# Padé Interpolation

Physics 342 Final Project

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## I. Theory

In standard notation, for two non-negative integers m and n, a Padé approximant [m/n] of a function f(x) is an approximation of f(x) by a rational function R(x), where R(x)=P(x)/Q(x) for polynomials P(x) of order m and Q(x) of order n.

[m/n] ≡ R(x) is an approximation of f(x) in the sense that f(0) = R(0) and the derivatives of f(x) and R(x) at 0 are identical up to the (m+n)th derivative. So long as we take the constant value of Q(x) to be 1, [m/n] is uniquely defined by f(x) and we can explicitly write [m/n] as:

$$[m/n]=\frac{p_0+p_1x+p_2x^2+...+p_mx^m}{1+q_1x+q_2x^2+...+q_nx^n} \tag{1}$$

When n = 0, we simply recover the first m terms of the Taylor series of f(x) at 0:

$$[m/0]=p_0+p_1x+p_2x^2+...+p_mx^m=f(0)+f'(0)+\frac{f''(0)}{2!}x^2+...+\frac{f^{(m)}(0)}{m!}x^m \tag{2}$$

Padé approximants are in many cases better approximations of f(x) than a number of terms from its Taylor series and sometimes remain close to f(x) outside of the Taylor series's radius of convergence.

A more interesting use of Padé approximation is “two-point Padé approximation” or Padé interpolation in which a Padé approximant for f(x) is constructed from two truncated Taylor series: one for when x is very small and one is for when x is very large. The Padé approximant in this method interpolates between the values at which f(x) is known. This method is directly applicable to perturbation theory.

Assume that $H_1$ and $H_2$ are two Hamiltonians for which energy eigenvalues of stationary states are already known, and which may both be treated as perturbations. Say that we then want to find energy eigenvalues for the combined Hamiltonian H:

$$H=H_1+H_2 \tag{3}$$

We then introduce an interpolation parameter λ > 0 (eventually to be set equal to 1) to create an interpolation Hamiltonian H(λ):

$$H(\lambda)=H_1+\lambda H_2 \tag{4}$$

Suppose $\lambda << 1$. Then $H(\lambda)$ is dominated by $H_1$, and we can treat $H_2$ as a perturbation. In this case perturbation theory can be used to expand an energy eigenvalue of H as a power series in terms of $\lambda$, up to order m:

$$E^{\lambda \ll 1} = a_0 + a_1\lambda + a_2\lambda^2 + ... + a_m\lambda^m \tag{5}$$

Now instead suppose $\lambda >> 1$. Then $H(\lambda)$ is instead dominated by $H_2$, and in particular we rewrite eq.(4) by:

$$H(\lambda) = \lambda(H_2 + \frac{1}{\lambda}H_1) \tag{6}$$

Expanding an energy eigenvalue of the terms inside in the parentheses as a power series in terms of $(1/\lambda)$, up to order n, gives us:

$$E^{\lambda \gg 1} = \lambda(b_0 + b_1(\frac{1}{\lambda}) + b_2(\frac{1}{\lambda})^2 + ... + b_n(\frac{1}{\lambda})^n) \tag{7}$$

We then want to use a Padé approximant to interpolate between the values for large $\lambda$ and small $\lambda$ for $E(\lambda)$. While in practice any values of n and m may be used, with different values giving better or worse approximations, in the literature eqs.(5) and (7) are typically taken with n=m, i.e. both approximations are taken to the same order in perturbation theory. In this case, and provided $b_0 \neq 0$, the relevant Padé approximant is of the form:

$$E^{PA} = \frac{p_0 + p_1\lambda + p_2\lambda^2 + ... + p_{n+1}\lambda^{n+1}}{1 + q_1\lambda + q_2\lambda^2 + ... + q_n\lambda^n} \tag{8}$$

The 2n+2 unknowns $p_i$ and $q_i$ above correspond to the 2n+2 $a_j$ and $b_j$ from eqs.(5) and (7). The first set of equations relating the two come from taking the Taylor series of eq.(8) with respect to $\lambda$ and matching values term-by-term against eq.(5).

