

## Low-energy scattering parameters for van der Waals perturbation theory

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The low-energy two-body scattering  $S$ - and  $P$ -wave parameters, together with a shape-dependent  $S$ -wave quantity, which appear in the well-known low-density expansions for the ground-state energy of many-boson and many-fermion systems, are accurately calculated for several central pair potentials for spin-polarized atoms, helium atoms, and nucleons. An integral-equation method allowing accurate determination of the coefficients of the above-mentioned parameters expanded in powers of the attraction strength of the pair potential is presented and applied. The results are needed for perturbation studies of ground-state energies of various quantum many-body systems.

### I. INTRODUCTION

Few Monte Carlo computer determinations,<sup>1</sup> whether of the variational or Green-function variety, for the ground-state energy as a function of particle density have become available for the various many-body systems interacting even via a simple two-body central potential. The reason is twofold: (a) The simulations are expensive in terms of computer time and (b) the Green-function case for fermions is still beset with serious theoretical difficulties.

In recent years, modern extrapolation techniques, such as the Padé approximant,<sup>2</sup> have been applied<sup>3</sup> to the well-known low-density expansions for the ground-state energy of many-boson<sup>4</sup> and many-fermion<sup>5</sup> systems in attempts to generate, at the necessary intermediate densities, reliable equations of state for such substances in a simple, inexpensive manner. The Padé techniques are widely known to be very efficient for this purpose even in cases where the original series are divergent.

For fermions the (at best asymptotic) expansion known to date for the energy per particle is

$$E/N \simeq \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \left[ 1 + C_1 k_F a + C_2 (k_F a)^2 + \left( \frac{1}{2} C_3 \frac{r_0}{a} + C_4 \frac{A_1(0)}{a^3} + C_5 \right) (k_F a)^3 + C_6 (k_F a)^4 \ln |k_F a| + \left( \frac{1}{2} C_7 \frac{r_0}{a} + C_8 \frac{A_0''(0)}{a^3} + C_9 \right) (k_F a)^4 + o((k_F a)^4) \right]. \quad (1)$$

Here  $m$  is the particle mass, and  $\hbar k_F$  is the Fermi momentum of the ideal gas at a particle density  $n = N/V = \nu k_F^3 / 6\pi^2$ , with  $\nu$  the number of different fermion species (i.e., spin and isospin degeneracy). The  $C_i$ 's are pure numbers as given in Ref. 6, while  $a$ ,  $r_0$ , and  $A_1(0)$  are the well-known scattering (potential-shape-independent) parameters of the effective range theory<sup>7</sup> which gives, for each partial wave  $l=0, 1, \dots$ , the low-energy result

$$k^{2l+1} \cot \delta_l(k) \simeq -\frac{1}{A_l(0)} + \frac{1}{2} r_l k^2 + O(k^4) \text{ as } k \rightarrow 0, \quad (2)$$

where  $A_0(0) \equiv a$  ( $S$ -wave scattering length) and  $\delta_l(k)$  is the  $l$ th partial-wave scattering phase shift. Also appearing in (1) is the shape-dependent  $S$ -wave quantity<sup>5</sup>

$$A_0''(0) \equiv -\frac{1}{3} \int_0^\infty dr r^3 v(r) u_0(r), \quad (3)$$

where  $v(r)$  is  $2\mu/\hbar^2$  times the central potential-energy function  $V(r)$  through which the particles interact,  $\mu \equiv m/2$ , and  $u_0(r)$  is the  $S$ -wave, zero-energy radial wave function.

The low-density expression for the energy per particle in the ground state of boson systems is analogous to (1) but somewhat simpler, although it involves an unknown coefficient in the term corresponding to the  $(k_F a)^4$  term for fermions. The unknown coefficient contains three-body cluster terms and thus depends on the shape of the boson-boson interaction (just as its counterpart for fermions is shape dependent), and an interesting form has been proposed for it.<sup>8</sup>

