SOLVING THE RADIAL SCHRÖDINGER EQUATION AT ENERGIES EXTREMELY CLOSE TO DISSOCIATION: BOUND STATES AND SCATTERING LENGTHS

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Studies of cold atomic and molecular systems often involve observation of very weakly bound levels which lie extremely close to dissociation and have outer turning points at distances of several tens, hundreds, or thousands of Å. Performing accurate calculations of the energies and other properties of such levels from a given potential energy function using conventional methods can be somewhat challenging. This paper shows that replacement of the normal radial integration variable r by a dimensionless variable of the form $y = (r^p - a^p)/(r^p + a^p)$, where p and a are constants, transforms the radial Schrödinger equation into a form in which treatment of levels lying extremely close to dissociation becomes just as straightforward and routine as treating levels in the lower part of the potential well. This approach also leads to a very straightforward, simple method of calculating scattering lengths.