For the remaining equations, define $\beta = 1/\lambda$ note that:

$$E^{PA} = \frac{\beta^{n+1}}{\beta^{n+1}} E^{PA} = \frac{p_0\beta^{n+1} + p_1\beta^n + p_2\beta^{n-1} + ... + p_{n+1}}{\beta^{n+1} + q_1\beta^n + q_2\beta^{n-1} + ... + q_n\beta} \tag{9}$$

Taking the Taylor series of eq.(9) with respect to $\beta = 1/\lambda$ then matching values term-by-term against eq.(7) yields the remaining equations.

This method also works when $\lambda$ represents an actual continuous physical quantity, in which case eq.(8) is presumed to be a valid approximation of the energy eigenvalue of a state over all $\lambda$, provided the terms in the denominator do not result in an unphysical singularity, a problem discussed later.

## II. Simple Padé interpolation

As explained in [1], one of the simplest examples of Padé interpolation is given in the case of a Hamiltonian that is the sum of two Pauli matrices, such as

$$H = \sigma_x + \lambda \sigma_z \tag{10}$$

Up to some scaling constant such a Hamiltonian could physically represent, for example, the interaction of a particle in a magnetic field in the x and z directions. Briefly, treating this problem as explained up to second-order in perturbation theory yields energy eigenvalues of.

$$\lambda >> 1: \quad E = \pm 1 \pm \frac{\lambda^2}{2} \qquad \lambda << 1: \quad E = \pm\lambda \pm \frac{1}{2\lambda} \tag{11}$$

For the higher and lower energy eigenstates, one can expand eqs.(8) and (9) to get:

$$E_+ = \frac{1 + 3/2\,\lambda + 3/2\,\lambda^2 + \lambda^3}{1 + 3/2\,\lambda + \lambda^2} \qquad E_- = \frac{-1 - 3/2\,\lambda - 3/2\,\lambda^2 - \lambda^3}{1 + 3/2\,\lambda + \lambda^2} \tag{12}$$

Finally, for this problem, the exact solutions may easily be calculated as:

$$E_\pm = \pm\sqrt{1 + \lambda^2} \tag{13}$$

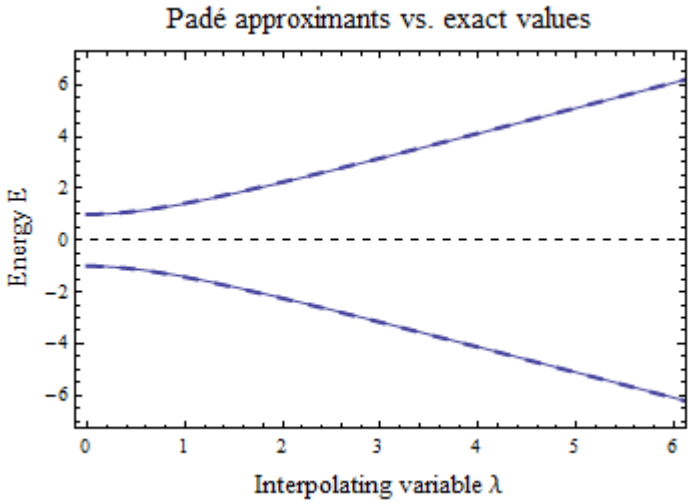


**Figure 1. Simple Padé interpolation**

Padé interpolation here provides an extremely accurate fit, with the approximations differing from the exact energy values by ~1% at most over all λ

## III. Padé interpolation for the Stark effect and shortcomings of method

A more interesting problem which appears nearly identical at first glance is one for which we already know the exact answer: the Stark effect for the $2S_{1/2}$ and $2P_{1/2}$ levels of hydrogen for an

electric field ε sufficiently weak that $e\varepsilon a_0$ is small compared to fine structure, and with the lamb shift δ taken into account (we solved this problem exactly and in the limits $e\varepsilon a_0 \ll \delta$ and $e\varepsilon a_0 \gg \delta$ in chapter 5, problem 13 of Sakurai). Defining $\alpha = 3ea_0$, the mixing between the two levels in the Stark effect can be shown to be described by the matrix H' defined as:

$$H' = \begin{pmatrix} \delta & \alpha\epsilon \\ \alpha\epsilon & 0 \end{pmatrix} \tag{14}$$

