

An efficient calculation of the scattering wavefunction and phase shift

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The scattering phase shift is a key characteristic of the colliding particles in quantum scattering theory. It is widely used to determine the metastable states, the scattering lengths as well as thermodynamic and transport properties of gases. The phase shift η_l is determined from the asymptotic form of the radial wavefunction $\psi(r) \simeq A \sin(kr + \eta_l + \pi l/2)$, where k is the relative wave vector of the colliding particles and l is the rotational quantum number. We show that if the wavefunction is represented in the form $f(r) \sin(kr) + g(r) \cos(kr)$, where $f(r) \simeq f_0 + f_1/r + \dots$ and $g(r) \simeq g_0 + g_1/r + \dots$ when $r \rightarrow \infty$, then the substitution of the radial variable $r = -(1+x)/x$ define the functions $f(r(x))$ and $g(r(x))$ in the finite domain $x \in [-1, 0]$ by the coupled equations

$$\begin{cases} -f''_{xx} - \frac{2}{x}f'_x + \frac{2k}{x^2}g'_x + \left[\frac{l(l+1)}{x^2} + \frac{2\mu V(r(x))}{\hbar^2 x^4} \right] f(x) = 0 \\ -g''_{xx} - \frac{2}{x}g'_x - \frac{2k}{x^2}f'_x + \left[\frac{l(l+1)}{x^2} + \frac{2\mu V(r(x))}{\hbar^2 x^4} \right] g(x) = 0 \end{cases}$$

which could be efficiently solved of by means of polynomial collocation method [1] (' denotes differentiation with respect x , $V(r)$ is interatomic potential). Thus it allows one to define the wavefunction $\psi(r)$ on the whole interval of interatomic distances $r \in [0, +\infty)$ and to determine the phase shift as $\eta_l = \arctan(g(x=0)/f(x=0))$ at the end of the interval. The mapping method has been already used for calculation bound levels and scattering lengths [2,3]. It poses the exponential convergence rate with respect to number of collocation points N (see Fig. 1). The multi-channel version of the method is applied for highly accurate calculation of the resonance position and width of quasi-bound levels above dissociation limits of KCs, RbCs and KRb molecules.

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References

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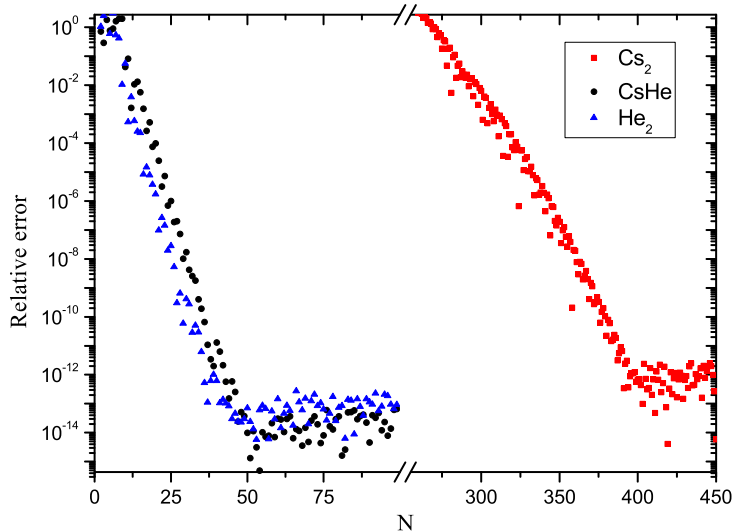


Figure 1: Relative errors in phase shift obtained for Cs_2 , $CsHe$ and He_2 potentials ($E=1000 \text{ cm}^{-1}$, $l=25$) as function of the number of grid points (N) used in the polynomial collocation method.