ADAPTIVE ANALYTIC MAPPING PROCEDURES FOR SIMPLE AND ACCURATE CALCULATION OF SCATTERING LENGTHS AND PHOTOASSOCIATION ABSORPTION INTENSITIES

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We have shown that one and two-parameter analytical mapping functions such as $r(y;\bar{r},\alpha) = \bar{r}\left[1 + \frac{1}{\alpha}\,\tan(\pi y/2)\right]$ and $r(y;\bar{r}) = \bar{r}\left[\frac{1+y}{1-y}\right]$ transform the conventional radial Schrödinger equation into equivalent alternate forms

$$\frac{d^2\phi(y)}{dy^2} \;=\; \left[\frac{\pi^2}{4} + \left(\frac{2\mu}{\hbar^2}\right) g^2(y)\,[E - U(r(y))]\right]\phi(y) \qquad \text{and} \qquad \frac{d^2\phi(y)}{dy^2} \;=\; \left(\frac{2\mu}{\hbar^2}\right) g^2(y)\,[E - U(r(y))]\,\phi(y)$$

respectively, in which $g(y) = dr(y)/dy$.[a] Such transformed equations are defined on the finite domain $y \in [-1, 1]$, and they may be solved routinely using standard numerical methods at all energies up to and including the potential asymptote. At the energy of the potential asymptote, the s-wave scattering length a_s can be expressed in terms of the logarithmic derivative of the wave function $\phi(y)$ at the right-hand boundary point:

$$a_s \;=\; \bar{r}\left[\frac{2}{\pi\alpha}\,\frac{1}{\phi(y)}\,\frac{d\phi(y)}{dy} + 1\right]_{y=1} \qquad \text{and} \qquad a_s \;=\; \bar{r}\left[2\,\frac{1}{\phi(y)}\,\frac{d\phi(y)}{dy} - 1\right]_{y=1}$$

The required logarithmic derivative of $\phi(y)$ can be obtained efficiently by direct outward integration of the differential equation all the way to the end point $y = 1$, which corresponds to the limit $r \to \infty$. This zero-energy wavefunction may also be combined with wavefunctions for ordinary bound states generated in the same manner[a] to calculate photoassociation absorption matrix elements using any appropriately modified Franck-Condon computer program.

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[a] V.V. Meshkov, A.V. Stolyarov, and R.J. Le Roy, *Phys. Rev. A* **78**, 052510 (2008).