Application of Padé interpolation to stationary state problems

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If the small and large coupling behavior of a physical system can be computed perturbatively and expressed respectively as power series in a coupling parameter $g$ and $1/g$, a Padé approximant embracing the two series can interpolate between these two limits and provide an accurate estimate of the system’s behavior in the generally intractable intermediate coupling regime. The methodology and validity of this approach is illustrated by considering several stationary state problems in quantum mechanics.

I. INTRODUCTION

A Padé approximation is a formal transformation of the first $n$ terms in the power series for a function $f(x)$ into a rational function. The rational function $R(x)$, known as the Padé approximant, typically comprises a ratio of two polynomials of $x$, chosen in a way that a Taylor expansion of $R(x)$ completely reproduces the original power series up to order $n$. In contrast to the truncated “mother” series, the Padé approximant is able to maintain remarkable fidelity to the true $f(x)$ for values of $x$ well beyond the radius of convergence of the original power series, although how accurate it is, or how large $|x|$ may be before the approximation fails is impossible to establish in general. Nevertheless, its extraordinary predictive power has in the past been exploited in areas of quantum field theory and statistical physics. In quantum electrodynamics and quantum chromodynamics, for example, the Padé method has been shown to be an effective means of both estimating unknown higher order terms as well as of summing the perturbation series for a physical observable that has been calculated to some finite order in the coupling constant.

In a recent paper, one of us has explored a different usage of the Padé approximation in which the Padé approximant, constructed from the truncated power series of $f(x)$ about two different points, serves to interpolate $f(x)$ between the two points of expansion. In particular, if one is able to compute perturbatively both the small $x$ and large $x$ behavior of $f(x)$ ($x > 0$), and express them respectively in a power series in $x$ and $1/x$, a Padé approximant that simultaneously satisfies the two perturbation series will provide an accurate estimation of $f(x)$ for the entire range of $x$, provided that $f(x)$ is a sufficiently smooth function in this range. This approach is known as the two-point Padé approximation and is especially savoring from the perspective of duality in supersymmetric gauge theories if one can infer perturbatively the strong coupling behavior of a theory from its weakly coupled dual theory, a Padé interpolation of this limit with the perturbative weak coupling limit of the original theory will then give us a handle on the behavior of the theory for all coupling strengths.

The Padé interpolation method may also be employed in some cases where there are no obvious expansion parameters. An example is a system for which the Hamiltonian $H$, although itself not exactly soluble, can be expressed as a sum of two constituent Hamiltonians, $H_1$ and $H_2$, both with known exact solutions. It was proposed in Ref. 2 that, by tagging either $H_1$ or $H_2$ with an interpolation parameter $\lambda$, the two required perturbative series in opposite limits of $\lambda$ could be generated, and an estimate for $H$ would correspond to evaluating the Padé approximant with $\lambda = 1$. This method was applied in Ref. 2 to heavy quarkonium systems with reasonable success.

The quarkonium example demonstrates the power and usefulness of Padé interpolation for treating a certain class of stationary state problems. The technique may serve as an improvement or a supplement to perturbation theory typically taught in courses on quantum mechanics. The purpose of this note is to present a pedagogical discourse of the methodology of Padé interpolation. For the examples considered below, the Padé interpolation method is shown to be stable to higher orders, and yield particularly good results when the usual perturbative method fails.

II. THE METHOD

Consider a system governed by a Hamiltonian $H$ that has no known solution, but which may be expressed as a sum of two parts: $H = H_1 + H_2$, where $H_1$ and $H_2$ are individually exactly soluble. We are interested in finding the spectrum of $H$. In order to implement the Padé interpolation for this purpose, we introduce the interpolation Hamiltonian

$$H(\lambda) = H_1 + \lambda H_2 ,$$

where the interpolation parameter $\lambda$ is real and positive. Suppose first that $\lambda \ll 1$. We may then regard $H_2$ as a perturbation, and calculate the eigenvalues of $H$ as power series in $\lambda$ (the subscript $j$ labels the eigenvalues):

