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Exact scattering length for a potential of Lennard-Jones type

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Abstract. For a modified Lennard-Jones interaction potential of the form $\sim[(r_0/r)^{2n-2} - (r_0/r)^n]$, an exact and simple expression for the s-wave scattering length is presented, and discussed in some detail. For heavy alkali atoms, which nowadays are routinely being employed to produce Bose-Einstein condensates, this potential is well compatible with known experimental data when $n = 6$.

PACS. 03.65.Nk Scattering theory – 34.20.Cf Interatomic potentials and forces

1 Introduction

When ultracold atoms scatter from each other, with de Broglie waves much longer than the extension of their interaction potential, knowledge of the full differential cross section is not required for a description of the scattering dynamics; it rather suffices to consider the s-wave scattering length a_{scatt}. This is reflected, for instance, by the fact that the leading terms of a density expansion of the ground-state energy of a Bose-Einstein condensate depend on the scattering length only [1–3]; non-universal contributions which do depend on the actual shape of the interaction potential emerge only in higher orders [4,5].

The relative motion of two particles is as usually described by the equivalent Schrödinger equation

$$E\varphi = -\frac{\hbar^2}{2m}\Delta\varphi + V\varphi \tag{1}$$

where m is the reduced mass and V the interatomic potential. In the case of low-energy collisions, as governing the interparticle interactions in ultracold atomic gases, the equation may be simplified, since contributions to the scattering amplitude for angular momenta $l > 0$ are normally negligible [2] and one can restrict oneself to the case $l = 0$. In addition, we can put $E = 0$, being interested in the scattering length a_{scatt} only and not in quantities like e.g. the effective range. These considerations lead together with the substitution $\varphi := rf\,(r)$ for the radial function to

$$\frac{d^2}{dr^2}f = \frac{2m}{\hbar^2}Vf := vf \tag{2}$$

where f has to satisfy the boundary condition $f(0) = 0$. Taking into account the asymptotic behaviour

$$f(r) \underset{r\to\infty}{\to} Ar + B \tag{3}$$

the (zero-energy s-wave) scattering length a_{scatt} follows as

$$a_{scatt} = -\frac{B}{A}. \tag{4}$$

The sign of a_{scatt} as the central quantity in low-energy scattering determines whether the interaction may be modelled by a repulsive ($a_{scatt} > 0$) or an attracting ($a_{scatt} < 0$) pseudopotential $V_{pseudo} = a_{scatt}\frac{2\pi\hbar^2}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}r$ [6,7]. The scattering cross section σ is given in this approximation as $\sigma = 4\pi a_{scatt}^2$.

The interatomic potential V is a function of the separation r of the two centers of mass. At short distances, this potential may not even be definable [2], but in the limit $r \to \infty$ it should be well approximated by the lowest-order van der Waals interaction $-C_6/r^6$ as the leading term of an expansion of the long-range part of V in inverse powers of r [8]. At smaller distances there is a repulsive core which, in the familiar Lennard-Jones potential described by a term $\sim r^{-12}$, usually is modelled by forms $\sim r^\alpha e^{-\beta r}$, cf. [9–11].

As far as analytical solutions of the zero-energy Schrödinger equation are concerned, only one van der Waals-like potential seems to have been considered so far; it is of the form $-C_n/r^n$ (in particular for the van der Waals potential, $n = 6$) for $r > r_{cut}$ and $V(r) = \infty$ for $r < r_{cut}$; for details see [9]. The main drawback of this model is the fact that there are no straight physical arguments where to place the cutoff radius r_{cut}. On the other hand, for more realistic potentials the wave function has to be calculated numerically and it is not easy to see how the scattering length depends on relevant potential parameters, e.g. the depth of the potential or the position of its minimum.