The exact eigenvalues for this problem are given by:

$$E = \frac{\delta}{2} \pm \sqrt{\frac{\delta^2}{4} + (\alpha\varepsilon)^2} \tag{15}$$

To try to approximate this solution using Padé interpolation, first note that we can write:

$$H' = \delta H_1 + \varepsilon H_2 \quad \text{for} \quad H_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad H_2 = \begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix} \tag{16}$$

In the limiting cases a) $\varepsilon \ll \delta$ and b) $\varepsilon \gg \delta$ we see:

$$\text{a)}\ \ H' = \delta\left(H_1 + \frac{\varepsilon}{\delta} H_2\right) \qquad \text{b)}\ \ H' = \varepsilon\left(H_2 + \frac{\delta}{\varepsilon} H_1\right) \tag{17}$$

In case a), we note $\delta H_1$ has eigenvalues $\lambda_{\varepsilon \ll \delta} = 0, \delta$, and that using these states to go up to second-order in perturbation theory, treating $(\varepsilon/\delta)H_2$ as a small perturbation then multiplying δ back in, yields second-order energy results for H' in terms of $(\varepsilon/\delta)$ of:

$$E_{\varepsilon \ll \delta} = -\delta a^2 \left(\frac{\varepsilon}{\delta}\right)^2, \delta + \delta a^2 \left(\frac{\varepsilon}{\delta}\right)^2 \tag{18}$$

In case b), we note $\varepsilon H_2$ has eigenvalues $\lambda_{\varepsilon \gg \delta} = \pm\alpha$, and that going to second-order in perturbation theory with $(\delta/\varepsilon)H_1$ yields result of:

$$\begin{aligned} E_{\varepsilon \gg \delta} &= \epsilon\left(a + \frac{1}{2}\frac{\delta}{\epsilon} + \frac{a}{2}\left(\frac{\delta}{\epsilon}\right)^2\right), \epsilon\left(-a + \frac{1}{2}\frac{\delta}{\epsilon} - \frac{a}{2}\left(\frac{\delta}{\epsilon}\right)^2\right) \\ &= \delta a \left(\frac{\delta}{\epsilon}\right)^{-1} + \frac{\delta}{2} + \frac{\delta a}{2}\left(\frac{\delta}{\epsilon}\right), -\delta a \left(\frac{\delta}{\epsilon}\right)^{-1} + \frac{\delta}{2} - \frac{\delta a}{2}\left(\frac{\delta}{\epsilon}\right) \end{aligned} \tag{19}$$

Note that eq.(18) and eq.(19) agree with our approximations of eq.(15) in Sakurai up to first order in δ. Furthermore the results from eq.(18) and eq.(19) allow us to calculate the Padé approximants in the form of eq.(8) for the two eigenvalues, with n = 2 and using $\lambda = E/\delta$.

In particular we find for the coefficients of the Padé approximant of the smaller eigenvalue, $E^-$:

(20) $$p_0=0 \quad p_1=0 \quad p_2=-\delta\alpha^2 \quad p_3=\frac{2\delta\alpha^3}{2\alpha^2-1} \quad q_1=\frac{2(\alpha^3-\alpha)}{2\alpha^2-1} \quad q_2=\frac{-2\alpha^2}{2\alpha^2-1}$$

And for the Padé approximant of the larger eigenvalue, $E^+$:

(21) $$p_0=\delta \quad p_1=\frac{2\delta(\alpha^3-\alpha)}{2\alpha^2-1} \quad p_2=\frac{\delta(2\alpha^4-3\alpha^2)}{2\alpha^2-1}$$
$$p_3=\frac{2\delta\alpha^3}{2\alpha^2-1} \quad q_1=\frac{2(\alpha^3-\alpha)}{2\alpha^2-1} \quad q_2=\frac{-2\alpha^2}{2\alpha^2-1}$$

The actual values of δ and α are largely irrelevant to our result, and we pick, for instance, δ=3, α=5 for graphing purposes, and plot the Padé approximants (dashed lines) against the exact results (solid lines) as functions of the field strength ε for small ε:

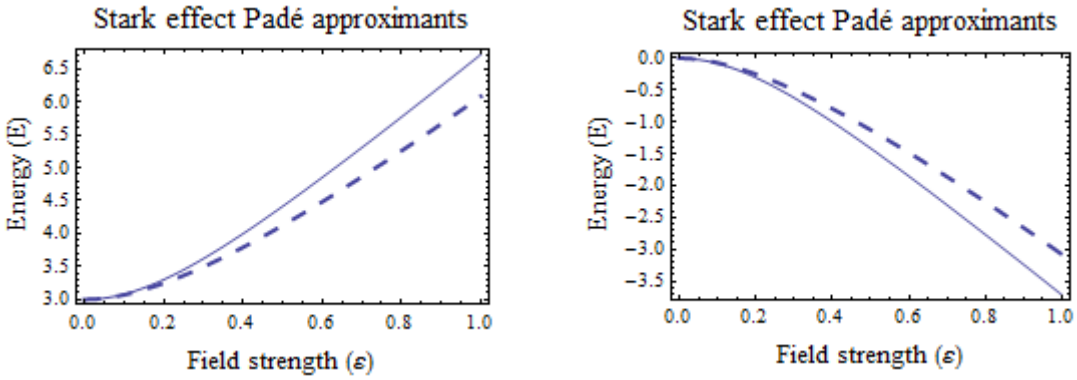


**Figure 2. Stark effect $2S_{1/2}$ and $2P_{1/2}$ weak field Padé approximants**

The Padé approximants here show good agreement with the exact values for very small ε, but quickly diverge significantly as ε grows larger, unlike in the previous example. However, by construction, the Padé approximants again rapidly converge to the exact values for large ε. The reason that the intermediate values don't match up well against the exact results is because the Padé approximants actually have singularities when ε=δα, as can be shown over a larger domain:

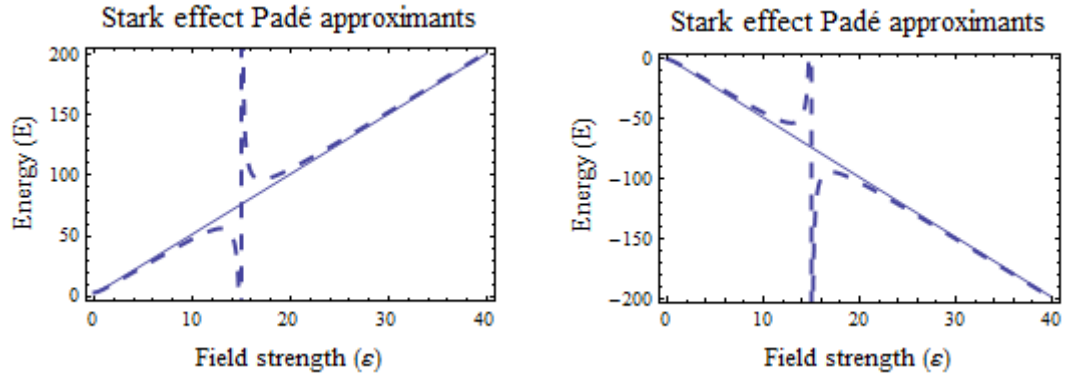


**Figure 3. Unphysical singularity in Stark effect Padé approximants**

In such cases, the fact that the Padé approximants eventually converge to the correct values (by ε=30, the Padé approximants are within 1% of the correct value) is of little consolation when they predict infinite energies at a seemingly arbitrary field strength. This result demonstrates one of the shortcomings of the Padé interpolation method: it is not possible in general to guarantee that the Padé approximant will have no unphysical singularities.

A glance at eq.(8) indicates that the problem may get worse as one uses higher and higher order results from perturbation theory, as a new singularity is potentially added each time one goes to the next highest order (unphysical unless the singularity occurs for a negative value of λ). In fact, this may often be the case; the fit quality of a result from Padé interpolation may improve as one goes to higher order in perturbation theory, but added unphysical singularities may cause it to rapidly diverge from the exact solution, at least in some small neighborhood (by construction it is guaranteed to converge to the correct result in the limit as λ goes to 0 or ∞).