$$E_j(\lambda) = c_0 + c_1 \lambda + c_2 \lambda^2 + \ldots + c_m \lambda^m .$$

In the opposite $\lambda \gg 1$ limit, we rewrite Eq. (1) as

$$H'(\lambda) = \lambda \left[ H_2 + \left( \frac{1}{\lambda} \right) H_1 \right] ,$$

where $H'$ is the "mother" series, the Padé approximant is able to maintain remarkable fidelity to the true $f(x)$ for values of $x$ well beyond the radius of convergence of the original power series, although how accurate it is, or how large $|x|$ may be before the approximation fails is impossible to establish in general. Nevertheless, its extraordinary predictive power has in the past been exploited in areas of quantum field theory and statistical physics. In quantum electrodynamics and quantum chromodynamics, for example, the Padé method has been shown to be an effective means of both estimating unknown higher order terms as well as of summing the perturbation series for a physical observable that has been calculated to some finite order in the coupling constant.

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In the opposite $\lambda \gg 1$ limit, we rewrite Eq. (1) as

$$H'(\lambda) = \lambda \left[ H_2 + \left( \frac{1}{\lambda} \right) H_1 \right] ,$$
and a second perturbative solution of $H(\lambda)$ follows from treating $1/\lambda$ as a small parameter:

$$E_j^\gamma(\lambda) = \lambda \left[ b_0 + b_1 \left( \frac{1}{\lambda} \right) + b_2 \left( \frac{1}{\lambda} \right)^2 + \ldots + b_n \left( \frac{1}{\lambda} \right)^n \right].$$  \hfill (4)

Note that both $H_1$ and $H_2$ must admit stationary states and be able to be treated as perturbations for the method to work. An example of a Hamiltonian that admits bound-state solutions but that cannot be treated as a perturbation is the Hamiltonian for an infinite rectangular potential well.

A generic Padé approximant for the energy eigenvalues has the form

$$E_j^{PA}(\lambda) = \frac{p_0 + p_1 \lambda + p_2 \lambda^2 + \ldots + p_N \lambda^N}{1 + q_1 \lambda + q_2 \lambda^2 + \ldots + q_M \lambda^M},$$  \hfill (5)

where the $N+M+1$ coefficients are determined by matching order by order the power series expansion of the Padé approximant with the perturbative results. For $b_0 \neq 0$, the nature of $E_j^\gamma(\lambda)$ in Eq. 4 demands that the polynomials in the numerator and the denominator of the Padé approximant differ by one degree such that $M = N - 1$. Furthermore, suppose that we solve $H(\lambda)$ for small and large $\lambda$ to the same order in perturbation theory, that is, $m = n$. (This case is just an illustration and is not a necessary condition for implementing the Padé interpolation, although the accuracy of the approximation will depend on $m$ and $n$.) Then Eqs. 2 and 4 together furnish $2n + 2$ simultaneous equations for the $2N$ unknown coefficients $p$ and $q$, and consequently the polynomials in the Padé approximant must satisfy $N = n + 1$ and $M = n$. The final step of setting $\lambda = 1$ in the Padé approximant yields an estimate for the eigenvalues of the original Hamiltonian $H$.

### III. EXAMPLES

We demonstrate here the validity of the Padé interpolation method by way of two examples. Consider first a simple two-state system described by the Hamiltonian

$$H = a \sigma_y + b \sigma_z,$$  \hfill (6)

where $a$ and $b$ are real parameters, and $\sigma_y$ and $\sigma_z$ are the Pauli matrices. For example, this Hamiltonian can represent the interaction energy of a charged spin-1/2 particle in a magnetic field $\vec{B} = (0, B_y, B_z)$. In this case,

$$a = -\frac{g\hbar B_y}{2} \quad \text{and} \quad b = -\frac{g\hbar B_z}{2},$$  \hfill (7)

where $g$ is the gyromagnetic ratio of the particle. This example is trivial in the sense that $H$ can be easily diagonalized to yield the exact eigenvalues

$$E_\pm = \pm \sqrt{a^2 + b^2}.$$  \hfill (8)

However, the comparison of these exact results with the approximate eigenvalues obtained below by Padé interpolation will provide a way to gauge the accuracy of the approximation method.