We present here a simple but nontrivial and realistic potential with two parameters. It not only allows for exact

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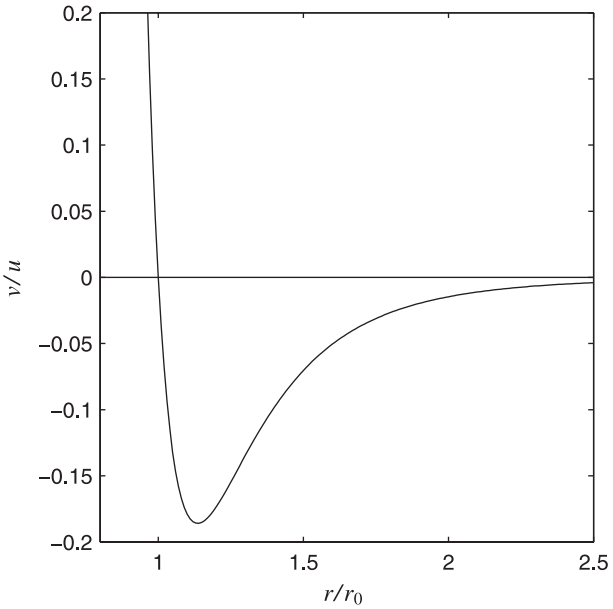

Fig. 1. Potential v/u for $n = 6$.

solutions for the scattering length but also, in addition, leads to very simple expressions for the scattering length by which analytical conclusions are possible. In spite of its simplicity, the results for this model agree well with experimental data as shown for the case of Rb^{85} and Rb^{87}.

All values are given in atomic units (a.u.), if not stated otherwise.

2 The potential and the scattering length

We consider here the potential of the Lennard-Jones type

$$v(r) = u\left[\left(\frac{r_0}{r}\right)^{2n-2} - \left(\frac{r_0}{r}\right)^{n}\right] \tag{5}$$

where n is not restricted to natural numbers. An example ($n = 6$) is shown in Figure 1. Note that the usual Lennard-Jones potential exhibits the exponents 12 and 6, or more generally $2n$ and n. At large distances v falls off $\simeq -r^{-n}$ with $n = 4$ for the interaction between an atom and an ion, $n = 6$ for neutral atoms and $n = 7$ for the Casimir-Polder potential between two neutral polarizable atoms.

The potential is zero for $r = r_0$ and achieves its minimum $v_{\min} = -u\frac{n-2}{2n-2}(\frac{n}{2n-2})^{\frac{n}{n-2}}$ at $r_{\min} = (\frac{2n-2}{n})^{\frac{1}{n-2}} r_0$.

The general solution of the radial equation (2) is given by

$$f(r) = Ce^{-\frac{1}{2}z}U(\alpha,\beta,z) + De^{-\frac{1}{2}z}M(\alpha,\beta,z) \tag{6}$$

with

$$\alpha = \frac{-r_0\sqrt{u}+n-1}{2n-4},\ \beta = \frac{n-1}{n-2},\ z = \frac{2r_0\sqrt{u}}{n-2}\left(\frac{r_0}{r}\right)^{n-2} \tag{7}$$

C and D are integration constants, and the Kummer functions $U(\alpha,\beta,z)$ and $M(\alpha,\beta,z)$ are defined as in [12]. In order to derive the scattering length we take into account the condition $f(0) = 0$ and the asymptotic behaviour of the Kummer functions. The condition $f(0) = 0$ requires $D = 0$ since for $z \to \infty$ ($r \to 0$) we have $M(\alpha,\beta,z) \sim z^{\alpha-\beta}e^z$. The remaining Kummer function $U(\alpha,\beta,z)$ may be expressed as

$$U(\alpha,\beta,z) = \frac{\pi}{\sin\pi\beta}\left[\frac{M(\alpha,\beta,z)}{\Gamma(1+\alpha-\beta)\,\Gamma(\beta)} - z^{1-\beta}\frac{M(1+\alpha-\beta,2-\beta,z)}{\Gamma(\alpha)\,\Gamma(2-\beta)}\right]. \tag{8}$$

