RESOLUTION OF A CONVERGENCE PROBLEM IN DIRECT-POTENTIAL-FIT DATA ANALYSES USING THE HERMAN-ASGHARIAN HAMILTONIAN

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The effective radial Schrödinger equation based on the Herman-Asgharian[a] Hamiltonian for a diatomic molecule in a $^1\Sigma$ state has the form

$$-\frac{\hbar^2}{2\mu}\left[1+\beta(r)\right]\frac{d^2\psi_{v,j}(r)}{dr^2}+\left\{\left[V_{\rm CN}(r)+\Delta V_{\rm ad}(r)\right]+\frac{\hbar^2}{2\mu\, r^2}\left[1+\alpha(r)\right]\left[J(J+1)\right]\right\}\psi_{v,j}(r) \;=\; E_{v,J}\;\psi_{v,j}(r) \qquad (1)$$

in which $\beta(r)$ and $\alpha(r)$ represent the effects of non-adiabatic corrections to the radial and angular kinetic energy operators, respectively, and $\Delta V_{\rm ad}(r)$ is the adiabatic correction to the "clamped nuclei" potential energy function function $V_{\rm CN}(r)$. An internal convergence problem encountered when utilizing wavefunction propagator methods for direct-potential-fit diatomic data analyses using this Hamiltonian is described and corrected. Improved Hamiltonian parameters for the ground states of GaH and ArH^+ will be reported.

[a] R. M. Herman and A. Asgharian, *J. Mol. Spectrosc.* **19**, 305 (1966).