Scattering Length for Helium Atom-Diatom Collision

E. A. Kolganova\textsuperscript{1,2}, A. K. Motovilov\textsuperscript{2}, and W. Sandhas\textsuperscript{3}

\textsuperscript{1} Max-Planck-Institut f"ur Physik komplexer Systeme, N"othnitzer str. 38, 01187 Dresden, Germany
\textsuperscript{2} Bogoliubov Laboratory of Theoretical Physics, JINR, Joliot-Curie 6, 141980 Dubna, Moscow Region, Russia
\textsuperscript{3} Physikalisches Institut, Universit"at Bonn, Endenicher Allee 11-13, D-53115 Bonn, Germany

Abstract. We present results on the scattering lengths of $^4\text{He}^-^4\text{He}_2$ and $^3\text{He}^-^4\text{He}_2$ collisions. We also study the consequence of varying the coupling constant of the atom-atom interaction.

1 Introduction

The two-body scattering length in a dilute gas of alkali atoms can be varied by changing the external magnetic field close to a Feshbach resonance \cite{1}. In this way one may force the two-body s-wave scattering length to go from positive to negative values through infinity. Therefore, the magnetic field should be an appropriate tool in modeling the Efimov effect. We recall that this effect occurs in case of infinite two-body scattering lengths, manifesting itself in an infinite number of three-body bound states.

This role of the magnetic field combined with a Feshbach resonance may be mimicked by varying the coupling constant of the two-body interaction within a three-body system that is not necessarily subject to a magnetic field \cite{2}. In this context the system of three $^4\text{He}$ atoms appears to be the best candidate. Actually, it has been shown that the excited state of the $^4\text{He}$ trimer is already of Efimov nature. To get the complete Efimov effect it suffices to weaken the He–He interatomic potential only by about 3%.

In the present work we extend the investigation of the three-atomic helium systems undertaken in \cite{3}, which was based on a mathematically rigorous hard-core version of the Faddeev differential equations. We calculate the scattering

\textsuperscript{*}Contribution to Proceedings of the International Workshop “Critical Stability of Few-Body Quantum Systems” (Dresden, October 17–22, 2005). This work was supported by the Deutsche Forschungsgemeinschaft (DFG), the Heisenberg-Landau Program, and the Russian Foundation for Basic Research.
lengths for \(^{3/4}\)He atoms - \(^4\)He dimer collisions. Under the assumption that weakening the potential mimics the behaviour of the scattering length in a magnetic field, we show the dependence of low-energy three-body scattering properties on the two-body scattering length.

Some of the results presented in this paper were reported already in [4] and [5].

2 Results

In our calculations we employed the hard-core version of the Faddeev differential equations developed in [3]. As He-He interaction we used the semi-empirical HFD-B [6] and LM2M2 [7] potentials by Aziz and co-workers, and the more recent, purely theoretically derived TTY [8] potential by Tang, Toennies and Yiu. For the explicit form of these polarization potentials we refer to the Appendix of Ref. [3]. As in our previous calculations we choose \(\hbar^2/m_{^{4}\text{He}} = 12.12 \text{ K A}^2\) and \(m_{^{3}\text{He}}/m_{^{4}\text{He}} = 0.753517\) where \(m_{^{3}\text{He}}\) and \(m_{^{4}\text{He}}\) stand for the masses of the \(^3\)He and \(^4\)He atoms, respectively. The \(^4\)He dimer binding energies and \(^4\)He-\(^4\)He scattering lengths obtained with the HFD-B, LM2M2, and TTY potentials are shown in Table 1. Note that the inverse of the wave number \(\kappa^{(2)} = \sqrt{|\epsilon_d|}\) lies rather close to the corresponding scattering length.