**IV. Padé interpolation for the Zeeman effect**

Here we show an example of the use of Padé interpolation to somewhat less trivial problems. For that we will interpolate between the strong-field and weak-field Zeeman effects in the n=2 shell of the hydrogen atom. Our total Hamiltonian is:

$$H = H_0 + H_{fs} + B H_Z \tag{22}$$

Where $H_0$ represents the basic Hamiltonian for the hydrogen atom (containing only the kinetic energy and Coulomb potential terms), $H_{fs}$ represents the fine structure potential including relativistic corrections and spin-orbit coupling, and $BH_Z$ represents the potential for the Zeeman effect with the hydrogen atom in a uniform external magnetic field, where we define:

$$H_z = -(\vec{\mu}_l + \vec{\mu}_s)\cdot\left(\frac{\vec{B}_{ext}}{|B_{ext}|}\right) \quad , \quad B = |B_{ext}| \tag{23}$$

Suppose B is very small; then $BH_Z$ may be treated as a perturbation. Using n=2 and the quantum numbers *l*, j, and $m_j$, the energy eigenvalues of $H_0 + H_{fs}$, along with the first order perturbative correction due to $H_Z$, are given by:

$$E_{l\,j\,m_j} = \frac{-13.6\,eV}{4}\left[1 + \frac{\alpha^2}{4}\left(\frac{2}{j+1/2} - \frac{3}{4}\right)\right] + \mu_B g_J B\, m_j \tag{24}$$

Calculating the energies for the eight n=2 kets is trivial, and a table is reproduced below, where we use the convention (nearly the same as that of [3]) ε = -3.4 eV (the unperturbed energy of an n=2 state), $\gamma = |\varepsilon|\alpha^2/16$, and $\beta = \mu_B B$.

| State $\|l,j,m_j\rangle$ | Energy |
|---|---|
| $\|0,1/2,+1/2\rangle$ | $\varepsilon - 5\gamma + \beta$ |
| $\|0,1/2,-1/2\rangle$ | $\varepsilon - 5\gamma - \beta$ |
| $\|1,1/2,+1/2\rangle$ | $\varepsilon - 5\gamma + (1/3)\beta$ |
| $\|1,1/2,-1/2\rangle$ | $\varepsilon - 5\gamma - (1/3)\beta$ |
| $\|1,3/2,+3/2\rangle$ | $\varepsilon - \gamma + 2\beta$ |
| $\|1,3/2,+1/2\rangle$ | $\varepsilon - \gamma + (2/3)\beta$ |
| $\|1,3/2,-1/2\rangle$ | $\varepsilon - \gamma - (2/3)\beta$ |
| $\|1,3/2,-3/2\rangle$ | $\varepsilon - \gamma - 2\beta$ |

**Table 1. Energies for n=2 states in the weak-field Zeeman effect**

Suppose B is very large; then we may take $H_0 + BH_Z$ as the primary Hamiltonian and treat $B(1/B)H_{fs}$ as our perturbation. Using n=2 and the quantum numbers $l$, $m_l$, $m_s$, along with the first order pertubative correction due to $H_{fs}$, are given by (with the term in {} going to 1 for $l$=0):

$$E_{l\,m_l m_s} = \frac{-13.6\text{eV}}{4}\left[1 - \frac{\alpha^2}{2}\left(\frac{3}{8} - \left\{\frac{l(l+1) - m_l m_s}{l(l+1/2)(l+1)}\right\}\right)\right] + \mu_B B(m_l + 2m_s) \tag{25}$$

As above, we provide an energy level for the eight n=2 kets using the new quantum numbers:

| State $\|l,m_l,m_s\rangle$ | Energy |
|---|---|
| $\|0,0,+1/2\rangle$ | $\varepsilon - 5\gamma + \beta$ |
| $\|0,0,-1/2\rangle$ | $\varepsilon - 5\gamma - \beta$ |
| $\|1,+1,+1/2\rangle$ | $\varepsilon - \gamma + 2\beta$ |
| $\|1,+1,-1/2\rangle$ | $\varepsilon - (11/3)\gamma$ |
| $\|1,0,+1/2\rangle$ | $\varepsilon - (7/3)\gamma + \beta$ |
| $\|1,0,-1/2\rangle$ | $\varepsilon - (7/3)\gamma - \beta$ |
| $\|1,-1,+1/2\rangle$ | $\varepsilon - (11/3)\gamma$ |
| $\|1,-1,-1/2\rangle$ | $\varepsilon - \gamma - \beta$ |