For $r \to \infty$ ($z \to 0$) we use the series expansion

$$M(\alpha,\beta,z) = 1 + \frac{\alpha}{\beta}z + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}z^2 + \ldots \tag{9}$$

In this way, we arrive for $U(\alpha,\beta,z)$ at the expression

$$U(\alpha,\beta,z) \underset{r\to\infty}{=} \frac{\pi}{\sin\pi\beta}\left[-\frac{r_0}{\Gamma(\alpha)\,\Gamma(2-\beta)}\left(\frac{2x}{n-2}\right)^{\frac{1}{n-2}} r + \frac{1}{\Gamma(1+\alpha-\beta)\,\Gamma(\beta)} + O\left(\frac{1}{r^{n-1}}\right)\right] \tag{10}$$

where we have introduced the short-hand notation $x := r_0\sqrt{u}$. The final result reads

$$a_{scatt} = r_0\left(\frac{2x}{n-2}\right)^{\frac{1}{n-2}} \frac{\Gamma\left(\frac{-x+n-1}{2n-4}\right)}{\Gamma\left(\frac{-x+n-3}{2n-4}\right)} \frac{\Gamma\left(\frac{n-3}{n-2}\right)}{\Gamma\left(\frac{n-1}{n-2}\right)}. \tag{11}$$

For the cases $n = 4$ and $n = 6$, the scattering length is shown in Figures 2 and 3. Note the different scales.

With (11), we have at our disposal a very simple and compact expression for the scattering length. We point out some of its properties.

(1) It is well-known that the constant cross section limit at zero energy is valid only for the potentials falling off faster than r^{-3} [13]. This is reflected by the fact that the scattering length goes to infinity when $n \to 3+$.

(2) Apart from the multiplicative factor r_0, the scattering length depends on two parameters only, namely n and x. In particular, this holds for the position of the poles and zeros. This fact allows for quite precise statements about the potential parameters especially in the case if scattering lengths are available for different isotopes, as shown below for ^{85}Rb and ^{87}Rb.

(3) Poles and zeros of the scattering length are given by the poles of $\Gamma(\frac{-x+n-1}{2n-4})$ and of $\Gamma(\frac{-x+n-3}{2n-4})$, respectively. Poles of a_{scatt} occur at

$$x_{pole} = (2n-4)N_b + n - 1; \quad N_b = 0,1,2,\ldots \tag{12}$$

where N_b denotes the number of bound states; there are N_b bound states for $(2n-4)(N_b-1)+n-1 < x < (2n-4)N_b + n - 1$. Zeros of a_{scatt} occur at

$$x_{zero} = (2n-4)M + n - 3; \quad M = 0,1,2,\ldots \tag{13}$$

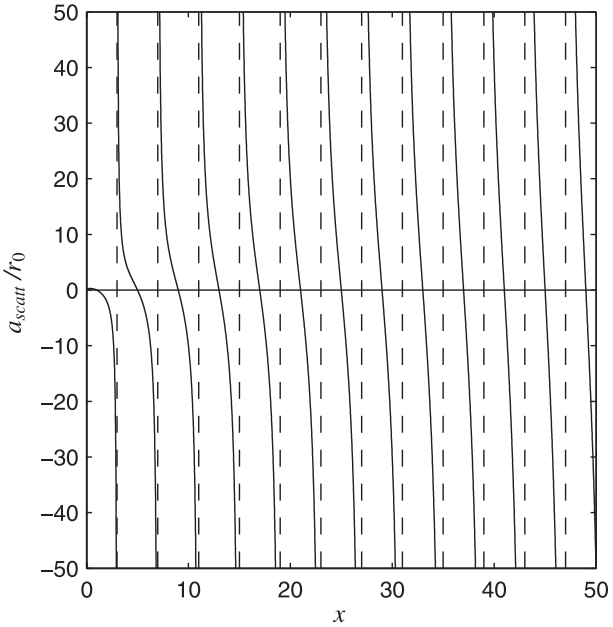

Fig. 2. Scattering length a_{scatt}/r_0 in dependence of the variable $x = r_0\sqrt{u}$ for the case $n = 6$. The dashed lines mark the positions of the poles.