For $|a| \gg |b|$, for example, if the magnetic field is almost aligned with the $y$-axis, the $b \sigma_z$ term in $H$ may be treated as a perturbation. To be more explicit, we may express the Hamiltonian as

$$H|a| \gg |b| = a \left( \sigma_y + \frac{b}{a} \sigma_z \right),$$  \hfill (9)

which has the form of Eq. 4, except that $\lambda$ is equal to $b/a$ and corresponds to a physical expansion parameter.

If we calculate the energy eigenvalues to second order in perturbation theory, we find

$$E_j^{[a] \gg |b|} = \pm |a| \left( 1 + \frac{b^2}{2a^2} \right).$$  \hfill (10)

For $|a| \ll |b|$, for example, if the magnetic field is almost parallel to the $z$-axis, the $a \sigma_y$ term in $H$ can be regarded as a perturbation. We find that, again to second order in perturbation theory (with $a/b$ as the expansion parameter), the eigenvalues of $H$ are now given by

$$E_j^{[b] \gg |a|} = \pm |b| \left( 1 + \frac{a^2}{2b^2} \right).$$  \hfill (11)

A Padé approximant that interpolates these two limits of the energy eigenvalues can now be constructed. For the eigenvalue $E_+$, we find

$$E_+^{PA} = \frac{|a|}{|b/a|} \left[ \frac{|b/a|^3}{|b/a|^3 + \frac{3}{2} |b/a|^2 + \frac{3}{2} |b/a| + 1} \right].$$  \hfill (12)

This Padé approximant is uniquely determined from the perturbative expansions for $E_+$ given in Eqs. 10 and 11. Table I compares this Padé interpolation result with the exact eigenvalue, Eq. 8, for various values of the parameter $|b/a|$. We see that the Padé interpolation yields an approximation that is within 1% of the exact result for all values of $|b/a|$. This simple example demonstrates the potential power of the Padé interpolation technique: by simply computing the leading perturbative corrections for small and large $|b/a|$, one obtains a very accurate approximation to the eigenvalues for all values of $|b/a|$.

As a second example, consider a single particle subject to a one-dimensional linear plus harmonic oscillator potential. (The Padé interpolation technique we shall use to solve this problem is similar to that applied in Ref. 2 to nonrelativistic quarkonium systems.) The Hamiltonian that describes the motion of the particle is

$$H = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \gamma x + \frac{1}{2} m \omega^2 x^2 + V(x),$$  \hfill (13)

where $\gamma > 0$. (The latter condition is necessary in order for the Hamiltonian $H_1$ in Eq. 13 to admit stationary
state solutions.)  \( V(x) \) represents the rigid wall potential:

\[
V(x) = \begin{cases} 
0 & x > 0 \\
\infty & \text{otherwise}
\end{cases}
\]  

(14)

The presence of \( V(x) \) restricts the particle’s motion to be along the positive \( x \)-axis.

The Hamiltonian in Eq. (13) without \( V(x) \) appears in many textbooks on quantum mechanics and can be easily solved by transforming to a new coordinate \( x’ \) with the origin at \( x = -\gamma/(m\omega^2) \). The presence of the rigid wall potential, however, requires all wave functions to vanish for \( x \leq 0 \) and renders such a coordinate redefinition useless. The Hamiltonian with \( \gamma = 0 \) is also a typical textbook problem that is exactly soluble; the boundary condition due to the rigid wall forces all energy eigenfunctions to vanish at the origin, which implies that only the harmonic oscillator states with odd parity are allowed.