**Table 2. Energies for n=2 states in the strong-field Zeeman effect**

Note that four energy values are repeated between Tables 1 and 2, specifically those for which $l$=0 or $|m_j| = 1/2$. In a sense these solutions are already "exact" for all B, at least up to first order in perturbation theory, thus Padé interpolation is unnecessary. The remaining four states mix, and it is not obvious which states from Table 1 connect to which states from Table 2 as B is increased, information we need to know for Padé interpolation to make sense.

In this case, we have an easy way out. Energy levels starting at points from the same y-intercept will not intersect under this potential as B is increased, and we may assume that one state which

eventually has slope 0 begins from each of the 2 y-intercepts from Table 1. This implies the states $|l{=}1,j{=}3/2,mj{=}{-}1/2\rangle$ and $|l{=}1,j{=}1/2,mj{=}{+}1/2\rangle$ connect to the states $|l,m_l,m_s\rangle$ with 0 slope in β, i.e. the two states with energy $\varepsilon - (11/3)\gamma$. By process of elimination the $|l{=}1,j{=}3/2,m_j{=}{+}1/2\rangle$ state connects to the $|l{=}1,m_l{=}0,m_s{=}{+}1/2\rangle$ state as B increases, and the $|l{=}1,j{=}1/2,m_j{=}{-}1/2\rangle$ state connects to the $|l{=}1,m_l{=}0,m_s{=}{-}1/2\rangle$ state as B increases. We have four sets of two points to interpolate between using Padé approximation.

First, we note that analytic solutions (in first-order perturbation theory) to these four sets are already known for all β, and are given in the following table (see [3]). These solutions will give us something to test the strength of our approximation against.

| State $\|l,j,m_j\rangle$ | Energy |
|---|---|
| $\|1,1/2,+1/2\rangle$ | $\varepsilon - 3\gamma + \beta/2 - \mathrm{sqrt}[4\gamma^2 + (2/3)\gamma\beta + \beta^2/4]$ |
| $\|1,1/2,-1/2\rangle$ | $\varepsilon - 3\gamma - \beta/2 - \mathrm{sqrt}[4\gamma^2 - (2/3)\gamma\beta + \beta^2/4]$ |
| $\|1,3/2,+1/2\rangle$ | $\varepsilon - 3\gamma + \beta/2 + \mathrm{sqrt}[4\gamma^2 + (2/3)\gamma\beta + \beta^2/4]$ |
| $\|1,3/2,-1/2\rangle$ | $\varepsilon - 3\gamma - \beta/2 + \mathrm{sqrt}[4\gamma^2 - (2/3)\gamma\beta + \beta^2/4]$ |

**Table 3. Energies for (non-linear with B) n=2 states in the Zeeman effect**

As an explicit example, consider the $|l{=}1,j{=}3/2,m_j{=}{+}1/2\rangle$ state. At low B it has energy $\varepsilon - \gamma + (2/3)\beta$, and as B increases it connects to a state with energy $\varepsilon - (7/3)\gamma + \beta$. As these are results from first-order perturbation theory, our Padé approximant looks like:

$$E = \frac{p_0 + p_1\beta + p_2\beta^2}{1 + q_1\beta} \tag{26}$$

We calculate:

$$p_0 = \epsilon - \gamma \qquad p_1 = \frac{3\epsilon + 5\gamma}{12\gamma} \qquad p_2 = \frac{1}{4\gamma} \qquad q_1 = \frac{1}{4\gamma} \tag{27}$$

