Effective-range fits for scattering phase shifts

D. G. Green, A. R. Swann, and G. F. Gribakin

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The Ps scattering phase shifts are determined from the Ps energy eigenvalues using the boundary condition on the Ps center-of-mass motion at the cavity wall, as described in Ref. [1]. Calculations were performed using cavity radii of 10, 12, 14, and 16 a.u. Effective-range-type fits were used to interpolate the S, P, and D phase shifts calculated at the discrete values of the Ps center-of-mass momentum K. These fits were used to determine the scattering length and the partial contributions to the elastic and momentum-transfer cross sections. This document details the fits for the phase shifts.

At low momenta K, the S-wave phase shift δ_0 behaves according to

$$K \cot \delta_0 \simeq -\frac{1}{A} + \frac{1}{2} r_0 K^2,$$

where A is the scattering length and r_0 is the effective range. This can be rearranged to give

$$\delta_0(K) = \tan^{-1} \frac{K}{a_0 + a_1 K^2} \pmod{\pi},$$

where $a_0 = -1/A$ and $a_1 = r_0/2$.

The P- and D-wave phase shifts behave according to

$$\delta_1 = \alpha K^3 + \beta K^4 + \gamma K^5 + \epsilon K^7 \ln K + O(K^7),$$
$$\delta_2 = \zeta K^4 + \eta K^5 + \lambda K^7 + \mu K^9 \ln K + O(K^9),$$

respectively, where α, β, γ, ϵ, ζ, η, λ, and μ are constants. We found that simple polynomial fits obtained by truncating these expansions tend to grow large as

$K \to 1$ a.u., so we used the following Padé-type fits instead:

$$\delta_1(K) = \frac{a_0 K^3}{1 + a_1 K^2 + a_2 K^4},$$
$$\delta_2(K) = \frac{a_0 K^4 + a_1 K^5}{1 + a_2 K^6}.$$

These fits have the correct leading-order behavior as $K \to 0$ and vary relatively slowly at large K, as observed in the calculated phase shifts.

The table below shows the values of the parameters of the fits for δ_L ($L = 0$, 1, 2) for He and Ne.

		Atom	
L	Parameter	He	Ne
0	a_0	−0.588	−0.568
	a_1	0.312	0.323
1	a_0	−1.90	−2.31
	a_1	3.41	2.86
	a_2	2.92	0.138
2	a_0	1.01	1.18
	a_1	−1.73	−2.25
	a_2	22.4	8.19

References

[1] A. R. Swann and G. F. Gribakin, Phys. Rev. A **97**, 012706 (2018).