PHYSICAL REVIEW
LETTERS

VOLUME 57 3 NOVEMBER 1986 NUMBER 18

Approximation Theory and the Calculation of Energies from Divergent Perturbation Series

L. S. Luo and J. Nuttall
Department of Physics, The University of Western Ontario, London, Ontario N6A 3K7, Canada
(Received 30 April 1986)

In problems such as the anharmonic oscillator and the H-atom Stark effect, the energies of bound states and resonances can be formally expressed in terms of series with a radius of convergence zero. We propose a method of rational approximation to sum such series and illustrate it by application to the anharmonic oscillator. In a certain sense this method is close to the best one possible.

PACS numbers: 03.65.Nk, 02.70.+d, 03.65.Ge

There are a number of interesting model problems[1] in which the energy of a bound state or a resonance is given formally in terms of a power series in a potential strength β which has a zero radius of convergence, i.e.,

$$E(\beta)=\sum_{k=0}^{\infty} a_k \beta^k, \tag{1}$$

where the coefficients a_k are real. In some cases (e.g., the anharmonic oscillator with $\beta>0$) $E(\beta)$ is real and represents a bound-state energy, but in others (e.g., the H-atom Stark effect) $E(\beta)$ is complex for real β, and corresponds to the energy of a resonance.

Here we describe a technique of rational approximation[2,3] which can be adapted to the calculation of $E(\beta)$ in both situations, and explain how a theorem from approximation theory shows that, in a certain sense, our method is close to the best one possible.

We illustrate our ideas by applying them to the anharmonic oscillator with Hamiltonian $H(\beta)=p^2+x^2+\beta x^4$, $-\infty<x<\infty$. For real $\beta>0$, we let $E(\beta)$ be the lowest bound-state energy. The coefficients in the series (1) are easy to calculate to high order from Rayleigh-Schrödinger perturbation theory. It has been shown[4] that $E(\beta)$ may be continued analytically along a path $\beta=|\beta|e^{i\theta}$, $0\le\theta\le\pi$, and we can interpret $E(-|\beta|)$, a complex number, as the energy of a resonance in the potential $x^2-|\beta|x^4$. $E(\beta)$ may be continued further into the third quadrant, but $E(\beta)$ has a set of branch points in that quadrant that approach $\beta=0$ from the direction of the negative imaginary axis. Similarly, $E(\beta)$ may be continued along the same path reflected in the real axis. The result is another value of $E(-|\beta|)$ which will be the complex conjugate of the previous one. We denote the two continuations of $E(\beta)$ in the neighborhood of the negative real axis by $E_1(\beta)$ and $E_2(\beta)$, and set $\Delta(\beta)=E_1(\beta)-E_2(\beta)$, so that $\Delta(\beta)$ is analytic in $\mathrm{Im}\beta<0$ except for the branch points referred to above.

For real $\beta>0$ it has been shown[5] that

$$\Delta(-\beta)=8i\pi^{-1/2}\beta^{-1/2}\exp(-2/3\beta)[1+O(\beta^{\lambda})],\quad \beta\to 0 \tag{2}$$

for some $\lambda>0$. The arguments used may be extended to show that (2) also holds for $0\le|\arg\beta|<\pi/2$. It is also known that $\Delta(\beta)=O(\beta^{1/3})$ as $\beta\to\infty$.

In what follows, it is more convenient to use $z=\beta^{-1}$ and write $\sigma(z)=\Delta(\beta)$, $\varepsilon(z)=E(\beta)$. The properties stated lead to the relation

$$\varepsilon(z)=\frac{1}{2\pi i}\int_{\Gamma(\pi)}\sigma(z')(z'-z)^{-1}dz',\quad z\notin\Gamma(\pi), \tag{3}$$

where $\Gamma(\alpha)=\{z=re^{i\alpha},\ 0\le r<\infty\}$. This representation can be of use in calculating the bound-state energy $\varepsilon(|z|)$, but we illustrate our method on the resonance case. Because of the analyticity of $\sigma(z)$, we can change $\Gamma(\pi)$ in (3) to $\Gamma(\pi+\alpha)$, $\alpha>0$, provided that α is small enough that no branch point of $\sigma(z)$ lies in the sector between $\Gamma(\pi)$ and $\Gamma(\pi+\alpha)$. Thus, for z_0 real negative we