### Table 1

| \(\epsilon_d\) (mK) | \(\ell_{sc}^{(1+1)}\) (Å) | Potential   | \(\epsilon_d\) (mK) | \(1/\kappa^{(2)}\) (Å) | \(\ell_{sc}^{(1+1)}\) (Å) |
|---------------------|--------------------------|-------------|---------------------|--------------------------|--------------------------|
| Exp. [2] 1.1\(^{+0.3}_{-0.2}\) 104\(^{+8}_{-18}\) | LM2M2 -1.30348 96.43 100.23 | TTY -1.30962 96.20 100.01 | HFD-B -1.68541 84.80 88.50 |

### Table 2

The \(^4\)He-\(^4\)He\(_2\) scattering length \(\ell_{sc}^{(1+2)}\) (Å) on a grid with \(N_{\rho} = N_{\theta} = 2005\) and \(\rho_{\text{max}} = 700\) Å.

| Potential  | \(l_{\text{max}}\) | This work   | [3] | [10] | [11] | [12] | [13] |
|------------|-------------------|-------------|-----|------|------|------|------|
| LM2M2      | 0                 | 158.2       | 168 | 158.2| 168  | 158.2| 168  |
|            | 2                 | 122.9       | 134 | 122.9| 134  | 122.9| 134  |
|            | 4                 | 118.7       | 131 | 126  | 115.4| 114.25| 113.1|
| TTY        | 0                 | 158.6       | 168 | 158.6| 168  | 158.6| 168  |
|            | 2                 | 123.2       | 134 | 123.2| 134  | 123.2| 134  |
|            | 4                 | 118.9       | 131 | 115.8| 115.8| 114.5| 114.5|
| HFD-B      | 0                 | 159.6       | 168 | 159.6| 168  | 159.6| 168  |
|            | 2                 | 128.4       | 138 | 128.4| 138  | 128.4| 138  |
|            | 4                 | 124.7       | 135 | 121.9| 121.9| 120.2| 120.2|

We have improved our previous calculations [3] of the scattering length by...
increasing the values of the grid parameters and cutoff hyperradius. The corresponding results are presented in Table 2. This table also contains the fairly recent results by Blume and Greene [10] and by Roudnev [11]. The treatment of [10] is based on a combination of the Monte Carlo method and the hyperspherical adiabatic approach. The one of Ref. [11] employs the three-dimensional Faddeev differential equations in the total angular momentum representation. Our results agree rather well with these alternative calculations.

For completeness we mention that besides the above \textit{ab initio} calculations there are also model calculations, the results of which are given in the last two columns of Table 2. The calculations of [12] are based on employing a Yamaguchi potential that leads to an easily solvable one-dimensional integral equation in momentum space. The approach of [13] represents intrinsically a zero-range model with a cut-off introduced to make the resulting one-dimensional Skornyakov-Ter-Martirosian equation [14] well defined. The cut-off parameter in [13] as well as the range parameter of the Yamaguchi potential in [12] are adjusted to the three-body binding energy obtained in the \textit{ab initio} calculations. In other words, these approaches are characterized by remarkable simplicity, but rely essentially on results of the \textit{ab initio} three-body calculations.

\begin{table}[h]
\centering
\begin{tabular}{cccc}
\hline
Potential & LM2M2 & TTY \\
\hline
$l_{\text{max}}$ & 0 & 2 & 4 \\
This work & 38.5 & 22.2 & 21.0 \\
[15] & 19.3 & & 19.6 \\
\hline
\end{tabular}
\caption{The $^3\text{He}^4\text{He}_2$ atom-dimer scattering length $\ell^{(1+2)}_{\text{sc}}$(in Å).}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{ccccccc}
\hline
$\lambda$ & $\epsilon_d$ & $\epsilon_d - E^{(1)}_{\text{ex}}$ & $\epsilon_d - E_{\text{virt}}$ & $\epsilon_d - E^{(2)}_{\text{ex}}$ & $\ell^{(1+2)}_{\text{sc}}$ & $\rho_{\text{max}}$(Å) \\
\hline
1.0 & -1.685 & 0.773 & - & - & 160 & 88.6 & 700 \\
0.995 & -1.160 & 0.710 & - & - & 151 & 106 & 900 \\
0.990 & -0.732 & 0.622 & - & - & 143 & 132 & 1050 \\
0.9875 & -0.555 & 0.222 & - & - & 125 & 151 & 1200 \\
0.985 & -0.402 & 0.518 & 0.097 & - & 69 & 177 & 1300 \\
0.982 & -0.251 & 0.447 & 0.022 & - & -75 & 223 & 1700 \\
0.980 & -0.170 & 0.396 & 0.009 & - & -337 & 271 & 2000 \\
0.9775 & -0.091 & 0.328 & 0.003 & - & -6972 & 370 & 3000 \\
0.975 & -0.036 & 0.259 & - & -0.002 & 7120 & 583 & 4500 \\
0.973 & -0.010 & 0.204 & - & -0.006 & 4260 & 1092 & 10000 \\
\hline
\end{tabular}
\caption{Dependence of the trimer energies (mK) and the scattering length (Å) on the potential strength $\lambda$ (for $l_{\text{max}} = 0$).}
\end{table}