This gives an extremely good fit, as shown on the next page. The solid curve is the analytic result from Table 3, the dashed curve is the result from Padé interpolation, and the dotted lines are the linear approximation results from Tables 1 and 2. The Padé variables for other three states are given below:

$$|l{=}1,j{=}3/2,m_j{=}{-}1/2\rangle: \quad p_0 = \epsilon - \gamma \qquad p_1 = \frac{3\epsilon - 11\gamma}{12\gamma} \qquad p_2 = 0 \qquad q_1 = \frac{1}{4\gamma}$$

$$|l{=}1,j{=}1/2,m_j{=}{+}1/2\rangle: \quad p_0 = \epsilon - 5\gamma \qquad p_1 = \frac{3\epsilon - 11\gamma}{12\gamma} \qquad p_2 = 0 \qquad q_1 = \frac{1}{4\gamma} \tag{28}$$

$$|l{=}1,j{=}1/2,m_j{=}{-}1/2\rangle: \quad p_0 = \epsilon - 5\gamma \qquad p_1 = \frac{3\epsilon - 13\gamma}{6\gamma} \qquad p_2 = \frac{-1}{2\gamma} \qquad q_1 = \frac{1}{2\gamma}$$

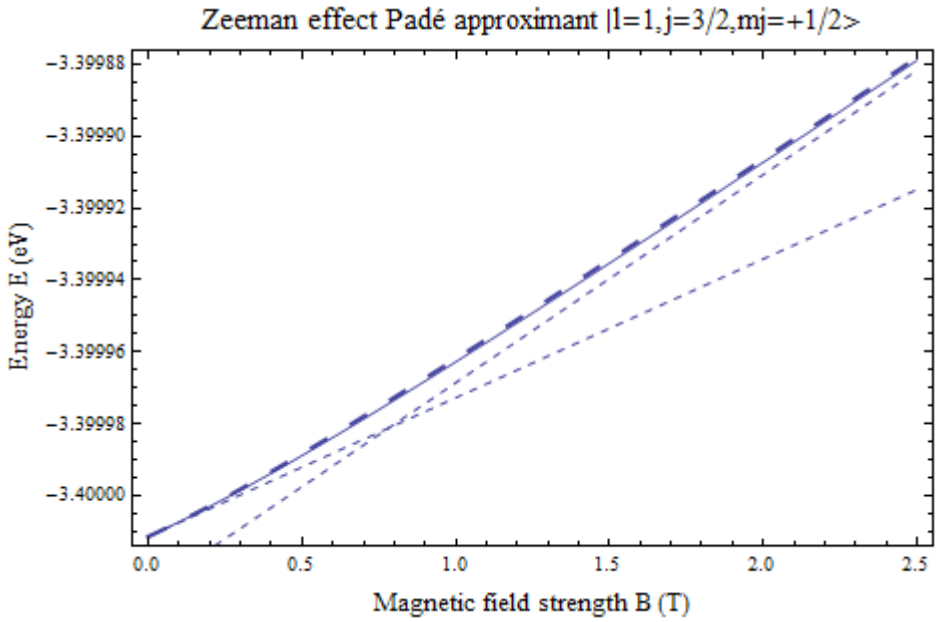


**Figure 4. Zeeman effect Padé approximant for $|l=1,j=3/2,m_j=+1/2\rangle$**

Padé interpolation in this case gives us a powerful fit, never more than 8.85 x $10^{-7}$ eV off the analytic result (reaching this point at about 1.43 T). Plotting all the approximations on the same graph also tells us that the strong-field Zeeman effect (Paschen-Back limit) requires extremely high external magnetic fields to be valid, stronger than 2 Tesla before its approximation begins to approach the analytic or Padé results.