For either case, fermion or boson, it is useful to separate the potential function  $v(r)$  into a positive part  $v_{\text{core}}(r)$  and a negative part  $v_{\text{att}}(r)$ , so that

$$v(r) = v_{\text{core}}(r) + \lambda v_{\text{att}}(r) \quad (4)$$

with  $\lambda$  a real, dimensionless parameter. The actual pair potential, of course, corresponds to the case  $\lambda=1$ . Expansion of  $a$ ,  $r_0$ ,  $A_1(0)$ , and  $A_0''(0)$  in powers of  $\lambda$ , and substitution into (1) or into the corresponding boson expression, clearly leads in either case to an energy expression

$$E/N \simeq \sum_{i=0}^{\infty} \varepsilon_i(n) \lambda^i \quad (5)$$

which is really a double series, in density  $n$  and in attractive coupling  $\lambda$ . The energy per particle is now in the form of a perturbation scheme not about the ideal gas, as in (1), but about a fluid of purely repulsive particles interacting via  $v_{\text{core}}(r)$ . The rearrangement (5) is essentially the perturbation treatment suggested, but never formulated, by van der Waals more than a hundred years ago. This scheme is actively being applied at present<sup>3,6</sup> but clearly requires knowledge of the various expansion coefficients for  $a$ ,  $r_0$ ,  $A_1(0)$ , and  $A_0''(0)$  for diverse two-body potentials. The  $\lambda$  power series of these parameters may or may not diverge for the physically relevant value  $\lambda=1$ ; this will be restricted in the double series (5) but later dealt with by Padé methods and generalizations thereof.

In this paper we conclude two previous studies that very precisely determined<sup>9</sup> these coefficients for several potentials and calculated<sup>10</sup> for the Lennard-Jones interaction between helium atoms the aforementioned expansion coefficients up to 14th order. In Sec. II we list the central potentials to be treated; in Sec. III we quote the values determined for the various scattering parameters. Section IV contains a new integral-equation method for calculating the corresponding expansion coefficients of these parameters and Sec. V states our results to sixth order. Results up to 19th order are available upon request from the University of Granada although perturbation studies carried out so far suggest the unlikelihood of having to go beyond sixth order.

## II. PAIR CENTRAL POTENTIALS

We shall be interested in solutions of the radial Schrödinger equation, with  $u_l(0)=0$ ,

$$u_l''(r) + \frac{m}{\hbar^2} [E - V(r)] u_l(r) - \frac{l(l+1)}{r^2} u_l(r) = 0 \quad (6)$$

for various pair central potentials  $V(r)$ , to be listed below. These potentials represent the interaction (a) between spin-polarized hydrogen H $\downarrow$ , deuterium D $\downarrow$ , and tritium T $\downarrow$  and (b) between  $^3\text{He}$  and  $^4\text{He}$  atoms, as well as (c) between nucleons. The values of  $\hbar^2/m$  used are given in Table I.

The pair central potentials  $V(r)$  considered in Eq. (1) are the following.

(a) The Lennard-Jones (LJ) potential, given by

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (7)$$

TABLE I. Values of  $\hbar^2/m$  for the different particles considered in Eq. (6), in units  $\text{K} \text{Å}^2$  for all cases except the last entry which is in  $\text{MeV F}^2$  ( $1 \text{ F} = 10^{-13} \text{ cm}$ ).

Particle	$\hbar^2/m$
H $\downarrow$	48.133 716
D $\downarrow$	24.078 181
T $\downarrow$	16.089 71
$^3\text{He}$	16.085 775
$^4\text{He}$	12.120 904
Nucleon	41.512 9306

with<sup>11</sup>  $\epsilon=6.46 \text{ K}$ ,  $\sigma=3.69 \text{ Å}$  for the spin-polarized atoms listed in Table I and  $\epsilon=10.22 \text{ K}$ ,  $\sigma=2.556 \text{ Å}$  for the helium atoms.

