Nonperturbative Quantum Physics from Low-Order Perturbation Theory

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The Stark effect in hydrogen and the cubic anharmonic oscillator furnish examples of quantum systems where the perturbation results in a certain ionization probability by tunneling processes. Accordingly, the perturbed ground-state energy is shifted and broadened, thus acquiring an imaginary part which is considered to be a paradigm of nonperturbative behavior. Here we demonstrate how the low order coefficients of a divergent perturbation series can be used to obtain excellent approximations to both real and imaginary parts of the perturbed ground state eigenenergy. The key is to use analytic continuation functions with a built-in singularity structure within the complex plane of the coupling constant, which is tailored by means of Bender-Wu dispersion relations. In the examples discussed the analytic continuation functions are Gauss hypergeometric functions, which take as input fourth order perturbation theory and return excellent approximations to the complex perturbed eigenvalue. These functions are Borel consistent and dramatically outperform widely used Padé and Borel-Padé approaches, even for rather large values of the coupling constant.

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Since the pioneering work of Dyson [1], the fundamental problem of how to reconstruct physical observables from divergent power-series expansions has remained an active area of research [2,3]. This problem has been encountered in virtually all areas of quantum physics, such as statistical [4–6], string [3], and quantum field theories [7–9], as well as in many-body problems of condensed matter physics [10,11] and quantum chemistry [12].

Simple examples can be found in single-particle quantum mechanics [2–4,9,13–17]. For instance, the perturbation expansion for the Stark Hamiltonian has zero radius of convergence [15–17]. The electronic ground state energy of hydrogen in a homogeneous electric field is shifted and broadened as the electric field intensity F increases. As a function of F, the perturbed ground state energy then has both a real part Δ and an imaginary part $\Gamma/2$, $E(F) = \Delta(F) - i\Gamma(F)/2$. The latter reflects the tunneling rate in and out of the Coulomb potential [18], which is very difficult to obtain perturbatively. To see this, let $f \equiv (F/4)^2$ and consider the perturbation expansion [16] for the ground state energy of hydrogen in powers of F around $F = 0$—we use atomic units (a.u.),

$$E(F) \sim -\frac{1}{2}\sum_{n=0}^{\infty} e_n f^n = -\frac{1}{2}(1 + 72f + 28\,440f^2 + 40\,204\,464f^3 + \cdots). \quad (1)$$

The same-sign expansion coefficients e_n are real and grow factorially with $2n$ and thus the series in Eq. (1) has zero radius of convergence. No matter how small F is, the series in Eq. (1) will never converge to $E(F)$, and so "$\sim$" is used in Eq. (1) to indicate that the rhs is an asymptotic expansion of the lhs. Furthermore, the rhs in Eq. (1) is real and therefore its partial sums cannot directly yield $-i\Gamma(F)/2$. Ultimately, the divergence of a perturbation expansion stems from the presence of singularities (poles and/or branch cuts) in $E(F)$ for complex F: the series in Eq. (1) diverges because $E(F)$ is not analytic at $F = 0$ which is a branch point. Physically the semidiscrete spectrum for $F = 0$ is replaced by a dense continuum of eigenvalues when $F \neq 0$; $E(F)$ is a complex resonance eigenvalue, characterizing the position (ReE) and width (ImE) of a peak in the density of states. To evaluate $E(F)$ for real F, it is necessary to approach the real F axis from above or below, corresponding to incoming or outgoing boundary conditions. The imaginary part of $E(F)$ discontinuously changes sign at Im$F = 0$.

Remarkably, accurate calculations of $\Gamma(F)$ have been achieved by a combining Eq. (1) with Borel-Padé (BP) resummation [17,19–21]. Often, for Stark-like problems these techniques require far too many coefficients for them to be reasonably accurate. Padé approximants (PAs) [22] and the techniques based on them—-such as BP—can account for poles in $E(F)$ but they are not well suited to mimic branch cuts, necessitating the calculation of very many coefficients. Resummation approaches that go beyond Padé remain virtually unknown by most users of perturbation theory: quadratic Padé approximants [23] are able to incorporate square-root branch cuts, but have been seldom used; modern resummation schemes that combine perturbation theory with large-order information [6] remain largely unexplored. Methods to reliably estimate quantities like $\Gamma(F)$ from low order perturbation theory are therefore badly needed: in practice one has available only low-order coefficients to work with.