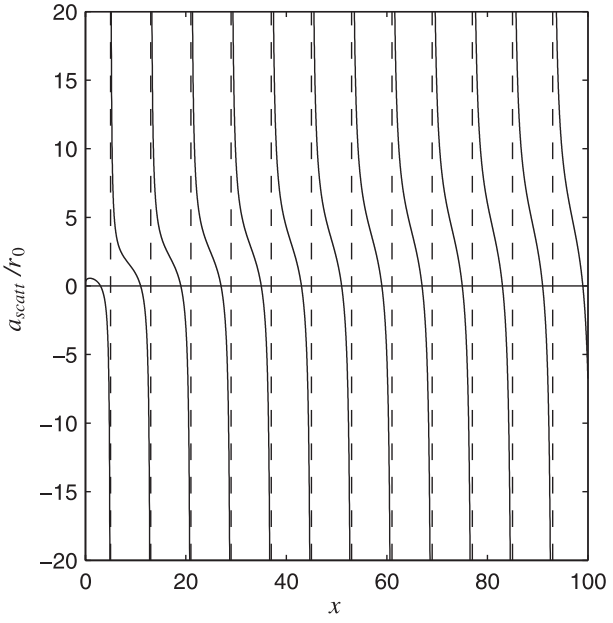

Fig. 3. Scattering length a_{scatt}/r_0 in dependence of the variable $x = r_0\sqrt{u}$ for the case $n = 6$. The dashed lines mark the positions of the poles.

(4) The relative proportion of positive and negative values of a_{scatt} is given by $\frac{n-3}{n-2}$ and $\frac{1}{n-2}$. For $n = 4$, we have an equipartition of positive and negative values of a_{scatt}, whereas for $n = 6$, positive values occur three times more often than negative ones. Similar conclusions hold for a potential described by an infinitely high hard-core plus long range r^{-6} [8] and for the semiclassical approximation of a general potential with long range r^{-6} [9]. See also Figures 2 and 3.

(5) If x happens to lie in the neighbourhood of a pole, any minor uncertainty in the shape of the potential can easily provoke big changes in the scattering length. On the other hand, this means that in this situation the potential parameters may be fixed very precisely even if the scattering length is known with a modest degree of accuracy.

3 Exact solution and semiclassical approximation

For potentials which fall off $\sim -C_n/r^n$, a semiclassical approximation for the scattering length was presented by [9]. It reads

$$a_{scatt}^{WKB} = r_0 \cos\left(\frac{\pi}{n-2}\right)\left(\frac{r_0\sqrt{u}}{n-2}\right)^{\frac{2}{n-2}} \frac{\Gamma\left(\frac{n-3}{n-2}\right)}{\Gamma\left(\frac{n-1}{n-2}\right)} \times \left[1 - \tan\frac{\pi}{n-2}\tan\left(\Phi - \frac{\pi}{2n-4}\right)\right] \quad (14)$$

with the phase $\Phi = \int_{r_0}^{\infty} \sqrt{|v(r)|}dr$. For the potential (5) it is given by

$$\Phi = \frac{\pi}{2n-4} r_0\sqrt{u}. \quad (15)$$

Because of $E = 0$ the classical turning point r_0 coincides with the zero of the potential (5). Note that with (15) the poles and zeros of a_{scatt}^{WKB} are exactly the same as for a_{scatt} as given in equations (12, 13).

