestimate it by a factor of 2.

# C. Atom-trimer scattering and excited tetramer state

Atom-trimer scattering calculations follow the same procedure as described in the previous subsection for the dimer-dimer scattering except that the AGS equations (6a) and (6b) around the energy  $E = -B_3$  are solved. The extrapolation to the limit of the original LM2M2 potential yields the <sup>4</sup>He atom-trimer scattering length  $A_{13} = 108.8(5)$  Å and the effective range  $R_{13} = 29.2(2)$  Å. The latter agrees well with the only available prediction  $R_{13} = 29.1$  Å in Ref. [7]. In contrast, there is nearly 5% difference with the prediction  $A_{13} = 103.7$  Å of Ref. [7] and a strong disagreement with  $A_{13} = 56$  Å of Ref. [5].

The binding energy of the excited tetramer state  $B_4^*$  is obtained looking for the energy corresponding to the pole of four-body transition operators at  $E = -B_4^*$  in Eqs. (6a) and (6b). The extrapolation to the LM2M2 point yields  $B_4^* = 127.46(2)$  mK or  $B_4^* - B_3 = 0.96(2)$  mK. The weak binding of the excited tetramer state with respect to the ground-state trimer causes a number of methods to fail heavily on  $B_4^* - B_3$ ,

despite quite accurate predictions for  $B_4$  [5,10]. Even the two most advanced calculations differ by 15%, with  $B_4^* - B_3 =$ 1.087 mK in Ref. [7] and 0.93 mK in Ref. [11]. The former is the estimation based on the effective-range expansion. The same approach using  $A_{13}$  and  $R_{13}$  of the present work yields a smaller value of  $B_4^* - B_3 = 0.97(2)$  mK, mainly due to a larger  $A_{13}$  than in Ref. [7]. Thus, the present results for  $B_4^* - B_3$  tend to support those of Ref. [11].

## VI. SUMMARY AND CONCLUSIONS

Calculations of weakly bound few-body atomic <sup>4</sup>He systems with realistic potentials are complicated due to the very strong repulsion at short distances. While the three-body system is still manageable using a number of methods, the four-body system requires a special treatment, especially in the continuum. The present work proposed a softening and extrapolation approach for dealing with the short-range repulsion and implemented it in the rigorous momentum-space framework for transition operators.

The strength of the short-range repulsion was gradually reduced by introducing one softening parameter, at the same time suppressing the high-momentum components by a nonlocal extension of the potential, adjusted to reproduce exactly the original dimer binding energy. This ensured that also other few-body observables deviate only mildly, within a few percent, from their original values. Furthermore, those deviations evolve smoothly with the softening parameter, allowing for the extrapolation back to the limit of the original potential. Sufficiently accurate solutions of momentum-space three- and four-body equations were obtained using the softened realistic LM2M2 potential. Binding energies of trimer and tetramer ground and excited states as well as the atom-dimer, atomtrimer, and dimer-dimer scattering lengths were calculated for a range of softening parameter values. Nearly linear correlations between all those three- and four-body quantities were observed, suggesting to use one of the easily calculable three-body quantities as the extrapolation variable, thereby essentially improving the accuracy of the extrapolation procedure. In particular, the linear correlation between the trimer binding energy and the dimer-dimer scattering was demonstrated, establishing an additional case of the Phillips line.

The tetramer ground-state energy, extrapolated to the limit of the original LM2M2 potential, agrees well with previous determinations by other methods. In the more controversial case of the excited tetramer state, my prediction for its binding energy is less than 1 mK with respect to the atom-trimer threshold, clearly supporting the results of Refs. [7,11] over those of Refs. [5,10]. There is a reasonable agreement with Ref. [7] in the case of the atom-trimer scattering length and effective range, though my slightly larger  $A_{13}$  value implies a slightly weaker binding for the excited tetramer state, in a better agreement with Ref. [11].

The most important result is the complex dimer-dimer scattering length. Its real part turns out to be very close to the atom-atom scattering length, while the imaginary part is smaller by more than a factor of 100. The latter determines the rate of <sup>4</sup>He trimer production via two-dimer collisions in ultracold gases. The universal zero-range theory is unable to reproduce accurately the imaginary part of the dimer-dimer scattering length and the trimer production rate, thereby indicating the importance of finite-range corrections.

- [1] V. Efimov, Phys. Lett. B 33, 563 (1970).
- [2] M. Kunitski et al., Science 348, 551 (2015).
- [3] P. Naidon and S. Endo, Rep. Prog. Phys. 80, 056001 (2017).
- [4] A. Kievsky, M. Gattobigio, L. Girlanda, and M. Viviani, Annu. Rev. Nucl. Part. Sci. 71, 465 (2021).
- [5] D. Blume and C. H. Greene, J. Chem. Phys. 112, 8053 (2000).
- [6] P. Barletta and A. Kievsky, Phys. Rev. A 64, 042514 (2001).
- [7] R. Lazauskas and J. Carbonell, Phys. Rev. A 73, 062717 (2006).
- [8] E. Kolganova, A. Motovilov, and W. Sandhas, Phys. Part. Nuclei 40, 206 (2009).
- [9] V. Roudnev and M. Cavagnero, J. Phys. B: At., Mol. Opt. Phys. 45, 025101 (2012).
- [10] T. K. Das, B. Chakrabarti, and S. Canuto, J. Chem. Phys. 134, 164106 (2011).
- [11] E. Hiyama and M. Kamimura, Phys. Rev. A 85, 022502 (2012).
- [12] A. Deltuva, Few-Body Syst. 56, 897 (2015).

- P. Grassberger and W. Sandhas, Nucl. Phys. B 2, 181 (1967);
   E. O. Alt, P. Grassberger, and W. Sandhas, JINR Report No. E4-6688, 1972.
- [14] A. Deltuva and A. C. Fonseca, Phys. Rev. Lett. 113, 102502 (2014).
- [15] R. A. Aziz and M. J. Slaman, J. Chem. Phys. 94, 8047 (1991).
- [16] M. Przybytek, W. Cencek, J. Komasa, G. Łach, B. Jeziorski, and K. Szalewicz, Phys. Rev. Lett. 104, 183003 (2010).
- [17] R. E. Grisenti, W. Schöllkopf, J. P. Toennies, G. C. Hegerfeldt, T. Köhler, and M. Stoll, Phys. Rev. Lett. 85, 2284 (2000).
- [18] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C 75, 061001(R) (2007).
- [19] O. A. Yakubovsky, Yad. Fiz. 5, 1312 (1967) [Sov. J. Nucl. Phys. 5, 937 (1967)].
- [20] A. Deltuva and A. C. Fonseca, Phys. Rev. C 75, 014005 (2007).
- [21] E. Hiyama and M. Kamimura, Phys. Rev. A 85, 062505 (2012).
- [22] A. Deltuva, Phys. Rev. A 84, 022703 (2011).