have

$$\varepsilon(z_0)=\frac{1}{2\pi i}\int_{\Gamma(\pi+\alpha)}\omega(z')\rho(z')(z'-z_0)^{-1}dz', \qquad (4)$$

where we have written $\omega(z)=|e^{-2z/3}|(1+|z|)^{3/2}$ and $\sigma(z)=\omega(z)\rho(z)$, $z\in\Gamma(\pi+\alpha)$. This will give the resonance energy $E_1(z_0^{-1})=\varepsilon(z_0)$. In view of the properties stated above,

$$\int_{\Gamma(\pi+\alpha)}|\rho(z')|^2|dz'|=C<\infty. \qquad (5)$$

To perform the rational approximation of $\varepsilon(z_0)$, we choose, as described below, a polynomial of degree n, $p(z)$, and calculate $q(z)$, another polynomial of degree n, by

$$q(z)=p(z)\varepsilon(z)+O(z^{-1}),\quad z\to\infty.$$

We approximate $\varepsilon(z)$ by $q(z)/p(z)$, and it may be shown[2] that

$$\delta_n(z_0)\equiv\varepsilon(z_0)-q(z_0)/p(z_0)=\frac{1}{2\pi i p(z_0)}\int_{\Gamma(\pi+\alpha)}\omega(z')\rho(z')p(z')(z_0-z')^{-1}dz'.$$

By the Schwarz inequality

$$|\delta_n(z_0)|^2\le\frac{C}{4\pi^2|p(z_0)|^2}\int_{\Gamma(\pi+\alpha)}\omega(z')^2|z'-z_0|^{-2}|p(z')|^2|dz'|.$$

The information which we are using is as follows: (i) analyticity of $\varepsilon(z)$ in $\mathbb{C}\backslash\Gamma(\pi+\alpha)$; (ii) the coefficients $a_0,\ldots,a_n$; and (iii) the fact that $\rho(z)$ satisfies (5). Without any further information, the best choice to use for $p(z)$ in this approximation scheme is the unique polynomial of degree n which minimizes

$$K_n(z_0)=|p(z_0)|^{-2}\int_{\Gamma(\pi+\alpha)}\omega(z')^2|z'-z_0|^{-2}|p(z')|^2|dz'|. \qquad (6)$$

It can be shown[6] that

$$\lim_{n\to\infty}[n^{-1/2}\ln K_n(z_0)]=-8(3^{-1}|z_0|\cos\alpha)^{1/2}\sin(\alpha/2),$$

so that, with the above choice of $p(z)$,

$$\lim_{n\to\infty}[n^{-1/2}\ln|\delta_n(z_0)|]\le-4(e^{-1}|z_0|\cos\alpha)^{1/2}\sin(\alpha/2) \qquad (7)$$

and, from what we known, $\rho(z)$ could be such that equality holds in (7).

Now each a_k is a linear functional of $\rho(z)$, as is $\varepsilon(z_0)$ given by (4), and the approximation $q(z_0)/p(z_0)$ is linear in $a_0,\ldots,a_n$, given the above information. There is a result in approximation theory[7-9] which states that, in these circumstances, no nonlinear algorithm is better than the best linear algorithm. This theorem suggests that there may be no point in using nonlinear approximations such as Borel-Padé, especially in view of the fact that no rigorous error bound is available in these cases. It must be stressed that for the actual $\rho(z)$ needed here, the error of a particular nonlinear algorithm could be less than the error of our method.

We have applied this method, modified slightly for convenience by replacing $|z'-z_0|^{-2}$ in (6) by $(1+|z'|)^{-2}$, which should not affect (7), to the case $z_0=-1$. The results for the choice $\alpha=\pi/4$ are shown in Fig. 1. The estimates of $\varepsilon(-1)$ appear to be converging to the correct value of $0.74775-i0.60998$, calculated by a variational method. This suggests that no branch point of $\sigma(z)$ lies in the sector between $\Gamma(\pi)$ and $\Gamma(\pi+\alpha)$.

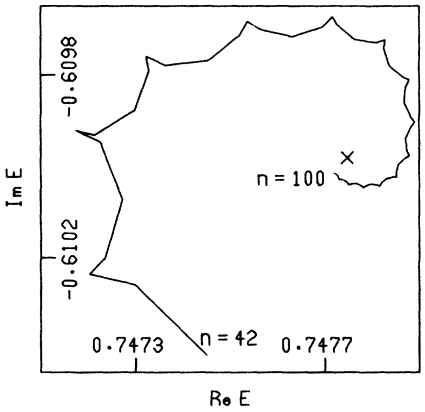

FIG. 1. Plot showing estimates of $\varepsilon(-1)$ corresponding to $n=42-100$, with $\alpha=\eta/4$. Successive points are joined by straight lines and the exact result is marked by a cross.