Due to the smaller mass of the $^3\text{He}$ atom, the $^3\text{He}^4\text{He}_2$ system is unbound. Nevertheless, the $^3\text{He}^4\text{He}_2$ trimer exists, though with a binding energy of about 14 mK (see [2] and references therein). And, in contrast to the symmetric case, there is no excited (Efimov-type) state in the asymmetric $^3\text{He}^4\text{He}_2$ system. Ta-
Table 3 contains our results for the $^3\text{He}^4\text{He}_2$ scattering length.

Following the idea that weakening the potential could imitate the action of a magnetic field on the scattering length, we multiply the original potential $V_{\text{HFD-B}}(x)$ by a factor $\lambda$. Decreasing this coupling constant, there emerges a virtual state of energy $E_{\text{virt}}$ on the second energy sheet. This energy, relative to the two-body binding energy $\epsilon_d$, is given in column 4 of Table 4. When decreasing $\lambda$ further, this state turns into the second excited state. Its energy $E_{\text{ex}}^{(2)}$ relative to $\epsilon_d$ is shown in the next column. These energy results are in a good agreement with the literature [16]. When the second excited state emerges, the $^4\text{He}^4\text{He}_2$ scattering length $\ell_{\text{sc}}^{(1+2)}$ changes its sign going through a pole, while the two-body scattering length $\ell_{\text{sc}}^{(1+1)}$ increases monotonically.

Acknowledgement. We are grateful to Prof. V. B. Belyaev and Prof. H. Toki for providing us with the possibility to perform calculations at the supercomputer of the Research Center for Nuclear Physics of Osaka University, Japan. One of us (E.A.K.) is indebted to Prof. J. M. Rost for his hospitality at the Max-Planck-Institut für Physik komplexer Systeme, Dresden.

References

1. R. A. Duine and H. T. C Stoof, Phys. Rep. 396, 115 (2004).
2. J. P. D'Incao and B. D. Esry, Phys. Rev. A 72, 032710 (2005).
3. A. K. Motovilov, W. Sandhas, S. A. Sofianos, and E. A. Kolganova, Eur. Phys. J. D 13, 33 (2001); arXiv: physics/9910010.
4. E. A. Kolganova, A. K. Motovilov, W. Sandhas, Phys. Rev. A 70, 052711 (2004); arXiv: physics/0408019.
5. W. Sandhas, E. A. Kolganova, Y. K. Ho, and A. K. Motovilov, Few-Body Systems 34, 137 (2004).
6. R. A. Aziz, F. R. W. McCourt, and C. C. K. Wong, Mol. Phys. 61, 1487 (1987).
7. R. A. Aziz and M. J. Slaman, J. Chem. Phys. 94, 8047 (1991).
8. K. T. Tang, J. P. Toennies, and C. L. Yiu, Phys. Rev. Lett. 74, 1546 (1995).
9. R. Grisenti, W. Schöllkopf, J. P. Toennies, G. C. Hegerfeld, T. Köhler, and M. Stoll, Phys. Rev. Lett. 85, 2284 (2000).
10. D. Blume and C. H. Greene, J. Chem. Phys. 112, 8053 (2000).
11. V. Roudnev, Chem. Phys. Lett. 367, 95 (2003).
12. F. M. Pen’kov, JETP 97, 536 (2003).
13. E. Braatem and H.-W. Hammer, Phys. Rev. A 67, 042706 (2003).
14. G. V. Skorniakov and K. A. Ter-Martirosian, Sov. Phys. JETP 4, 648 (1956).
15. V. Roudnev, private communication.
16. B. D. Esry, C. D. Lin, and C. H. Greene, Phys.Rev.A 54, 394 (1996).