These considerations lead us to the following question: Can we calculate $\Gamma(F)$ accurately with just a few coefficients? In this Letter, we demonstrate that low-order approximations can, paradoxically, reproduce nonperturbative quantities like $\Gamma(F)$ with excellent accuracy even for rather large values of the perturbation strength. This is achieved by using Bender-Wu dispersion relations [13] to guess the branch cut structure of $E(F)$, and designing approximants with the desired branch-cut structure "built in" and with flexible branch points. For the Stark problem the branch cut structure is indeed known from Bender-Wu dispersion relations [13]: $E(F)$ possesses branch points at $F = 0$ and $F \to \pm\infty$; hypergeometric functions are shown to well reproduce this double branch cut, yielding accurate low order approximations for Stark-like problems and showcasing an alternative approximating philosophy where knowledge of the convergence-limiting singularity structure in the complex-F plane is exploited to design accurate low order approximants.

Let us then start by trying to calculate $E(F)$ from Eq. (1). Traditionally, the first choice is to calculate PAs [22]. These are parametrized rational approximations, $E(F) \approx E_{L/M}(F)$, where $E_{L/M}(F) = (\sum_{n=0}^{L} p_n f^n)/(1 + \sum_{n=1}^{M} q_n f^n)$, and the parameters p_n and q_n are determined by equating each order up to $L + M = N$ in the Taylor and asymptotic series of $E_{L/M}(F)$ and $E(F)$, respectively, so that $E(F) = E_{L/M}(F) + O(f^{L+M+1})$. PAs and other similarly simple sequence transformations [24–26] are valuable tools for analytic continuation (AC), and can work well in many cases [27]. They provide a family of rational functions that are easily built order by order: the first-order PAs are $E_{1/0}$ and $E_{0/1}$; the second-order ones are $E_{2/0}$, $E_{0/2}$, and $E_{1/1}$; etc. By studying the resulting Padé table, one can in many cases extract good approximations to the expectation value of interest. However, by approximating $E(F)$ with a rational function of F, one is imposing an asymptotic behavior for large values of F which is in general not physical. Approximating $\Delta(F)$ can be difficult because the denominator in $E_{L/M}$ can vanish for specific values of the interaction strength. More importantly, $E_{L/M}(F)$ is a real number for real F, and therefore $\Gamma_{L/M}(F) = 0$; i.e., the standard PAs cannot work for our problem as they fail to give $\Gamma(F) \neq 0$ [17,19]. $\Gamma(F) \neq 0$ arises from evaluating $E(F)$ "on" the branch cut, where known sequence transformations fail [7,25,26]; such techniques are known to work well for a strictly alternating series [2,3] while the coefficients in Eq. (1) are all of the same sign.

Nevertheless, the idea behind PAs is general and it can be used to propose new approximations. For example, one can choose a parametrized analytic function $\mathcal{E}(F) = \mathcal{E}(\{h_i\}; F)$ to approximate $E(F)$, fixing the parameters $\{h_i\}$ so that the Taylor series for $\mathcal{E}(F)$ is equal to the asymptotic series of $E(F)$ up to the desired order—for an example, see Ref. [28]. Since here we are concerned with the determination of $\Gamma(F)$, we initially aimed for a function $\mathcal{E}(F)$ with the following desirable properties: (i) it is a complex function of real F, with the ability to mimic the branch cut structure discussed above; (ii) it can be built from low-order perturbation theory, as PAs are built; (iii) it is amenable to generalization by being a member of a more general family of "higher order" functions; and (iv) is itself general and flexible including many other functions as particular cases. A possible candidate satisfying all desirable properties (i)–(iv) is the Gauss hypergeometric function ${}_2F_1(h_1, h_2, h_3; h_4 f)$. It satisfies (i) and (ii) as it is complex and has a branch cut for $h_4 f > 1$, and it contains at most four parameters so it can be built from the coefficients e_{1-4}. It also satisfies condition (iii) because there are hypergeometric functions of higher order ${}_pF_q$ which generalize to the so-called Meijer-G function [29]. Finally, ${}_2F_1$ satisfies condition (iv) as it is well known that many functions are particular cases of ${}_2F_1$.