It is to be expected that if more information about $\varepsilon(z)$ were to be used a better result would be found. Thus, if we set $z=t^2$, $\eta(t)\equiv\varepsilon(z)$, and apply the method to $\eta(t)$ using a contour $\Gamma(\beta)\cup\Gamma(-\beta)$, with $\pi/2<\beta<3\pi/4$, we shall be incorporating the knowledge that $\varepsilon(z)$ is analytic on more than one sheet of the z plane. An asymptotic analysis for the corresponding polynomials,[10] indeed, gives a smaller bound than (7) for large n. We have an asymptotically better method for calculating the resonance energy (t pure imaginary) and also a method for the bound state that is better than the Padé method. To illustrate this point we compare in Table I the results of calculating $E(1)=\varepsilon(1)=\eta(1)$ with diagonal Padé ap-

TABLE I. Errors in calculation of $E(1)$ using diagonal Padé approximants and rational approximation to $\eta(t)$.

Number of coefficients a_k used	Error in diagonal Padé approximant	Error in method of text
3	0.12	0.19×10^{-1}
7	0.19×10^{-1}	0.45×10^{-2}
11	0.43×10^{-2}	0.38×10^{-3}
15	0.12×10^{-2}	-0.12×10^{-5}
19	0.41×10^{-3}	0.66×10^{-5}
23	0.15×10^{-3}	0.16×10^{-5}
27	0.62×10^{-4}	0.17×10^{-7}
31	0.27×10^{-4}	0.80×10^{-7}
35	0.12×10^{-4}	0.22×10^{-7}

proximants[11] and rational approximation of $\eta(t)$ with denominator $p(t)$ chosen to minimize

$$K_n(1) = |p(1)|^{-2}\int_{\Gamma(\beta)\cup\Gamma(-\beta)} |\exp(\tfrac{4}{3}t^2)|\,|p(t)|^2\,|dt|$$

with $\beta=5\pi/8$. Approximants which use the same number of coefficients a_k are compared. The correct value $E(1)=1.392\,351\,641\,5$ has been calculated by Biswas *et al.*[12]

We note that the Padé method apparently can be improved.[13] If the information that has gone implicitly into this improvement could be incorporated into our method, then presumably it also could be made better.

There are other problems, such as the high-energy expansion for a disordered medium, which have a mathematical formulation similar to that described here, and this method of rational approximation could be appropriate.

We are grateful to W. P. Reinhardt and G. M. Trojan for helpful conversations, and to K. Aashamar for the use of his multiple-precision arithmetic code GENPREC. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.

[1]B. Simon, Int. J. Quantum Chem. **21**, 3 (1982).

[2]R. T. Baumel, J. L. Gammel, and J. Nuttall, J. Comput. Appl. Math. **7**, 135 (1981).

[3]G. M. Trojan, Constr. Approx. **2**, 101 (1986).

[4]B. Simon, Ann. Phys. (N.Y.) **58**, 76 (1970).

[5]E. Harrell and B. Simon, Duke Math. J. **47**, 845 (1980).

[6]E. A. Rakhmanov, Mat. Sb. **119**, 161 (1982) [Math. USSR-Sb. **47**, 155 (1984)].

[7]K. Y. Osipenko, Mat. Zametki **19**, 29 (1976) [Math. Notes **19**, 17 (1976)].

[8]C. A. Michelli and T. J. Rivlin, in *Optimal Estimation in Approximation Theory,* edited by C. A. Michelli and T. J. Rivlin (Plenum, New York, 1976).

[9]J. F. Traub and H. Woźniakowski, *A General Theory of Optimal Algorithms* (Academic, New York, 1980).

[10]L. S. Luo and J. Nuttall, "Asymptotic Behavior of the Christoffel Function Related to a Certain Unbounded Set," to be published.

[11]Note that the Padé approximants given in Ref. 4 are successively more inaccurate from $N=10$ onwards.

[12]S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, J. Math. Phys. (N.Y.) **14**, 1190 (1973).

[13]J. Cizek and E. R. Vrscay, Int. J. Quantum Chem. **21**, 27 (1982).