Solving the complete Hamiltonian is a somewhat more challenging task. In particular, if the linear and quadratic potentials are comparable, conventional perturbative methods are not applicable. We shall therefore resort to the method outlined in Sec. II to find its eigenvalues. Note that as long as we confine the particle’s motion to the positive \( x \) branch, and impose the boundary condition that all eigenfunctions vanish at \( x = 0 \), we may drop the rigid wall potential \( V(x) \) in Eq. (13). The resulting Hamiltonian can then be cast in the form of Eq. (1), with

\[
H_1 = -\frac{1}{4} \frac{d^2}{dx^2} + \gamma x,
\]

and

\[
H_2 = -\frac{1}{4} \frac{d^2}{dx^2} + \frac{1}{4} x^2,
\]

(15)

(16)

where, for simplicity, we have set \( \hbar = 1 \), \( m = 1 \) and \( \omega = 1 \) such that the arbitrary parameter \( \gamma \) alone regulates the relative importance of the two potential energy terms. Note that it is also necessary to split the kinetic energy term. Here, we have arbitrarily put half of the original kinetic energy term into each of the sub-Hamiltonians in Eqs. (14) and (15). As we will see (in the last paragraph of this section), better accuracy will generally be achieved in Padé interpolation if a larger fraction of the kinetic energy is included in the sub-Hamiltonian containing the dominant potential energy term.

The solutions to \( H_1 \) are the familiar Airy functions \( Ai(z) \), with \( z = (2/\gamma)^{2/3}(\gamma x - \epsilon_j^x) \); the energy eigenvalues \( \epsilon_j^x \) are determined by the roots of \( Ai(z) \). On the other hand, \( H_2 \) is solved by \( \exp(-\xi^2/2)h_j(\xi) \), where \( h_j(\xi) \) are the Hermite polynomials of degree \( j \), \( \xi = 2^{1/4}x \), \( \epsilon_j^x = (j + 1/2)/\sqrt{2} \) are the allowed energies, and the index \( j \) must be an odd integer in order to satisfy the boundary condition \( \psi_j(0) = 0 \), where \( \psi_j(x) \) denotes the stationary state wave functions.

We now proceed to perform the relevant perturbative calculations. We have evaluated to first, second, and third order in \( \lambda \) and \( 1/\lambda \) the approximate ground and first excited state energies for \( \gamma = 1 \), that is, when the linear and quadratic potential energy terms are comparable, and have formed the unique Padé approximant for each instance. Because closed-form expressions for integrals involving Airy functions generally do not exist, we did the exercise numerically. As an illustration, the analysis of the ground state generates the two series,

\[
E_0^< = 1.47292 + 1.06950\lambda - 0.0131354\lambda^2 + \ldots, (17)
\]

\[
E_0^\gamma = 1.06006\lambda + 1.47918 - 0.00467253\frac{1}{\lambda} + \ldots (18)
\]

The first (second) order Padé approximant,

\[
E_{0,1st}^{PA} = \frac{1.47292 + 3.14779\lambda + 1.49659\lambda^2}{1 + 1.41100\lambda},
\]

\[
E_{0,2nd}^{PA} = \frac{1.47292 + 5.36462\lambda + 6.07765\lambda^2 + 2.14021\lambda^3}{1 + 2.91607\lambda + 2.01781\lambda^2},
\]

(19)

(20)

follows from manipulating the first two (three) terms of Eqs. (17) and (18). Tables IV and V contain a summary of the results for the ground and first excited states.

It is instructive to compare these results with those one would obtain from conventional perturbative calculations alone. Because there is no preference for either of the two potential energy terms, we consider both of the following parameterizations of the Hamiltonian:

\[
H(\alpha) = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \alpha \gamma x + V(x),
\]

and

\[
H(\beta) = -\frac{1}{2} \frac{d^2}{dx^2} + \gamma x + \beta \frac{1}{2} x^2 + V(x),
\]

(21)

(22)

where \( \alpha \) and \( \beta \) are the small parameters that are eventually set to 1. As seen in Tables VI and VII, the Padé interpolation gives by far the most stable results. A further comparison with exact solutions from the numerical integration of the Schrödinger equation, also given in Tables VI and VII, exemplifies the validity of the method. We have also checked the accuracy of the method for higher excited states. The approximate energies obtained, even to first order in the perturbation parameters, are always accurate to within 1% of their exact values.