(b) The Kolos-Wolniewicz (KW) potential is found in the form of numerical tables in the literature.<sup>12</sup> However, a simple parametrization is the so-called Silvera fit given by Friend and Etters<sup>13</sup> and is of the form

$$V(r) = A e^{-(a_1 r + a_2 r^2)} - B f(r) \left[ \frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}} \right], \quad (8)$$

$$f(r) \equiv e^{-(D/r-1)^2} \quad (r \leq D)$$

$$\equiv 1 \quad (r \geq D),$$

where the constants  $A$ ,  $B$ ,  $D$ ,  $a_1$ ,  $a_2$ ,  $C_6$ ,  $C_8$ , and  $C_{10}$  are found in Ref. 13. A more accurate representation of the KW data of Ref. 12 has been devised by Uang and Stwalley<sup>14</sup> who use a cubic spline fit. It has the form [with  $x \equiv r/R$  and  $R$  defined so that  $V(R) \equiv 0$ ]

$$V(r) = A e^{-a_1(x-1)} + B \quad (0 \leq x \leq a)$$

$$= \sum_{\alpha=0}^3 A_{i\alpha} (x - x_i)^\alpha \quad (a \leq x \leq b)$$

$$= - \left[ \frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}} \right] \quad (r \geq b), \quad (9)$$

the values of the dimensionless parameters (rounded off to nine digits) being  $A=76\,384.2397$ ,  $B=43\,130.2264$ ,  $a_1=17.531\,772\,16$ ,  $C_6=18.418\,0095$ ,  $C_8=7.326\,268\,46$ ,  $C_{10}=4.021\,440\,56$ ,  $a=0.144\,156\,961$ ,  $b=1.729\,883\,53$ . We have further refined the spline parameters  $A_i, x_i$  of Ref. 14 so as to yield 16-digit instead of only 10-digit accuracy.

(c) The Aziz *et al.* potential, presently considered the most accurate He-He potential, is of the form, with  $x \equiv r/r_m$  and  $r_m=2.9673 \text{ Å}$ ,

$$V(r) = \epsilon A e^{-ax} - F(x) \left[ \frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}} \right], \quad (10)$$

$$F(x) = \begin{cases} e^{-(D/x-1)^2} & (x \leq D) \\ 1 & (x \geq D) \end{cases},$$

with the unspecified parameters given in Ref. 15.

(d) The two-Gaussian nucleon-nucleon potential, which is of the form

$$V(r) = 2200 e^{-1.5r^2} - 66 e^{-0.1449r^2} \text{ MeV} \quad (11)$$

TABLE II. Interparticle separation  $R$  at which the various pair central potentials change sign, in Å except for the last entry, which is in F (1 F =  $10^{-13}$  cm). For LJ potentials,  $R = \sigma$  by inspection of Eq. (7).

Potential	$R$
KW (Sil)	3.687 4439
KW (Stw)	3.670 8394
Aziz <i>et al.</i>	2.638 5037
Two-Gaussian	1.608 6251

if  $r$  is in Fermi (F) units. It was devised in Ref. 16 as a model nuclear potential for the various reasons given there.

In Table II we list the values of  $R$  at which the above-mentioned potentials change sign, i.e.,  $V(R)=0$ . We note a difference as of the third digit between the two parametrizations of the KW potential, with "Sil" referring to Ref. 13 and "Stw" to Ref. 14.

### III. DIRECT DETERMINATION OF SCATTERING PARAMETERS

The usual way of determining  $a$ ,  $r_0$ , and  $A_1(0)$  for a given potential involves first calculating the phase shift  $\delta_l(k)$  for small wave number  $k$  by solving the Schrödinger equation for small scattering energies. Second, one graphs the left-hand side of Eq. (2) versus  $k^2$  for small  $k$ ; the slope yields  $r_0/2$  while the intercept at  $k^2=0$  gives  $-1/A_1(0)$ . This graphical method<sup>14</sup> is indirect and not very accurate. Far more accurate is the *direct* method which employs for  $a$ ,  $r_0$ , and  $A_1(0)$  integral expressions similar to Eq. (3). This was carried out for the LJ, KW, and Aziz *et al.* potentials in Ref. 9. In Ref. 10 were calculated, in addition, the coefficients up to order 14 of the  $\lambda$  expansion of  $a$ ,  $r_0$ ,  $A_1(0)$ , and  $A_0''(0)$  for the LJ potential for  $^3\text{He}$  and  $^4\text{He}$ . The method used in Ref. 10 for the determination of these expansions depends critically on the special structure of the LJ potential and cannot be used for the other (physically more interesting) interactions which require a straight numerical approach to be discussed in Sec. IV. However, the fact that the LJ potential is asymptotically of the same form as most of the other potentials has made Ref. 10 of great help in ascertaining the goodness of the various numerical approaches. From these comparisons the integral-equation method turned out to be precise and stable, thus ensuring that noise arising from numerical approximations is negligible in all results to be presented below.

