Padé Interpolation:

Methodology and Application to Quarkonium

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Abstract

A novel application of the Padé approximation is proposed in which the Padé approximant is used as an interpolation for the small and large coupling behaviors of a physical system, resulting in a prediction of the behavior of the system at intermediate couplings. This method is applied to quarkonium systems and reasonable values for the c and b quark masses are obtained.

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The Padé approximation seeks to approximate the behavior of a function, $f(x)$, by a ratio of two polynomials of x. This ratio is referred to as the Padé approximant. Compared to the usual perturbative power series approximation, the Padé approximant has the advantage that it deviates less rapidly from the true values of $f(x)$ as x becomes large. Recently, the Padé approximation has been applied to quantum field theories to estimate the next order term in a perturbation series [1]. The method involves calculating a certain physical quantity perturbatively to nth order in the coupling constant and then forming a Padé approximant which, when expanded in a power series of the coupling constant, reproduces the perturbative result. The $(n+1)$th order term in the expansion of the Padé approximant yields an estimate of the $(n+1)$th order term in the perturbation series for the physical quantity. It turns out one can obtain reasonably good estimates from this approach.

In this paper a different usage of the Padé approximation is proposed. We observe that, because of the nature of the Padé approximant, it can be expanded in a power series in x when x is small as well as in a power series in $\frac{1}{x}$ when x is large. It is therefore interesting to ask the question: in cases when both the small x (e.g., weak coupling) and the large x (e.g., strong coupling) behaviors of a theory can be computed perturbatively, is it possible to form a single Padé approximant which interpolates the weak and strong coupling behaviors, and if so, how well does this Padé interpolation approximate the behaviors of the theory at intermediate values of the coupling constant? This is a particularly timely question since, with the advance of duality in supersymmetric gauge theories [2], we may someday be able to compute the strong coupling behaviors of a theory from its dual theory. The Padé interpolation will then provide a means to estimate the behaviors of the theory for the entire range of the coupling constant.

The method proposed here goes beyond interpolating the strong and weak coupling behaviors of a system. For example, the expansion parameter x can be the temperature, the strength of an applied field, or, as discussed below in the application to heavy quarkonia, a parameter introduced to implement the Padé interpolation.

We have tested the Padé interpolation method with examples in which the exact result is

known, with encouraging success. To see how accurate the Padé interpolation can be and to illustrate the methodology involved, let us consider a simple quantum mechanical two-state system with the Hamiltonian,

$$H = \sigma_x + \lambda\sigma_z, \tag{1}$$

where the σ's are the Pauli matrices and the coupling constant λ is assumed to be positive. For $\lambda \ll 1$, the σ_z term may be treated as a perturbation and we find, to second order in perturbation theory, the eigenvalues of H are

$$E_{\pm}^{<} = \pm 1 \pm \frac{\lambda^2}{2}. \tag{2}$$

For $\lambda \gg 1$, the Hamiltonian can be written as $H = \lambda(\sigma_z + \frac{1}{\lambda}\sigma_x)$, and the σ_x term can be treated as a perturbation. We find, again to second order in perturbation theory, the eigenvalues of H are now

$$E_{\pm}^{>} = \pm\lambda \pm \frac{1}{2\lambda}. \tag{3}$$

A Padé approximant which interpolates the small and large λ behaviors of the energies can now be constructed. For the higher energy level E_+, we find

$$E_{+}^{(\mathrm{PA})} = \frac{\lambda^3 + \frac{3}{2}\lambda^2 + \frac{3}{2}\lambda + 1}{\lambda^2 + \frac{3}{2}\lambda + 1}. \tag{4}$$

This Padé approximant is uniquely determined from the perturbative expansions for E_+ given in (2) and (3). The large λ behavior indicates that the polynomial in the numerator must be one degree higher than the polynomial in the denominator and that the coefficient for the highest order term in λ must be the same for the two polynomials. Without loss of generality, we may choose this coefficient to be 1. If the numerator is a polynomial of degree d, there will be a total of $(2d-1)$ coefficients to be determined for the Padé approximant. Because the small λ behavior requires the numerator and the denominator to have the same constant (i.e., λ-independent) term, there are only $(2d-2)$ remaining coefficients to be determined. Expanding the Padé approximant and matching against the perturbation series in (2) and (3) provide an additional four conditions, which selects $d = 3$.

In Figure 1, the approximate result generated from Padé interpolation is compared with the exact result, $E_+ = \sqrt{\lambda^2 + 1}$. We see that the Padé approximant (open squares) tracks the exact result (solid curve) for all values of the coupling constant. In fact, $E_+^{(\mathrm{PA})}$ differs from E_+ by no more than about 1% for the entire range of λ. For example, for $\lambda = 0.5$, 1.0, 2.0, and 4.0, $E_+^{(\mathrm{PA})}$ is larger than E_+ by 0.63%, 1.02%, 0.62%, and 0.18%, respectively. One may improve the approximation by calculating more terms in the perturbation series for $E_+^<$ and $E_+^>$ and constructing the corresponding Padé approximant. However, our example suffices to demonstrate the potential power of the Padé interpolation method in that very few terms in the perturbation expansions can yield a very accurate approximation to the exact result for the entire range of the coupling constant.

