Scattering length and effective range in two dimensions; application to adsorbed hydrogen atoms

B J Verhaar, J P H W van den Eijnde, M A J Voermans and M M J Schaffrath

Department of Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Abstract. The concepts of scattering length (a) and effective range (r_e) are introduced in two dimensions for an isotropic finite-range potential. Application to mutual scattering of pairs of hydrogen atoms in the triplet state adsorbed at a liquid helium surface shows the usefulness of a description in terms of two parameters. The values derived for this case are $a = 2.468a_0$ and $r_e = 11.62a_0$.

It is generally believed that the introduction of the concepts of scattering length and effective range meets with grave difficulties in two dimensions. Certain logarithmic effects in the numerically calculated elastic and inelastic scattering of pairs of slowly moving H atoms adsorbed at a liquid helium film (Ahn *et al* 1982, 1983, van den Eijnde *et al* 1983) prompted us to start a study in this direction with the ultimate aim of describing the two-dimensional low-energy scattering with simple expressions, as is possible in three dimensions.

We restrict ourselves to the simple case of scattering of a particle with mass μ from a circularly symmetric potential $V(r)$ of finite range r_0. Writing a partial wave solution in the usual way as $(u(r)/\sqrt{r}) \exp im\phi$, the radial wave equation for $m = 0$ reads in customary notation

$$\mathrm{d}^2 u/\mathrm{d}r^2 + [k^2 - (2\mu/\hbar^2) V(r) + \tfrac{1}{4}/r^2] u = 0. \tag{1}$$

A preliminary study (Shaffrath *et al* 1982) led us to the following results for the phase shift $\delta(k) \equiv \delta_{m=0}(k)$ and the radial function $u(r; k)$ beyond $r = r_0$:

$$\delta(k) = (\tfrac{1}{2}\pi/\log ka)[1 + \mathrm{O}(1/\log ka)], \tag{2}$$

$$u(r; k) = -(\sqrt{k}/\log ka)[(\pi r/2)^{1/2} \log r/a + \mathrm{O}(1/\log ka)], \tag{3}$$

for $k \to 0$, where a is the scattering length. The approximation corresponding to (2) has been mentioned previously by Kagan *et al* (1982). A numerical application to the case of two-dimensional H–H scattering, where for all practical purposes the potential may be neglected beyond $r_0 \simeq 15a_0$, confirmed (2), but also showed that the convergence to the first term for $k \to 0$ is so slow that the practical usefulness is strongly reduced. This is illustrated in figure 1 (dotted and full curves). At energies corresponding to temperatures of 0.01 to 0.1 K the deviations are of the order of 10%. In the case of the radial wavefunction the convergence to the behaviour described by the first term of (3) turned out to be even worse. This slow convergence only enabled us to derive a rough estimate for the scattering length. We therefore used the more accurate value
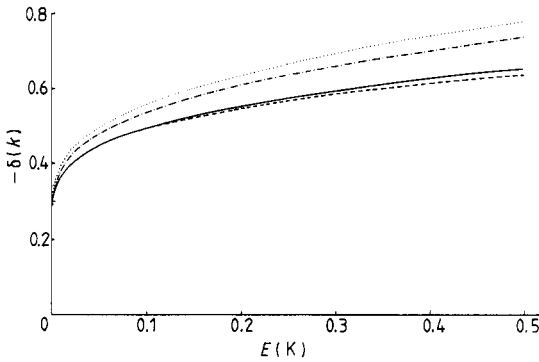
Figure 1. Two-dimensional triplet H–H scattering phase-shift (full curve), compared with various low-energy approximations; $-\frac{1}{2}\pi/\log ka$: dotted curve; $-\frac{1}{2}\pi/(\gamma + \log \frac{1}{2}ka)$: chain curve; $\tan^{-1}[-\frac{1}{2}\pi/(\gamma + \log \frac{1}{2}ka)]$: broken curve. The latter approximation including the effective-range term is indistinguishable from the full curve on this scale.

$a = 2.468a_0$, to be derived in the following more satisfactory analysis, to calculate the dotted curve in figure 1.