The Taylor series for ${}_2F_1$ is given by

$$ {}_2F_1(h_1, h_2, h_3; h_4 f) = \sum_{n=0}^{\infty} \frac{(h_1)_n (h_2)_n}{n!(h_3)_n} h_4^n f^n, \qquad (2) $$

where $(h_i)_n = h_i(h_i + 1)\cdots(h_i + n - 1)$. To obtain the h_i, one equates each order in the asymptotic series for $E(F)$ with the corresponding order in the Taylor series for $\mathcal{E}(F)$ to obtain a system of four equations with four unknowns

$$ e_n = \frac{(h_1)_n (h_2)_n h_4^n}{(h_3)_n n!}, \qquad 1 \leq n \leq 4. \qquad (3) $$

Once the coefficients h_i are determined, hypergeometric approximations $E(F) \approx \mathcal{E}(F)$ for, e.g., the Stark case can be constructed as

$$ \mathcal{E}(F) = -\frac{1}{2} {}_2F_1(h_1, h_2, h_3, h_4 f), \qquad (4) $$

where ${}_2F_1$ is evaluated "on the cut" by taking the limit as $\mathrm{Im}F \to \pm 0$, and choosing the sign so that $\mathrm{Im}E(F) < 0$ and $\Gamma > 0$, consistent with the usual outgoing-wave boundary conditions. We apply this scheme to three Hamiltonians from single-particle quantum mechanics, with divergent perturbation expansions: the Stark Hamiltonian, $\hat{H} = -\nabla^2/2 - 1/r + Fz$, with asymptotic series expansion described [16,17] by Eq. (1); the cubic one-dimensional anharmonic oscillator with real perturbation [30], $\hat{H} = -(\partial^2/\partial x^2)/2 + \lambda x^2/2 + Fx^3$, and imaginary perturbation [31,32], $\hat{H} = -(\partial^2/\partial x^2)/2 + \lambda x^2/2 + iFx^3$. Here, λ is the force constant taken as $1/4$ in the numerical analysis below. Furthermore, the perturbed ground-state eigenvalue has $\Gamma(F) \neq 0$ in the first two cases, while in the third case one has a $\mathcal{PT}$-symmetric [31,32] Hamiltonian with $\Gamma(F) = 0$. For simplicity, all equations are written assuming the Stark Hamiltonian problem. We stress that Eqs. (3) are nonlinear and multiple solutions are