For comparison, we have also plotted in Figure 1 the perturbative result for small λ, $E_+^<$ (dotted curve). As expected, it only agrees with the exact result for small values of λ and diverges significantly from the exact result when λ becomes large. Similarly, $E_+^>$ will diverge from the exact result for small λ. In contrast, by interpolating $E_+^<$ and $E_+^>$, the Padé approximant is constrained not to deviate too far from the exact result for the full range of the coupling constant. In this way, the Padé interpolation method can yield a very good approximation, provided the quantity we try to approximate is a smooth, continuous function of the coupling constant.

When applying the Padé interpolation, one should beware of potential unphysical singularities coming from the zeroes of the polynomial in the denominator of the Padé approximant. This complication may limit the scope of applicability of the method. On the other hand, this property may prove useful in some applications. For instance, when interpolating the high and low temperature behaviors of a system for which a phase transition takes place at some intermediate temperature, one may try to construct a Padé-like approximant (perhaps involving fractional powers in the polynomials) which mimics the singular behavior near the phase transition point.

Another way to implement the Padé interpolation method is in cases when the Hamiltonian can be expressed as $H = H_1 + H_2$, where the exact solutions for H_1 and H_2 (but not

H) are known. Introducing the interpolating Hamiltonian,

$$H(\beta) \equiv H_1 + \beta H_2, \tag{5}$$

where β is a positive constant, we can then treat H_2 as a perturbation when $\beta \ll 1$ and treat H_1 as a perturbation when $\beta \gg 1$, in exactly the same way as in the example (1). A Padé approximant is formed interpolating the perturbative results for large and small β. Finally, an approximate solution for the original Hamiltonian H is obtained by setting β equal 1 in the Padé approximant. This method will be applied below to calculate quarkonium spectra. Reasonable values for the c and b quark masses are obtained by fitting the calculated levels to their measured values, which demonstrates the legitimacy of this Padé interpolation approach.

Quarkonium refers to the bound state of a heavy quark Q (e.g., c or b quark) with its antiquark $\bar{Q}$. It is well known that such systems can be described reasonably well using nonrelativistic quantum mechanics [3]. Various potential energy functions have been used to model the $Q\bar{Q}$ interaction. It has been found that the potential description is flavor independent, i.e., the same potential describes equally well the $c\bar{c}$ and the $b\bar{b}$ systems. We consider here a central potential consisting of an attractive Coulomb term and a confining linear potential [4]:

$$V(r) = -\frac{\alpha}{r} + \lambda r, \tag{6}$$

where α and λ are positive coupling constants. We shall focus on the S states for the purpose of testing the proposed interpolation method. In this case, the Hamiltonian for the radial Schrödinger equation is simply

$$H_r = -\frac{1}{2\mu}\frac{d^2}{dr^2} - \frac{\alpha}{r} + \lambda r, \tag{7}$$

where μ is the reduced mass for the heavy quark Q, $\mu = m_Q/2$. Note that H_r can be expressed as the sum of two exactly solvable Hamiltonians: a Hamiltonian for the Coulomb potential,

$$H_C = -\frac{1}{4\mu}\frac{d^2}{dr^2} - \frac{\alpha}{r}, \tag{8}$$

and a Hamiltonian for the linear potential,

$$H_L = -\frac{1}{4\mu}\frac{d^2}{dr^2} + \lambda r. \tag{9}$$

We have split the kinetic energy term in half so that the "effective mass" that appears in H_C and in H_L is $2\mu = m_Q$.

We may now form the interpolating Hamiltonian, $H_r(\beta) = H_C + \beta H_L$, and perform perturbative calculations for small β as well as for large β. We shall summarize the results of our calculation here. Details of the calculation can be found in Ref. [5] where the calculation including the quarkonium P states is also discussed. (For the P states, the centrifugal pontential energy term, $\frac{l(l+1)}{2\mu r^2}$, should be included with H_C, resulting in a solvable "hydrogen-like" Hamiltonian. Because of the half kinetic energy term, care must be taken to redefine the orbital angular momentum quantum number in order to extract the energy eigenvalues.)

The bound state energies for the S states of $H_r(\beta)$ are computed for small β as well as for large β to the same order in perturbation theory. Wherever necessary (e.g., integrals involving the Airy functions, the eigenfunctions of H_L), terms in the perturbation series are evaluated numerically. In addition, for second and higher order calculations, the infinite series that appear in the perturbation expansions are estimated using the method of acceleration of convergence [6,5]. A separate Padé approximant is formed interpolating the small and large β results from our first, second, and third order calculations. Our estimates for the S state energies are obtained by letting β equal 1 in the respective Padé approximant. These are fitted to the corresponding measured values treating α, λ, m_c, m_b as well as the zero-point energies V_c (for charmonium) and V_b (for bottomonium) as free parameters. We used the data for the J/ψ(1S), J/ψ(2S), Υ(1S), Υ(2S), and Υ(3S) given in Ref. [7]. When performing the fit, care must be taken to avoid the artificial singularities of the Padé approximant.