Let us compare the two scattering lengths a_{scatt}^{WKB} and a_{scatt}. With equation (11) it follows with $x = r_0\sqrt{u}$:

$$\xi := \frac{a_{scatt}^{WKB}}{a_{scatt}} = \left(\frac{x}{2n-4}\right)^{\frac{1}{n-2}} \frac{x-n+1}{x-n+3} \frac{\Gamma\left(\frac{x-n+1}{2n-4}\right)}{\Gamma\left(\frac{x-n+3}{2n-4}\right)}. \quad (16)$$

Obviously, $\xi \to 0$ for $x \to 0$ whereas for $x \to \infty$ we have

$$\xi \underset{x\to\infty}{=} 1 - \frac{(n-1)(n-3)}{6(n-2)}\frac{1}{x^2} + O\left(\frac{1}{x^3}\right). \quad (17)$$

According to the last equation, the ratio ξ differs from 1 more than 1% if $x \lesssim 10\sqrt{\frac{(n-1)(n-3)}{6(n-2)}}$. On the other hand, the first singularity in a_{scatt} occurs at $x = 3n-5$, see equation (12). Since $10\sqrt{\frac{(n-1)(n-3)}{6(n-2)}} < 3n-5$ for $n > 3$, one can conclude that a_{scatt} and a_{scatt}^{WKB} are practically identical if one or more bound states exist.

4 Comparing the potential with existing data

In this section, we check to which extent the assumed parametrization (5) of the interaction potential is compatible with known experimental data for heavy alkalis,

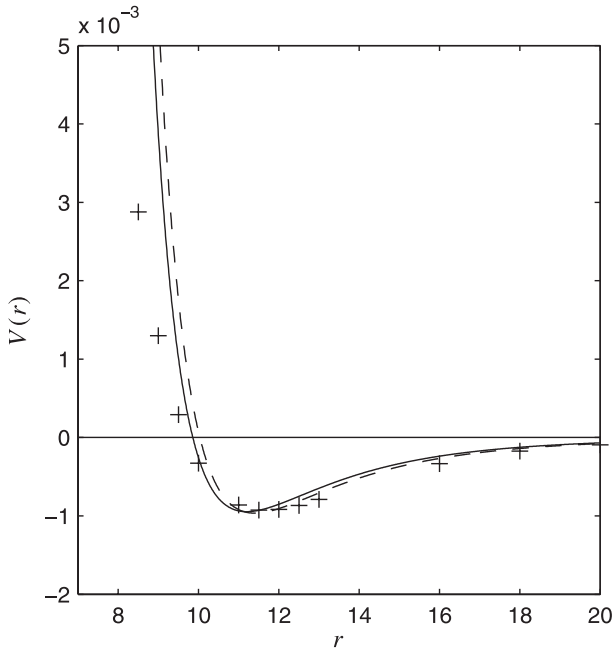

Fig. 4. Comparison of data points from [14] with the potential $V(r)$ for Rb_2 $\left({}^3\Sigma_u^+\right)$ for $n = 6$ and the parameters $S_1 = \left(11.2, 9.46 \times 10^{-4}\right)$ and $S_2 = \left(11.4, 9.65 \times 10^{-4}\right)$ (dashed).

which are favourite atomic species for the production of Bose-Einstein condensates [8].

Numerically computed values for the interatomic potential are found e.g. in [14] where tables for the energy curves of some alkali diatomics are given. We choose Rb_2 $\left({}^3\Sigma_u^+\right)$ as an illustrative example. Interpolating the lowest four data points of [14] leads to $r_{\min} \approx 11.67$ and $|V_{\min}| \approx 9.3 \times 10^{-4}$. However, the potential (5) fits better for slightly different values. Since there is no unique prescription how to fit these data in an optimal manner, we use in the following two exemplary sets of parameters $(r_{\min}, |V_{\min}|)$, namely $S_1 = \left(11.2, 9.46 \times 10^{-4}\right)$ and $S_2 = \left(11.4, 9.65 \times 10^{-4}\right)$, as shown in Figure 4. With the first set the potential (5) fits somewhat better for smaller, with the second for medium values of r.