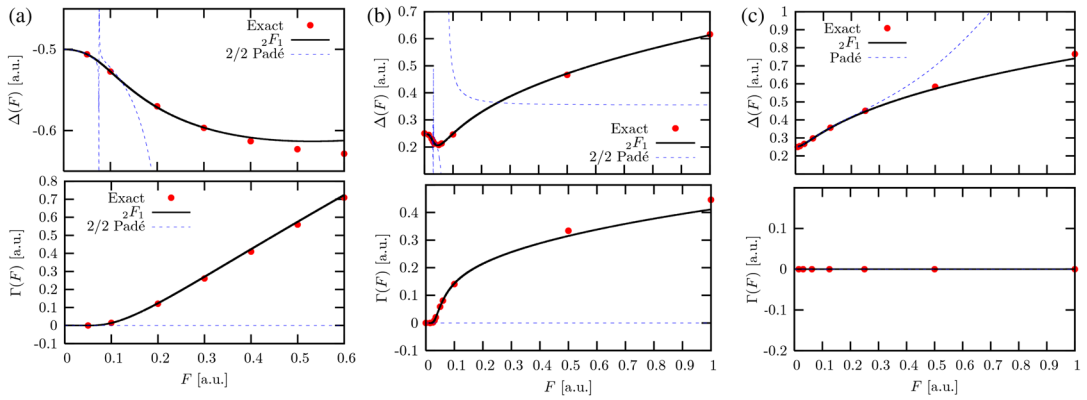

FIG. 1 (color online). Real $\Delta(F)$ and imaginary $\Gamma(F)$ part of the perturbed ground state energy of: (a) the Stark Hamiltonian as a function of the electric field strength F; (b) the anharmonic oscillator with real perturbation Fx^3; and (c) the anharmonic oscillator with imaginary perturbation iFx^3. We compare numerically exact values (dots) [30,31,34], with the fourth-order hypergeometric approximant ${}_2F_1$ (solid line) and Padé approximants (dashed line). In all three cases the ${}_2F_1$ approximant improves over Padé approximants [of the same-order in panels (a) and (b); and of much higher order in panel (c)] for the calculation of both $\Delta(F)$ and $\Gamma(F)$.

possible. For these examples, however, only two solutions are found (h_1, h_2, h_3, h_4) and (h_2, h_1, h_3, h_4), which correspond to the same hypergeometric function, as follows from Eq. (2). The numerical values of h_{1-4} obtained for the Stark problem are $h_1 \approx 0.319$, $h_2 \approx -0.162$, $h_3 \approx 118.193$, and $h_4 \approx 164961$ [33].

Figure 1 shows $\Delta(F)$ [top panels] and $\Gamma(F)$ [bottom panels] as a function of F for these three Hamiltonians. In Fig. 1(a), values of $\Delta(F)$ and $\Gamma(F)$ are shown for the Stark Hamiltonian. Exact results taken from Ref. [34] are compared with those calculated using the simple hypergeometric approximant ${}_2F_1$ and the same-order $2/2$ Padé approximant. The simple ${}_2F_1$ approximant introduced here provides excellent approximations to both $\Delta(F)$ and $\Gamma(F)$, while the $2/2$ Padé approximant fails to approximate either quantity. In Fig. 1(b) a similar comparison is made for the cubic anharmonic oscillator with real perturbation, taking the exact numerical values from Ref. [30]. Once again the ${}_2F_1$ approximant dramatically outperforms the $2/2$ Padé approximant. Finally, in Fig. 1(c) we see the results obtained from the cubic anharmonic oscillator with imaginary perturbation. In this case, both Padé and exact results are taken from Ref. [31]. The Padé results have been obtained in Ref. [31] by means of a Cesaro sum of the energies obtained from the $22/22$ and $22/23$ Padé approximants. Figure 1(c) shows that ${}_2F_1$ outperforms large-order Padé $(N = 44)$ for the calculation of $\Delta(F)$, and they both reproduce the exact value of $\Gamma(F) = 0$. Therefore, the hypergeometric approximant offers an excellent fourth-order approximation, likely to outperform Padé approximants of much higher order. Note that a single hypergeometric approximant yields the results shown in Figs. 1(b) and 1(c), just by replacing F by iF.

A comparison between the hypergeometric approximant and PAs is admittedly not very fair. To obtain $\Gamma(F) \neq 0$ from PAs, the standard procedure [17] thus far has been to employ the BP method [2]. In this method, one starts from a large number of coefficients e_n and evaluates the Borel-transformed coefficients $b_n = e_n/n!$, which are then employed to calculate PAs $B_{L/M}(f)$ and Laplace transforms $\mathcal{F}_{L/M}(f) = \int_0^\infty dt B_{L/M}(ft)e^{-t}$, leading to the BP approximation, $E(F) \approx -\frac{1}{2}\mathcal{F}_{L/M}(f)$. The Borel method removes $n!$ from the coefficients, sums the transformed series, and puts $n!$ back into the series by means of the Laplace transform. The essence of the BP method [2] is to perform AC on the Borel transformed coefficients and use the resulting analytic function to evaluate the Laplace transform. While the BP method allows accurate calculations of $\Gamma(F)$ from the perturbation series, it also requires [17] very large orders of perturbation theory that are unavailable in practice.