This slow convergence being related to the slow decrease of $1/\log ka$ for decreasing k, in a further study (Voermans *et al* 1982) we tried to collect all logarithmic effects in the zero-order term. This attempt turned out to be successful. The idea is simply to replace (2) and (3) by expressions in which the log ka contributions are the same as for scattering from a hard (two-)sphere (HS) of radius a. For that case it is easily shown that (Morse and Feshbach 1953)

$$\cot \delta_{HS}(k) = (N_0(ka)/J_0(ka)) = (2/\pi)(\gamma + \log \tfrac{1}{2}ka) + O(k^2), \tag{4}$$

$$u_{HS}(r; k) = -(\gamma + \log \tfrac{1}{2}ka)\left(1 + \frac{\pi^2/4}{(\gamma + \log \tfrac{1}{2}ka)^2}\right)^{1/2}$$

$$\times (\pi r/2)^{1/2}(\log r/a)[1 + O(k^2 r^2)], \tag{5}$$

where γ is Euler's constant: $\gamma = 0.577\ 215\ 665\dots$.

It can be shown that for the more general potential $V(r)$ similar expressions can be derived. The argument goes as follows. We compare two solutions of (1), both of which satisfy the regularity condition at the origin but which differ in normalisation. The first one, $u(r; k)$, is normalised to amplitude 1 at infinity:

$$u(r; k) = (\pi kr/2)^{1/2}(J_0(kr)\cos \delta(k) - N_0(kr)\sin \delta(k)), \qquad r > r_0. \tag{6}$$

The normalisation of the second one, $u_1(r; k)$, is prescribed by a normalisation condition at the origin:

$$u_1(r; k)/\sqrt{r} = 1 + o(1), \qquad r \to 0. \tag{7}$$

In imposing this boundary condition we assume the potential to be well behaved up to the origin. If we assume the potential to have a hard core within some radius R_0, such as is possible in practice for low-energy H–H scattering, we can replace (7) by the conditions

$$u_1(R_0; k) = 0, \qquad u_1'(R_0; k) = 1, \tag{8}$$

which are also energy independent. Here and in the following the prime denotes radial

differentiation. As in the three-dimensional case (Newton 1982) it can be shown (de Alfaro and Regge 1965) from the k independence of the boundary condition that $u_1(r; k)$ as well as $u_1'(r; k)$ is for each fixed radius r an entire analytic function of k^2. As a consequence, for $k \to 0$

$$u_1(r; k) = u_1(r; 0) + O(k^2), \qquad u_1'(r; k) = u_1'(r; 0) + O(k^2). \qquad (9)$$

On the other hand, $u_1(r; 0)$ can for $r > r_0$ always be written as a linear combination of the basis solutions:

$$u_1(r; 0) = \alpha\sqrt{r} + \beta\sqrt{r}\log r \equiv \beta\sqrt{r}\log r/a. \qquad (10)$$

This defines the two-dimensional scattering length a.

We relate the normalisations of the two solutions by an unknown function $c(k)$, i.e.

$$u_1(r; k) = c(k)u(r; k). \qquad (11)$$

Differentiating (6) with respect to r at some $r > r_0$, solving for $\sin \delta(k)$ and for $\cos \delta(k)$, taking the ratio of these expressions and making use of (11), we find

$$\cot \delta(k) = (2/\pi)(\gamma + \log \tfrac{1}{2}ka) + O(k^2). \qquad (12)$$

We note that in $\cot \delta(k)$, as well as in $\sin \delta(k)$, $\cos \delta(k)$ and $\tan \delta(k)$, the slow log ka dependence can thus be completely included in the zero-order term. Note that the approximation $\tfrac{1}{2}\pi/(\gamma + \log \tfrac{1}{2}ka) + n\pi$ for $\delta(k)$ which one might be inclined to consider on the basis of (12) does not show a clear improvement compared with (2), the correction containing an $O(1/\log^2 \tfrac{1}{2}ka)$ contribution. This is again illustrated in figure 1 (chain curve).