### IV. INTEGRAL-EQUATION METHOD

A scheme more powerful and elegant than that used in Ref. 10 for the calculation of the  $\lambda$ -expansion coefficients of  $a$ ,  $r_0$ ,  $A_1(0)$ , and  $A_0''(0)$  will now be presented and applied. The method can be illustrated in some detail for one of the necessary parameters,  $a$ , the  $S$ -wave scattering length. We start with the zero-energy  $S$ -wave radial function, which from Eq. (6) satisfies

$$\begin{aligned} u_0''(r) &= v(r)u_0(r), \\ v(r) &\equiv \frac{m}{\hbar^2} V(r). \end{aligned} \quad (12)$$

The radial function must obey the conditions

$$u_0(0)=0 \quad \text{and} \quad \lim_{r \rightarrow \infty} u_0(r) = r - a, \quad (13)$$

so that the above partial-wave equation may be recast into integral form as

$$\begin{aligned} u_0(r) &= r - \int_0^r dr' r' v(r') u_0(r') \\ &\quad - r \int_r^\infty dr' v(r') u_0(r'). \end{aligned} \quad (14)$$

From the integral equation, as the  $r \rightarrow \infty$  limit is taken, the scattering length  $a$  can clearly be identified as

$$a = \int_0^\infty dr r v(r) u_0(r). \quad (15)$$

This expression for  $a$  suggests that once the expansions of  $v(r)$  and  $u_0(r)$  in powers of  $\lambda$  are known, the expansion of  $a$  will also be known. More explicitly, combining Eq. (4) with the expansion

$$u_0(r) = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} u_{0k}(r), \quad (16)$$

we have

$$v(r)u_0(r) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} [v_{\text{core}}(r)u_{0n}(r) + n v_{\text{att}}(r)u_{0n-1}(r)]. \quad (17)$$

If

$$a = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left[ \frac{d^n a}{d\lambda^n} \right]_{\lambda=0},$$

then Eqs. (15) and (17) give

$$\begin{aligned} \left[ \frac{d^n a}{d\lambda^n} \right]_{\lambda=0} &= \int_0^R dr r v_{\text{core}}(r) u_{0n}(r) \\ &\quad + n \int_R^\infty dr r v_{\text{att}}(r) u_{0n-1}(r). \end{aligned} \quad (18)$$

To complete the scheme  $u_{0n}(r)$  must be found. For the determination of  $u_{0n}(r)$  one may contemplate using either the differential or the integral equation satisfied by  $u_0(r)$ . For all  $u_{0n}(r)$  inside the range of the repulsive core,  $r \leq R$ , the differential-equation approach proves useful. By substituting the expansion for  $u_0(r)$  into the partial-wave equation one obtains

$$u_{0n}''(r) = \begin{cases} v_{\text{core}}(r)u_{0n}(r) & (r \leq R) \\ n v_{\text{att}}(r)u_{0n-1}(r) & (r \geq R). \end{cases} \quad (19)$$

Since  $u_0(r)$  and  $u_0'(r)$  are both continuous in  $r$ , one must insist on continuity for  $u_{0n}(r)$  and  $u_{0n}'(r)$ , even at  $r=R$ . From Eq. (19) it is immediately clear that for  $r \leq R$  the  $u_{0n}(r)$  are proportional to each other for all  $n$  if  $u_{0n}(0)=0$ , which follows from  $u_0(0)=0$ . Numerical integration may be used to obtain  $u_{00}(r)$  which is determined fully if  $u_{00}(0)=0$  and  $[u_{00}'(r)]_{r=R}=1$  are imposed. The latter condition is necessary since  $u_{00}''(r)=0$  and