In the BP method, the analytic function is a PA. In the same spirit, we use hypergeometric functions as analytic functions to construct the Borel-hypergeometric method, by performing hypergeometric AC of the Borel-transformed series, calculating the h_i coefficients that define the hypergeometric function ${}_2F_1(h_1, h_2, h_3; h_4 f)$ from $e_n/n!$. The Borel-hypergeometric approximation, $E(F) \approx \mathcal{E}(F)$, is then

$$\mathcal{E}(F) \approx -\frac{\alpha}{2}\int_0^\infty dt e^{-\alpha t}\,{}_2F_1(h_1, h_2, h_3, \alpha h_4 f t), \qquad (5)$$

and $\alpha = \sqrt{i}$ specifies the integration contour [17]. An expression somewhat similar to Eq. (5) was used in Ref. [6] as the starting point to construct convergent strong-coupling expansions, while requiring the knowledge of both $e_{n\to\infty}$ and $E(F \to \infty)$.

We now apply the Borel-hypergeometric method to approximate $\Delta(F)$ and $\Gamma(F)$ for the same three Hamiltonians studied in Fig. 1. Figure 2 demonstrates that in all three problems considered the Borel-hypergeometric

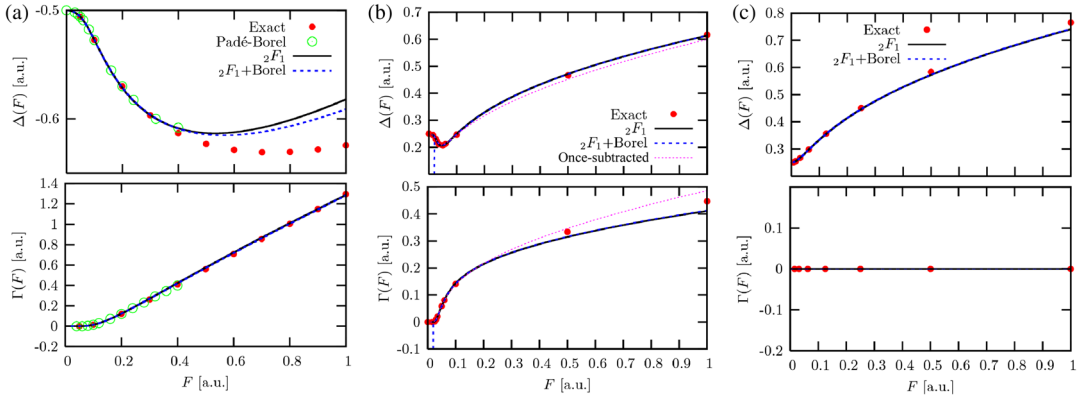

FIG. 2 (color online). Panels (a)–(c) are as in Fig. 1, but calculated using the fourth-order hypergeometric approximant $_2F_1$ (solid line), Borel-hypergeometric method (dashed line) in Eq. (5), and the numerically exact values taken from the literature (filled dots) [30,31,34]. In panel (a) we also show the Padé-Borel results (empty dots) from Ref. [17]. The Borel-hypergeometric and hypergeometric methods are in excellent agreement, both yielding excellent approximations to both $\Delta(F)$ and $\Gamma(F)$ in all three cases.

method gives excellent approximations to both $\Delta(F)$ and $\Gamma(F)$, and reproduces the results given by the hypergeometric approximant. Comparing Borel-hypergeometric and hypergeometric approximants reveals that the hypergeometric approximant is *Borel consistent* to a very good approximation. It is well known that a convergent sum and its Borel resummation give the same result. The hypergeometric approximations discussed here satisfy this desirable property to a good approximation. We note that in Fig. 2(b) the Borel-hypergeometric sum diverges for very small F. This is not a problem since the simple hypergeometric approximant is already well behaved for $F \to 0$. Alternatively, one can calculate one extra order of perturbation theory and build the Borel-hypergeometric approximant from the coefficients of the once-subtracted series, $[E(F) - E(0)]/(e_1 f)$. As shown in Fig. 2(b) that procedure mitigates this minor problem, while leading to similarly accurate overall results.