Whereas the correspondence is quite satisfying for $r \gtrsim 10$, it is seen that the potential is too steep for smaller r. However, one may expect that the details of the potential in this region will not play a crucial role, since the wave function is damped out in the region with positive potential.

Another possibility to fix parameters of the potential (5) is furnished by the experimentally determined values of the dispersion coefficient C_6, as given e.g. in [10] and [11] by $4619 \lesssim C_6 \lesssim 4635$ and $4698 \lesssim C_6 \lesssim 4703$. Taking into account the equation $C_6 = 2.5\,|V_{\min}|\, r_{\min}^6$, we get for S_1 and S_2 the dispersion coefficients $C_6 = 4668$ and 5295. The last value is somewhat too large, but this should not be overinterpreted since due to the high exponent in $r_{\min}^6$ the coefficient C_6 depends very sensitively on the precise value of $r_{\min}$.

Finally, for given $(r_{\min}, V_{\min})$ the number of bound states N_b may be calculated by means of equation (12). For S_1 one arrives at 34/35 bound states for $^{85}Rb/^{87}Rb$. For S_2 we have with 35/36 the same result as given in [10]. In [11] one finds 40/41; however, these high values are out of reach for the potential (5) since the number of bound states is restricted to $33 \leq N_b \leq 37$ for ^{85}Rb on condition that the quite reasonable inequalities $11 < r_{\min} < 12$ and $9 \times 10^{-4} < |V_{\min}| < 10^{-3}$ hold; cf. Figure 4.

5 Comparing the scattering length with existing data

We now check if the scattering length (11) is compatible with existing data, confining ourselves to the discussion of the triplet scattering length of ^{85}Rb and ^{87}Rb. The masses are $m^{85} = 84.912$ amu and $m^{87} = 86.909$ amu as given by [15]. For $n = 6$, the mass-dependent variable $x = r_0\sqrt{u}$ in (11) reads $x = 5/\sqrt{6} r_{\min}\sqrt{2m\,|V_{\min}|}$ where m is the reduced mass. Introducing the notations x^{85} and x^{87}, we have $x^{85} = 803.08 r_{\min}\sqrt{|V_{\min}|}$ and $x^{87} = 812.47 r_{\min}\sqrt{|V_{\min}|}$.

In the literature, there exist different values for the scattering lengths. In e.g. [16] one finds $-520 < a_{scatt}^{85} < -315$ and $101 < a_{scatt}^{87} < 108$, in [10] $-1200 < a_{scatt}^{85} < -324$ and $107 < a_{scatt}^{87} < 119$ and in [11] $-388 < a_{scatt}^{85} < -387$ and $98.98 < a_{scatt}^{87} < 98.99$. For our model, the data set S_1 leads to $a_{scatt}^{85} = -480$ and $a_{scatt}^{87} = 116$, and the data set S_2 to $a_{scatt}^{85} = -255$ and $a_{scatt}^{87} = 126$. The agreement of these results with the experimental data is satisfying, all the more since, due to the neighbouring singularity, the gradients of the scattering amplitude are very large which results in a numerically quite delicate situation.

To get more information, we take into account in a first step just the structure of the given data and, in a second step, the actual numerical values.

In the first step we argue as follows: since the experimentally given values of the scattering length for ^{85}Rb are large negative and for ^{87}Rb large positive numbers and in view of the small mass difference between the two isotopes, it is reasonable to assume that x^{85} has to lie between a zero and the following pole, and $x^{87} = 1.0117 x^{85}$ between this pole and the next zero of the scattering length; cf. Figure 3. This leads to the two inequalities [I1] $8N_b + 3 < x^{85} < 8N_b + 5$ and [I2] $8N_b + 5 < x^{87} < 8\,(N_b + 1) + 3$ with N_b and $N_b + 1$ bound states for ^{85}Rb and ^{87}Rb. Since for $21 \leq N_b \leq 63$ [I1] is stronger than [I2] we arrive at

$$\frac{8N_b + 3}{803.08} < r_{\min}\sqrt{|V_{\min}|} < \frac{8N_b + 5}{803.08} \tag{18}$$

which leads for instance to the conditions

$$N_b = 34 \Rightarrow 0.3424 < r_{\min}\sqrt{|V_{\min}|} < 0.3449 \tag{19}$$

$$N_b = 35 \Rightarrow 0.3524 < r_{\min}\sqrt{|V_{\min}|} < 0.3549. \tag{20}$$

Note that inequality (18), which confines the allowed range of the potential parameters, holds irrespectively of