For completeness, we have examined situations in which one potential energy term is dominant, and perturbative calculations on the smaller term alone are expected to yield reasonably accurate results. This is certainly the case. However, as seen in Tables VII and VIII, the Padé interpolation is able to do a better job, provided that the original kinetic energy term is distributed among the two sub-Hamiltonians in a way that reflects the relative significance of the two potential energy terms. We have also studied the effects of distributing the kinetic energy unevenly between the two sub-Hamiltonians in the \( \gamma = 1 \) case. As shown in Tables VII and VIII, rather good estimates of the exact results can be achieved regardless of how the kinetic energy
is distributed, particularly if one goes to higher order. However, the best accuracy is obtained if somewhat less kinetic energy (40% to be precise) is included in $H_1$, especially for the first excited state. This result can be understood from Tables II and III which show that the perturbation series for $H'(\lambda)$ converges faster than $H(\lambda)$ to the exact result. This behavior in turn suggests that for $\gamma = 1$, the linear potential is weaker than the quadratic potential. Hence, according to the results in Tables IV and V, a more accurate Padé approximant will be obtained by underweighting the kinetic energy in $H_1$. Unfortunately, there are no quantitative rules for how the kinetic energy should be distributed among the two Hamiltonians. Tables VI and VII suggest that a 50 : 50 split should produce reasonably good estimates.

IV. CONCLUSION

The stationary state problems considered here provide a good illustration of the power of Padé interpolation for problems for which exact solutions are difficult to obtain and ordinary perturbation methods are not applicable. For practice, the interested reader may wish to apply the method to interpolate the strong-field and weak-field Zeeman effects in hydrogen. Exact results for the $n = 2$ level can be found in Ref. 6. They involve square-root functions of the expansion parameter (the magnitude of the magnetic field), similar to the first example discussed in Sec. III. See also Ref. 7 which discusses the case of the two-dimensional hydrogen atom.

The use of Padé interpolation is of course not limited to quantum mechanical problems, because all that is needed is an expansion parameter, be it a physical one as in Eq. (9) or an artificial one such as the interpolation parameter in Eq. (1), for which the behavior of the physical system can be calculated or measured when the parameter is small as well as when it is large. We encourage the reader to find other applications of this useful approximation scheme.

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### Table I: The eigenvalue $E_+$ (in units of $|a|$) of the two-state system for various values of the parameter $|b/a|$.

| $|b/a|$ | Padé    | Exact   |
|-------|---------|---------|
| 0.1   | 1.00517 | 1.00499 |
| 0.5   | 1.12500 | 1.11803 |
| 1     | 1.42857 | 1.41421 |
| 2     | 2.25000 | 2.23607 |
| 10    | 10.0517 | 10.0499 |
TABLE II: Ground state energy, $\gamma = 1$. Columns two to five display the first, second, and third order perturbative solutions to the Hamiltonians $H(\alpha)$, $H(\beta)$, $H(\lambda)$, and $H'(\lambda)$, where the perturbation parameters $\alpha$, $\beta$, $\lambda$, and $1/\lambda$ are all set to unity. Results from the Padé interpolation of $H(\lambda)$ appear in column six. These are to be compared with the exact energy, shown in the bottom, obtained from numerical integration of the Schrödinger equation.

|       | $H(\alpha)$ | $H(\beta)$ | $H(\lambda)$ | $H'(\lambda)$ | Padé   |
|-------|--------------|-------------|--------------|---------------|--------|
| 1st order | 2.62838      | 2.77411     | 2.54242      | 2.53984       | 2.53724 |
| 2nd order | 2.51908      | 2.30374     | 2.52928      | 2.53517       | 2.53720 |
| 3rd order | 2.54121      | 2.88137     | 2.54998      | 2.53882       | 2.53720 |
| Exact   | 2.53720      |             |              |               |        |