The approximation for $\cot \delta(k)$ based on (12) is much better. It is also illustrated in figure 1 (broken curve). The value of the scattering length which turns out to correspond to the low-energy behaviour of $\delta(k)$ is $a = 2.468a_0$. At 0.1 K the approximate phase-shift differs from the exact one by 1% and at 0.5 K by 3%. The agreement is further improved by including an effective-range k^2 term. In analogy to the usual derivation in three dimensions (Newton 1982) it is possible to derive

$$\cot \delta(k) \simeq (2/\pi)(\gamma + \log \tfrac{1}{2}ka) + (2\pi)^{-1}r_e^2k^2, \qquad (13)$$

the effective range r_e in two dimensions being defined by

$$r_e^2 = 4a \int_0^\infty dr \, (\phi^2(r; k=0) - \psi^2(r; k=0)). \qquad (14)$$

Here, $\psi(r; k)$ is apart from normalisation identical to $u(r; k)$:

$$\psi(r; k) = u(r; k)/(k^{1/2}a^{1/2}\sin \delta(k)), \qquad (15)$$

while $\phi(r; k)$ is the free wavefunction identical to $\psi(r; k)$ outside r_0 and in general singular at $r = 0$. With the coefficient $1/2\pi$ of the k^2 term in (13) the effective range is so normalised that its value for scattering from a hard sphere is the corresponding radius. For H–H scattering, including the k^2 term with an effective range $r_e = 11.62a_0$, we find that we approach the exact phase-shift in figure 1 to within 0.003% at 0.1 K and to within 0.7% at 0.5 K.

We now turn to the radial wavefunction. Especially in view of distorted-wave calculations, it is useful to dispose of a simple expression for $u(r; k)$ with the normalisation defined by (6). A k-dependent factor in this expression to be derived for the

region beyond $r = r_0$ will also determine the k dependence of $u(r; k)$ for $r < r_0$. To derive it we substitute expressions for $\cos \delta(k)$ and $\sin \delta(k)$ following from (12) in (6). The result is

$$u(r; k) = \frac{-(k\pi/2)^{1/2}}{(\gamma + \log \frac{1}{2}ka)[1 + \frac{1}{4}\pi^2/(\gamma + \log \frac{1}{2}ka)^2]^{1/2}} \sqrt{r}(\log r/a)[1 + O(k^2)], \tag{16}$$

for $k \to 0$. Again the $\log ka$ contributions have been included in the zero-order expression. It should be noted that the highest k value for which the latter gives a satisfactory description depends on r: the larger r, the smaller the highest k value allowed. For the example of H–H scattering (16) describes the radial wavefunction at $r = 20a_0$ to within 3.5% up to energies corresponding to 0.1 K. At $r = 40a_0$, on the other hand, the maximum energy allowed to obtain a similar maximum deviation corresponds to 0.02 K.

For a fixed r interval contributing to some distorted-wave integral, the k-dependent factor $f(k)$ in (16) for the initial channel and a similar one, $f(k')$, for the final channel determine the energy dependence of the distorted-wave matrix-element via the product $f(k)f(k')$. For this method to be practically useful, the range of the interaction causing the inelastic transition should be sufficiently small. Otherwise, the above-mentioned non-uniform convergence of the radial wavefunctions for decreasing k and k' will limit the energy interval where the energy dependence is predicted satisfactorily to rather low energies. An example is the inelastic scattering of pairs of adsorbed H atoms, undergoing a transition among the two lowest hyperfine levels in a strong magnetic field (Ahn *et al* 1982). The transition between these so-called a and b levels, which plays a crucial role in the stabilisation of atomic hydrogen, is due to the interatomic magnetic dipole interactions among electron and proton spins. Up to energies in the b channel corresponding to 10 mK the product $f(k)f(k')$ describes the energy dependence within 0.5%, but at 0.1 K the deviation is already 40%. In this example of a long-range inelastic interaction, however, the above-mentioned method can still be used with advantage in calculating the energy integral over the lower part of the Maxwell–Boltzmann distribution where the radial integrals still show a strong energy-dependence.

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