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SOLUTION OF THE SCHRÖDINGER EQUATION USING PADÉ APPROXIMANTS TO SUM ASYMPTOTIC SERIES

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In physics one is frequently interested in finding solutions to a Schrödinger Equation which contains a potential falling off as r^{-n} at large distances. An r^{-4} potential, for example, corresponds to the polarization of an atom by a distant charged particle. In the case of the interaction of an electron with an excited hydrogen atom there is an r^{-2} potential at large r. In these cases, the solutions for the long range behavior (Mathieu and Bessel functions, respectively) are known.

However, in many cases the solutions are not known, except in terms of a divergent series in $1/r$. A good example is the Coulomb three body problem where it has been only very recently that Stagat, Nuttall, and Hidalgo [1] have found such an asymptotic series for the three body wave function for the vth excited level of hydrogen in the presence of a distant electron for zero angular momentum.

For small distances the long ranged potential is usually modified by a different short ranged behavior. Our idea is to use Padé approximants to sum the asymptotic series in $1/r$ to a form which at large r might be used as the basis for a variational trial wave function. For small r we suggest using other wave functions and looking for a region of overlap where the two pieces of the wave function match.

Let us now consider radial Schrödinger equation:

$$\left(- \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + V(r) - k^2 \right) \psi(r) = 0. \tag{1}$$

In most cases one knows (or pretends to know) the asymptotic form of the wave function, namely

$$\lim_{r \to \infty} \psi(r) = \frac{a_1}{r}. \tag{2}$$

This is the first term in a power series expansion in r^{-1},

$$\psi(r) = \sum_{n=1}^{\infty} \frac{a_n}{r^n}. \tag{3}$$

Substituting this expansion into the differential equation and equating like inverse powers of r, we may find relations among the a_n's. For

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