TABLE III: First excited state energy, $\gamma = 1$. See Table II caption for a detailed description.

|       | $H(\alpha)$ | $H(\beta)$ | $H(\lambda)$ | $H'(\lambda)$ | Padé   |
|-------|--------------|-------------|--------------|---------------|--------|
| 1st order | 5.19257      | 6.05194     | 5.20217      | 5.13559       | 5.10483 |
| 2nd order | 5.09417      | 3.67756     | 4.90789      | 5.08365       | 5.10380 |
| 3rd order | 5.08881      | 8.19137     | 5.53588      | 5.11655       | 5.10333 |
| Exact   | 5.10382      |             |              |               |        |
TABLE IV: Perturbation theory versus Padé interpolation: dominant quadratic potential, \( \gamma = 0.1 \). Columns two and three show respectively the results from standard perturbative calculations with the linear potential as the perturbation, and the corresponding estimates from the Padé interpolation of \( H(\lambda) \), where the original kinetic energy term is distributed among the sub-Hamiltonians (15) and (16) in the ratio 1 : 9. The exact energies, obtained from numerically integrating the Schrödinger equation, are also displayed.

|                  | Perturbation Theory | Padé  |
|------------------|---------------------|-------|
| Ground state     |                     |       |
| 1st order        | 1.61284             | 1.61174 |
| 2nd order        | 1.61174             | 1.61177 |
| 3rd order        | 1.61177             | 1.61177 |
| Exact            | 1.61177             |       |
| First excited state |                 |       |
| 1st order        | 3.66926             | 3.66844 |
| 2nd order        | 3.66827             | 3.66828 |
| 3rd order        | 3.66827             | 3.66828 |
| Exact            | 3.66828             |       |

TABLE V: Perturbation theory versus Padé interpolation: dominant linear potential, \( \gamma = 10 \). Columns two and three show respectively the results from standard perturbative calculations with the quadratic potential as the perturbation, and the corresponding estimates from Padé interpolation of \( H(\lambda) \), where the original kinetic energy term is distributed among the sub-Hamiltonians (15) and (16) in the ratio 9 : 1. The exact energies, obtained from numerically integrating the Schrödinger equation, are also displayed.

|                  | Perturbation Theory | Padé  |
|------------------|---------------------|-------|
| Ground state     |                     |       |
| 1st order        | 8.81152             | 8.80704 |
| 2nd order        | 8.80681             | 8.80706 |
| 3rd order        | 8.80708             | 8.80706 |
| Exact            | 8.80706             |       |
| First excited state |                 |       |
| 1st order        | 15.6650             | 15.6432 |
| 2nd order        | 15.6412             | 15.6431 |
| 3rd order        | 15.6433             | 15.6431 |
| Exact            | 15.6431             |       |
### TABLE VI: Comparisons similar to the last three columns in Table II except the original kinetic energy is distributed among the sub-Hamiltonians (15) and (16) in the ratios indicated.

| Ratio | 1st Order | 2nd Order | 3rd Order |
|-------|------------|------------|-----------|
| 1:9   | 3.64332    | 2.60113    | 2.54126   |
| 2:8   | -2.96766   | 2.52016    | 2.53730   |
| 3:7   | 33.5854    | 2.54173    | 2.53721   |

### TABLE VII: Comparisons similar to the last three columns in Table III except the original kinetic energy is distributed among the sub-Hamiltonians (15) and (16) in the ratios indicated.

| Ratio | 1st Order | 2nd Order | 3rd Order |
|-------|------------|------------|-----------|
| 1:9   | 6.62887    | 5.15343    | 5.10321   |
| 2:8   | -3.53137   | 5.09570    | 5.10468   |
| 3:7   | 80.5535    | 5.09344    | 5.10330   |

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