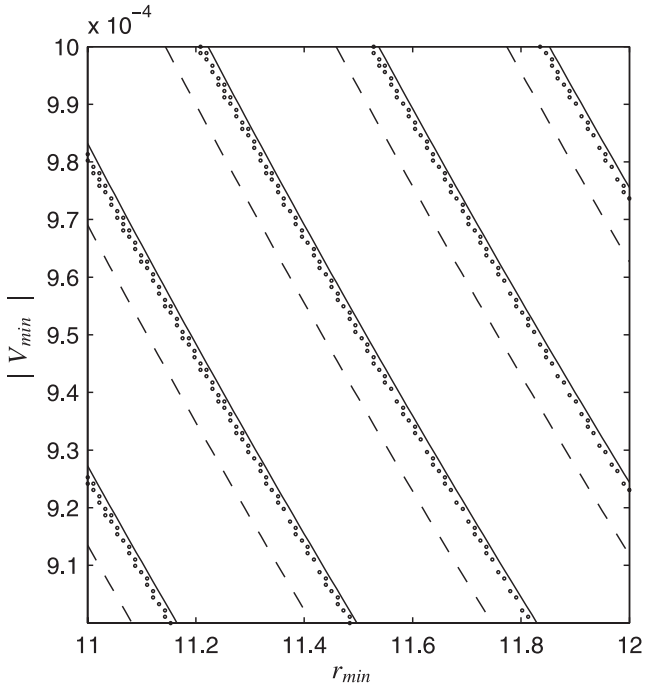

Fig. 5. Points in the $(r_{\min}, |V_{\min}|)$-plane for which the scattering lengths fulfill inequalities 21). The lines are the bounds given in (18) for $N_b = 33 \ldots 37$ (from left to right) where the dashed lines mark the lower bounds.

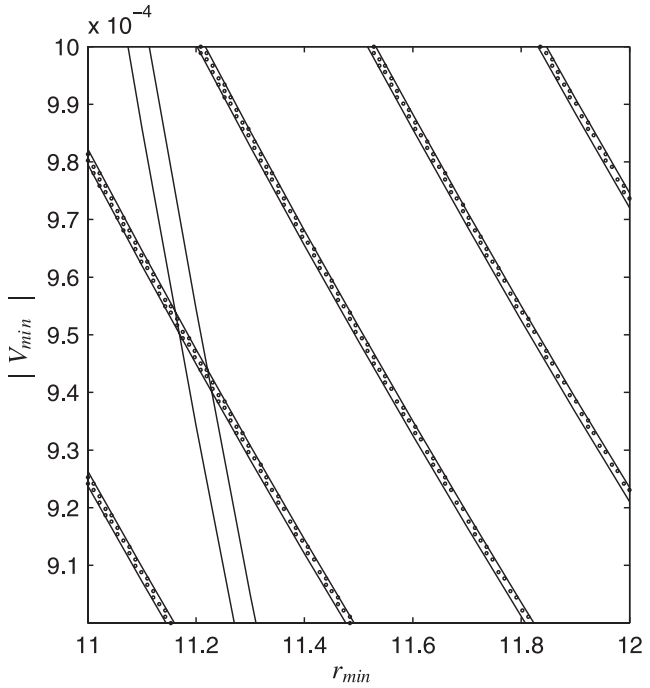

Fig. 6. Points in the $(r_{\min}, |V_{\min}|)$-plane for which the scattering lengths fulfill inequalities (21). The lines are the bounds given as in (18) for $N_b = 33 \ldots 37$ (from left to right). The steeper lines stem from the inequality (24) for the dispersion coefficient.

the actual experimental values, provided that the interaction may described by the potential (5). For our parameter set S_1 with $N_b = 34$ we have $r_{\min}\sqrt{|V_{\min}|} = 0.3445$ and for S_2 with $N_b = 35$ we have $r_{\min}\sqrt{|V_{\min}|} = 0.3541$.