$u_{00}(r)=r-a_0$  for  $r \geq R$  by convention in normalization. Now from Eq. (15),  $a_0$ , the unperturbed  $S$ -wave scattering length, is given by

$$a_0 = \int_0^R dr r v_{\text{core}}(r) u_{00}(r). \quad (20)$$

But consistency requires that

$$u_{0n}(r) = u_{00}(r) [u'_{0n}(r)]_{r=R}. \quad (21)$$

It is important to note that from the integral equation (14) satisfied by  $u_0(r)$  one has

$$[u'_0(r)]_{r=R} = 1 - \int_R^\infty dr v(r) u_0(r), \quad (22)$$

which upon expansion in powers of  $\lambda$  gives

$$[u'_{0n}(r)]_{r=R} = -n \int_R^\infty dr' v_{\text{att}}(r') u_{0n-1}(r'). \quad (23)$$

With the help of this relation and Eq. (18) an important term in  $(d^n a / d\lambda^n)_{\lambda=0}$  may be rewritten as

$$\int_0^R dr r v_{\text{core}}(r) u_{0n}(r) = -n a_0 \int_R^\infty dr v_{\text{att}}(r) u_{0n-1}(r), \quad (24)$$

so that

$$(d^n a / d\lambda^n)_{\lambda=0} = n \int_R^\infty dr (r - a_0) v_{\text{att}}(r) u_{0n-1}(r). \quad (25)$$

Now it clearly becomes important to find  $u_{0n}(r)$  outside the repulsive core of the two-body interaction  $r \geq R$ . From the integral equation (14) for  $u_0(r)$  with  $r \geq R$ , upon expansion in powers of  $\lambda$  one gets for  $n \geq 1$

$$u_{0n}(r) = -n(r - a_0) \int_r^\infty dr' v_{\text{att}}(r') u_{0n-1}(r') - n \int_R^r dr' (r' - a_0) v_{\text{att}}(r') u_{0n-1}(r') \quad (26)$$

with the help of Eq. (24). Clearly, starting with  $u_{00}(r)=r-a_0$  for  $r \geq R$ , it is possible to generate successively all  $u_{0n}(r)$  and, through Eq. (25), all derivatives of  $a$ .

It is now straightforward to use the  $u_{0n}(r)$  and the various pieces in finding the expansion in powers of  $\lambda$  for the effective range<sup>7</sup>

$$r_0 \equiv \frac{2}{a^2} \int_0^\infty dr [(r - a)^2 - u_0^2(r)] \quad (27)$$

as well as for  $A_0''(0)$  given by Eq. (3). For example,

$$\left[ \frac{d^n A_0''(0)}{d\lambda^n} \right]_{\lambda=0} = -n \int_R^\infty dr \left[ \frac{r^3}{3} + A_0''(0) \right] v_{\text{att}}(r) u_{0n-1}(r), \quad (28)$$

where

$$A_0''(0) \equiv -\frac{1}{3} \int_0^R dr r^3 v_{\text{core}}(r) u_{00}(r). \quad (29)$$

The development for the  $P$ -wave scattering length  $A_1(0)$  is analogous to that of  $a$ . By definition<sup>7</sup>

$$A_1(0) \equiv \frac{1}{3} \int_0^\infty dr r^2 v(r) u_1(r), \quad (30)$$

where  $u_1(r)$  is the zero-energy  $P$ -wave radial function satisfying Eq. (6) with  $E=0$ . The boundary conditions here are  $u_1(0)=0$  and  $u_1(r) \rightarrow r^2/3 - A_1(0)/r$ , as  $r \rightarrow \infty$ . Then

$$\left[ \frac{d^n A_1(0)}{d\lambda^n} \right]_{\lambda=0} = n \int_R^\infty dr \left[ \frac{r^2}{3} - \frac{A_{10}(0)}{r} \right] v_{\text{att}}(r) u_{1n-1}(r), \quad (31)$$

where

$$A_{10}(0) \equiv \frac{1}{3} \int_0^R dr r^2 v_{\text{core}}(r) u_{10}(r), \quad (32)$$

and

$$u_{1n}(r) = -n \left[ \frac{r^2}{3} - \frac{A_{10}(0)}{r} \right] \int_r^\infty \frac{dr'}{r'} v_{\text{att}}(r') u_{1n-1}(r') - n \frac{1}{r} \int_R^r dr' \left[ \frac{(r')^2}{3} - \frac{A_{10}(0)}{r'} \right] v_{\text{att}}(r') u_{1n-1}(r'), \quad (33)$$

provided  $r \geq R$  and

$$u_{10}(r) = \frac{r^2}{3} - \frac{A_{10}(0)}{r} \quad \text{for } r \geq R.$$

On the other hand, for  $r \leq R$  one simply has to solve

$$u_0''(r) - \left[ \frac{2}{r^2} + v_{\text{core}}(r) \right] u_{10}(r) = 0. \quad (34)$$

