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

J. H. McGUIRE, J. E. GOLDEN AND J. NUTTALL

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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example $d^2/dr^2 - k^2$ will relate a_{n+2} to a_n. Using these recursion relations, and knowing the first coefficient a_1, the entire series in r^{-n} may be generated.

Unfortunately this series is not useful. Generally one finds that the series is an asymptotic series with a zero radius of convergence. It is therefore a good patient for Padé approximants.

In order to test this idea of using Padé approximants to find solutions to the Schrödinger Equation, we tried the technique for the potential $V(r) = V_0/r^2$. The exact solution in this case is known, namely

$$\psi(r) = r^{1/2} J_v(kr), \qquad v^2 = \ell(\ell + 1) + \tfrac{1}{4} + V_0. \tag{4}$$

Since Gargantini and Henrici [2] have related $K_v(z)$ to a series of Stieltjes for $-\frac{1}{2} \leqq v \leqq \frac{1}{2}$, we choose to work with the $K_v(z)$ functions. For real v we have been able to show [3] that $K_v(z)$ is proportional to a series of Stieltjes plus a polynomial whose degree is equal to the integer part of v. Hence we were able to prove the convergence of the Padé approximants obtained from the asymptotic series. We also determined the rate of convergence.

If the potential is sufficiently attractive v can become imaginary. For complex v, $K_v(z)$ is not related to a series of Stieltjes nor any function for which a proof of convergence now exists. However, the Padé approximants converge at a rate similar to v real. For both real and imaginary v the number of Padé approximants required increases as $r \to 0$.

Our example for a $1/r^2$ potential suggests the value of using Padé approximants to sum an asymptotic series for $\psi(r)$ in general. However, the usefulness of this technique for computing physical observables such as cross sections involving integrals over $\psi(r)$ remains open to question.

References

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Dept. of Physics, Kansas State University, Manhattan, Kansas 66502

Dept. of Physics, Texas A&M University, College Station, Texas 77843

Dept. of Physics, University of Western Ontario, London, Ontario, Canada