In the second step we take into account the actual numerical ranges for a_{scatt} as given above. Again, we confine the considerations to the ranges $11 < r_{\min} < 12$ and $9 \times 10^{-4} < |V_{\min}| < 10^{-3}$. For these ranges the scattering lengths of the potential (5) cannot lie strictly in the intervals given by [11,16], whereas the interval given by [10] is accessible. In view of the simplicity of our potential (5) we permit somewhat more generous limits, namely

$$-1200 \leq a_{scatt}^{85} \leq -300; \quad 96 \leq a_{scatt}^{87} \leq 120. \tag{21}$$

Together with the lines defined by (18), Figure 5 shows some points in the $(r_{\min}, |V_{\min}|)$-plane for which the scattering lengths fulfill the inequalities (21).

In order to describe this behaviour more closely we note that the ratio $a_{scatt}^{85}/a_{scatt}^{87}$ depends only on $r_{\min}\sqrt{|V_{\min}|}$ and not on the single parameters. With the inequalities (21) we have $-12.5 \leq a_{scatt}^{85}/a_{scatt}^{87} \leq -2.5$. These last inequalities may be numerically solved for $r_{\min}\sqrt{|V_{\min}|}$ in the range $33 \leq N_b \leq 38$. We note here just the result for the two cases $N_b = 34$ and $N_b = 35$:

$$N_b = 34 \Rightarrow 0.3443 < r_{\min}\sqrt{|V_{\min}|} < 0.3447 \tag{22}$$

$$N_b = 35 \Rightarrow 0.3542 < r_{\min}\sqrt{|V_{\min}|} < 0.3549. \tag{23}$$

These inequalities are substantially sharper than (19), (20). They form, as may be seen in Figure 6, the limiting lines of the hits. In addition, Figure 6 shows the bounds induced by the inequalities for the dispersion coefficient

$$4610 \leq C_6 \leq 4710. \tag{24}$$

In the case $N_b = 34$ (i.e. for S_1) there exists a region where the potential parameters satisfy both inequalities (21) *and* (24). The four corner points of this trapezoid have the coordinates $(r_{\min}, |V_{\min}|) = (11.161, 9.54 \times 10^{-4})$, $(11.168, 9.50 \times 10^{-4})$, $(11.221, 9.44 \times 10^{-4})$ and $(11.228, 9.40 \times 10^{-4})$.

Of course, we do not claim that we can fix the parameters of the potential (5) (let alone the real interaction) which such an accuracy. The point is rather that with the potential (5) we have a plain and simple model which, for a natural choice of the parameter values, is able to fulfill (at least approximately) all conditions imposed, though the numerical conditions are quite delicate. This means that our simple potential mirrors the essential features of the real interaction at least for low energy scattering, i.e. $E = 0$.

6 Conclusion

The parametrization (5) for an interatomic interaction potential, which for $n = 6$ leads to a 6-10-potential and thus differs from the usual 6-12-Lennard-Jones form by a somewhat softer core, allows for an exact analytical determination of the s-wave scattering length, as given by

equation (11). For the strongly polarizable heavy alkali atoms, which are characterized by a large van der Waals coefficient C_6 and, correspondingly, give rise to interaction potentials with a substantial number of bound states, the assumed form (5) is well compatible with experimental data. It is hoped that the availability of an exact expression for a realistic, nontrivial interaction potential will be found useful in other cases as well.

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