We emphasize that the hypergeometric and Borel-hypergeometric approaches are fourth-order approximations and thus much simpler and less expensive than the widely used BP method [2], while being of comparable accuracy. For instance, in the case of the Stark Hamiltonian with $F = 0.4$ a.u., some 70 orders of perturbation theory were required in Ref. [17] by the BP scheme to produce $E(F = 0.4) = -0.608 - 0.200i$, which can be contrasted with our result $\mathcal{E}(F = 0.4) = -0.609 - 0.212i$, and with numerically exact data [34] $\mathcal{E}(F = 0.4) = -0.613 - 0.205i$. For the Stark Hamiltonian, $F = 0.4$ a.u. $\simeq 2 \times 10^3$ MV cm^{-1} corresponds to a rather large electric field. We have also checked (data not shown) that $_2F_1$ performs better than fifth-order quadratic PAs.

It is easy to understand why the hypergeometric and Borel-hypergeometric method dramatically outperform the traditional BP method [2]. To obtain $\Gamma(F) \neq 0$ one needs approximants with a branch cut in the complex F plane with branch points at $F = 0$ and $F = \pm\infty$ [13,19]. Padé approximants typically have both poles and zeros on the real F axis, thereby lacking the correct analytic structure of $E(F)$ that is essential for rapid convergence. The function $_2F_1(h_1, h_2, h_3; h_4 f)$ has a branch cut running from $h_4 f = 1$ to $h_4 f = \infty$. When calculating $\{h_i\}$ from the low-order coefficients $e_1, \ldots, e_4$, we typically obtain a large value for h_4, thus mimicking the correct branch cut structure in $E(F)$, as illustrated in Fig. 3. We note that the tip of the cut is not exactly positioned, but for the examples considered this poses no real problems as h_4 is very large and Γ is extremely small. Nevertheless, hypergeometric approximants with exactly positioned cuts are possible and might be needed in some cases [35].

Our study illustrates the potentially immense advantages of supplementing the low-order information with an AC function able to mimic the convergence-limiting singularity structure on $E(F)$. The approach here could have applications in nonequilibrium many-body perturbation theory [36] for condensed matter systems where partial resummations are often used [37–41]. Such approximations are

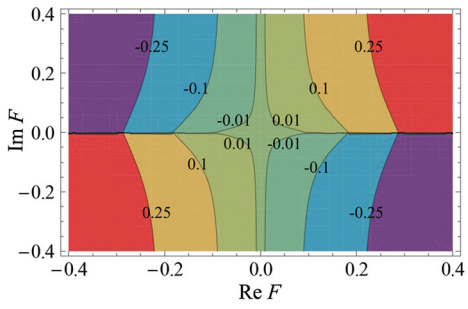

FIG. 3 (color online). Imaginary part of $_2F_1(h_1, h_2, h_3, h_4 f)$ calculated for the Stark Hamiltonian in the complex F plane. The built-in branch cut extends from $(h_4)^{-1}$ to ∞, and is essential to obtain $\Gamma(F) \neq 0$. The h_i are determined from the first four coefficients of the perturbation expansion. These yield $h_4 \approx 164961$.

uncontrolled because an error is "summed" to all orders (starting from second order) [27,41]. An alternative could be to build exact diagrammatic series—including vertex corrections—at low orders [10,11], and then use a suitable AC technique. In Ref. [42] the approach put forward in this Letter has been used to obtain the critical exponents for the two-dimensional Bose-Hubbard model. Our results should encourage interested readers to explore perturbation theory beyond the second order, to study the analytic structure in the complex coupling-constant plane and to try hypergeometric functions as approximants.

In conclusion, by analogy with traditional Padé and Borel-Padé techniques we have developed a fourth-order hypergeometric approximant and its natural Borel extension which are able to mimic convergence-limiting branch cuts, evade the calculation of a large number of coefficients, and dramatically outperform standard Padé and Borel-Padé approaches. Nonperturbative physics can be obtained from the low-order coefficients of a divergent perturbation series, as long as a carefully tailored analytic continuation technique is implemented.

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