## V. RESULTS

Using the method just outlined, one can very accurately deduce the coefficients of the  $\lambda$  expansions of  $a$ ,  $r_0$ ,  $A_1(0)$ , and  $A_0''(0)$  for the various potentials listed in Sec. II. Tables III–XI list the results, rounded off to nine significant digits, for up to order 6 in the  $\lambda$  expansions given by

$$a = \sum_{n=0}^{\infty} a_n \lambda^n, \quad r_0 = \sum_{n=0}^{\infty} r_{0n} \lambda^n, \quad (35)$$

$$A_1(0) = \sum_{n=0}^{\infty} A_{1n}(0) \lambda^n, \quad A_0''(0) = \sum_{n=0}^{\infty} A_{0n}''(0) \lambda^n.$$

We have not listed the results for <sup>3</sup>He and <sup>4</sup>He with the LJ potential as these are found in Ref. 10. Note, however, that in this latter reference lengths are in  $\sigma=2.556$ -A units, whereas in the present paper they are in angstrom units.

TABLE III. First seven coefficients of the  $\lambda$  expansions [Eq. (36)] for two spin-polarized hydrogen atoms  $H\downarrow$ , interacting via the LJ potential [Eq. (7)].

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.841 295 47	1.891 451 63	-7.909 573 81	7.665 481 13
1	-1.507 830 58	6.786 841 81	65.767 049 7	-29.937 699 5
2	-0.476 483 64 8	11.043 137 1	12.182 032 4	-2.703 228 33
3	-0.170 703 769	14.126 017 3	4.223 951 29	-0.487 168 762
4	-0.061 960 378 2	16.178 095 50	1.527 012 95	-0.093 252 633 2
5	-0.022 529 621 6	17.410 577 2	0.554 926 659	-0.018 032 626 5
6	-0.008 194 182 1	18.007 293 5	0.201 813 809	-0.003 493 961 88

TABLE IV. Same as Table III but for  $D\downarrow$ .

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.957 065 31	1.969 458 82	-8.854 661 2	8.634 230 00
1	-2.796 731 38	11.985 066 2	128.124 374	-58.734 458 6
2	-1.640 771 78	35.031 120 5	43.726 110 8	-10.016 120 1
3	-1.097 728 28	81.039 343 8	28.264 084 7	-3.442 052 52
4	-0.744 955 410	168.116 389	19.096 541 3	-1.259 401 45
5	-0.506 570 565	327.907 944	12.977 227 5	-0.465 817 639
6	-0.344 573 948	614.842 214	8.826 344 84	-0.172 666 736

TABLE V. Same as Table III but for  $T\downarrow$ .

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	3.020 356 09	2.012 042 87	-9.401 217 45	9.197 170 70
1	-4.014 670 86	16.793 787 3	189.018 731	-86.952 912 5
2	-3.379 372 89	69.254 424 0	92.187 366 0	-21.462 020 6
3	-3.254 343 09	226.859 185	85.689 722 2	-10.731 901 2
4	-3.181 058 90	666.996 981	83.372 860 0	-5.721 482 71
5	-3.116 138 45	1844.418 98	81.614 267 1	-3.084 716 75
6	-3.053 567 09	4903.801 26	79.966 650 1	-1.666 905 58

TABLE VI. Same as Table III but for the KW (Stw) potential of Eq. (9).

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.728 958 57	1.814 327 01	-7.154 182 43	6.806 801 32
1	-1.359 259 15	5.392 474 21	51.238 712 9	-23.709 769 9
2	-0.427 170 825	8.490 991 55	9.569 206 27	-2.220 311 48
3	-0.149 354 116	10.472 737 1	3.269 309 43	-0.394 442 635
4	-5.273 748 15	11.524 831 1	1.151 581 84	-7.370 872 89
5	-1.864 432 33	11.900 523 1	0.407 129 911	-1.388 224 59
6	-6.592 298 87	11.801 549 0	0.144 000 064	-2.618 252 86

TABLE VII. Same as Table VI but for two  $D\downarrow$  atoms.