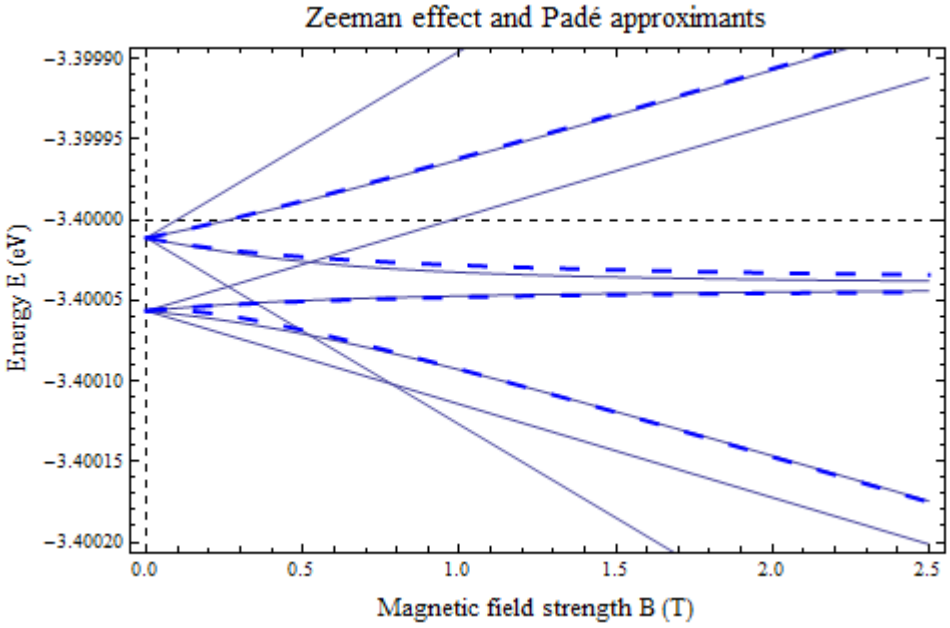


**Figure 5. Zeeman effect Padé approximants for states non-linear in B**

While these Padé approximants are not quite as good fits as the one in the explicit example, they still track the analytic values closely and the difference between their approximate and analytic

solution remains small compared to the differences in energy level between different states.

## V. Conclusions

Given a Hamiltonian with two components that may be treated perturbatively with an added interpolating variable, or a Hamiltonian which already contains a simple dependence on a physical variable that may be treated as the interpolating variable, Padé interpolation is an attractive feature because when successful it allows using a single formula to represent the results of approximations at different extremes which may even be valid in the intermediate region, as was the case with the Stark effect. Moreover, these results are possible even when going only to first-order in perturbation theory.

Furthermore, although the problems looked at here involved problems with known solutions to demonstrate the validity of the approach, it has applications to many other problems; for example, in [1], Leung and Murakowski use Padé interpolation to calculate quarkonium spectra from a simple potential and compare their findings against experimental values. In [1] and [2] Leung also uses a technique not discussed here in which the kinetic energy term of the Hamiltonian is split up between the sub-Hamiltonians (see eq.(4)) when each sub-Hamiltonian is exactly solvable, which may give more accurate results than the approach taken in the treatment of Zeeman effect above (giving all the kinetic energy to the term with the dominant potential).

That being said, Padé interpolation still has several problems that make it difficult to take advantage of. While first-order Padé interpolation may appear to be more powerful than first-order perturbation theory in a problem like the Zeeman effect because it works outside of just one limit, it only works as well as it does because it is guaranteed by construction to reduce to first-order perturbation theory in those limits. Standard perturbation theory at intermediate values, where it is possible (as in the analytic solutions for the Zeeman effect from [3]), will likely yield more accurate results where it is performed, even though it may be more difficult. Furthermore while in perturbation theory one can get progressively more accurate results by going to higher and higher order, in general Padé interpolation cannot be assumed to become more accurate as higher and higher order perturbative results are used due to the increased likelihood of unphysical singularities. Finally, Padé interpolation is only useful in problems where the different components of the Hamiltonian may actually be treated as perturbations; for example, Padé interpolation obviously should fail if one of the sub-Hamiltonians contains an infinite square-well potential.

When Padé interpolation does work, however, it typically gives surprisingly accurate results. Because of its potential for high accuracy and its general ease of use – the only extra work is solving a system of equations – Padé interpolation could be of great use in approximating and making predictions about the behavior of a complicated system with simple limiting cases.

## VI. References

[1] C.N. Leung and J.A. Murakowski, JMP 41, 2700-2705 (2000).
[2] C.N. Leung and Y.Y. Yvonne, Am.J.Phys. 70, 1020-1024 (2002).
[3] Griffiths, “Introduction to Quantum Mechanics 2nd Ed.,” 277-283 (2005).