The details of the fit results are presented in Table 1. We see that the first-order approximation already produces a rather good fit to the measured S-state energies, although

the best fit values for m_c and m_b are somewhat high. The second-order approximation improves the fit quality, reproducing all of the quarkonium S-levels. The fit quality, defined as $\sum_i \left(m_i^{(\text{experiment})} - m_i^{(\text{calculated})} \right)^2$, worsens (from less than 1 to 240) as we go to the third-order approximation, primarily due to the increased difficulty to avoid a larger number of unphysical singularities from the Padé approximant in performing the fit. Using the second-order results, our best fit values for m_c and m_b are 1.521 GeV and 5.046 GeV, respectively, to be compared with the values given in Ref. [7]: $m_c = 1.0$ to 1.6 GeV; $m_b = 4.1$ to 4.5 GeV. The best fit values for the parameters in the quarkonium potential (6), $\alpha = 0.4984$ and $\lambda = 0.1771$ GeV^2, also compare favorably with earlier results: $\alpha = 0.520$ and $\lambda = 0.183$ GeV^2 in Ref. [8]; $\alpha = 0.507$ and $\lambda = 0.169$ GeV^2 in Ref. [3].

We have also performed a fit with the constraint $V_b - V_c = 2(m_b - m_c)$ on the model parameters. The results are presented in Table 2. The fit quality in this case is comparable to that of the unconstrained fit and the best fit values of the model parameters differ somewhat from the best fit values of the unconstrained fit, indicating that the found minimum is not sharp and allows for some variation of the quark masses as long as their difference remains equal to half of the difference between the zero-point energies V_b and V_c. The model parameters appear to be more stable than before as we go from first to second-order Padé interpolation, which corroborates the physical significance of the constraint.

As a final check, we have integrated numerically the Schrödinger equation for the quarkonium systems with the second-order best fit values of the parameters to obtain the energy levels. The results are shown in the last column of Table 1. This verifies the validity of the Padé interpolation method.

In conclusion, using quarkonia and a simple two-state model as our testing grounds, we have shown that Padé interpolation can be a powerful method for estimating physical quantities at intermediate values of the coupling constant where perturbative calculations are not reliable. There are many areas for which this method may be applicable. One of which is the K-meson system. The strange quark mass, m_s, has the value such that neither chiral perturbation theory (for small quark masses) nor heavy quark effective theory (for large

quark masses) gives a good description of K-meson properties. With Padé interpolation we may be able to obtain a more accurate estimate of the K-meson properties by interpolating the small m_s and large m_s behaviors which can be obtained perturbatively through chiral perturbation theory and heavy quark effective theory, respectively. These issues are being examined by one of us and the results will be reported in the near future [9].

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Table 1. Fit results from Padé interpolation.

Enrgy level	Measured	1st order	2nd order	3rd order	Numerical
$J/\psi(1S)$ [MeV]	3097	3097	3097	3089	3097
$J/\psi(2S)$ [MeV]	3686	3686	3686	3694	3687
$\Upsilon(1S)$ [MeV]	9460	9459	9460	9464	9456
$\Upsilon(2S)$ [MeV]	10023	10026	10023	10028	10020
$\Upsilon(3S)$ [MeV]	10355	10353	10355	10347	10356
Fit quality [MeV^2]		13	< 1	240	
Fit parameters					
α		0.4600	0.4984	0.7510	0.4984
λ [GeV^2]		0.1834	0.1771	0.1344	0.1771
V_c [MeV]		2767	2765	2953	2765
V_b [MeV]		9573	9585	9761	9585
m_c [MeV]		1719	1521	1253	1521
m_b [MeV]		5538	5046	4143	5046

Table 2. Fit results from Padé interpolation with the constraint $V_b - V_c = 2(m_b - m_c)$.

Enrgy level	Measured	1st order	2nd order
$J/\psi(1S)$ [MeV]	3097	3097	3098
$J/\psi(2S)$ [MeV]	3686	3686	3685
$\Upsilon(1S)$ [MeV]	9460	9459	9460
$\Upsilon(2S)$ [MeV]	10023	10026	10022
$\Upsilon(3S)$ [MeV]	10355	10353	10356
Fit quality [MeV^2]		13	3
Fit parameters			
α		0.4850	0.4964
λ [GeV^2]		0.1741	0.1784
V_c [MeV]		2770	2773
V_b [MeV]		9571	9574
m_c [MeV]		1560	1572
m_b [MeV]		4960	4972

FIGURE CAPTION

Figure 1: see description in the text.