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.868 862 48	1.505 163 56	-8.191 539 21	7.893 752 57
1	-2.471 570 00	7.805 089 49	98.957 446 5	-46.221 997 1
2	-1.422 846 91	22.044 947 9	33.412 878 1	-8.083 123 67
3	-0.917 776 498	48.564 240 9	21.011 487 4	-2.718 703 32
4	-0.598 624 571	95.164 143 5	13.657 601 9	-0.964 591 364
5	-0.391 039 424	174.727 259	8.915 788 90	-0.345 170 415
6	-0.255 500 703	307.867 667	5.823 890 46	-0.123 711 582

TABLE VIII. Same as Table VI but for two  $T_{\downarrow}$  atoms.

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.943 335 29	1.959 846 28	-8.786 561 57	8.518 281 03
1	-3.512 685 50	12.679 333 1	145.342 748	-68.190 456 8
2	-2.882 082 11	48.584 533 3	69.444 633 6	-17.148 712 3
3	-2.660 088 76	148.290 369	62.395 862 0	-8.358 129 42
4	-2.484 843 09	405.190 903	58.036 015 7	-4.304 284 31
5	-2.325 347 58	1040.081 13	54.237 756 9	-2.236 570 50
6	-2.177 098 85	2565.407 50	50.729 731 6	-1.164 118 87

TABLE IX. Same as Table III but for two  ${}^3\text{He}$  atoms interacting via the Aziz *et al.* potential of Eq. (10).

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.111 661 65	1.406 130 41	-3.240 267 54	3.145 351 34
1	-2.144 038 78	7.714 196 76	45.461 968 4	-21.332 165 6
2	-1.468 454 51	25.126 056 4	18.487 059 2	-4.545 390 79
3	-1.144 238 45	64.800 491 3	13.960 067 7	-1.880 348 72
4	-0.903 612 578	149.681 756	10.981 792 5	-0.822 171 617
5	-0.714 883 057	324.867 555	8.683 100 53	-0.362 747 291
6	-0.565 725 722	677.586 700	6.870 535 82	-0.160 318 810

TABLE X. Same as Table IX but for two  ${}^4\text{He}$  atoms.

$n$	$a_n$ (Å)	$r_{0n}$ (Å)	$A''_{0n}(0)$ (Å <sup>3</sup> )	$A_{1n}(0)$ (Å <sup>3</sup> )
0	2.146 317 58	1.429 516 16	-3.389 850 06	3.301 526 88
1	-2.749 828 42	9.720 278 48	59.595 586 9	-28.039 097 5
2	-2.416 360 79	40.058 670 1	30.976 478 6	-7.714 739 53
3	-2.422 435 75	131.178 615	30.071 334 9	-4.142 017 59
4	-2.462 570 34	385.064 680	30.447 280 8	-2.353 158 64
5	-2.508 167 99	1062.389 34	30.993 239 1	-1.349 383 63
6	-2.555 334 03	2817.206 31	31.573 376 4	-0.775 160 422

TABLE XI. Same as Table III but for two nucleons interacting via the two-Gaussian potential defined in Eq. (11).

$n$	$a_n$ (F)	$r_{0n}$ (F)	$A''_{0n}(0)$ (F <sup>3</sup> )	$A_{1n}(0)$ (F <sup>3</sup> )
0	0.988 877 189	0.643 620 820	-0.404 350 425	0.334 752 409
1	-4.810 029 16	23.360 193 2	30.183 046 8	-13.419 901 8
2	-7.922 969 33	377.914 898	44.281 274 3	-7.114 278 30
3	-13.645 341 3	3931.851 37	75.362 673 7	-4.626 582 56
4	-23.610 663 8	35 236.824 8	130.213 444	-3.121 940 15
5	-40.877 131 2	292 554.639	225.397 213	-2.123 868 07
6	-70.775 738 3	2318 362.37	390.249 402	-1.447 660 19

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