PROPERTIES OF NEARLY ONE-ELECTRON MOLECULES: A GREEN'S FUNCTION APPROACH

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We present an improved procedure to determine the collision theory reaction matrix (K matrix) and bound state energy levels in an effective one-electron calculation. As a first illustration, we consider the scattering of an electron from a monopole and a point dipole [J. K. G. Watson, Mol. Phys. 81, 277 (1994).] and obtain excellent agreement with the exact results. In the second illustration, the spectral quantum defects for the $^2\Sigma^+$ states of CaF are computed using the effective potential of [M. Arif, Ch. Jungen, and A. L. Roche, J. Chem. Phys. 106 4102 (1997)], obtaining results close to the experimental data. We show that other representations of the ion-core are compatible with our treatment.