Energy calculations of low-$|m|$ diamagnetic hydrogen states with dimensional perturbation theory

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In a previous article [J. R. Walkup, M. Dunn, and D. K. Watson, Phys. Rev. A **58**, 4668 (1998)] dimensional perturbation theory (DPT) was applied to circular Rydberg states of diamagnetic hydrogen to investigate avoided crossings in its energy spectrum as both the field strength and magnetic quantum number m were swept. Because the DPT perturbation parameter $\delta=1/(D+2|m|+1)$, where D is the dimensionality of the system, is inversely related to m, one might assume that for a given field strength DPT would be effective only when m is large. However, the field-strength expression used in DPT is scaled as a function of m, so it is not obvious *a priori* whether the effectiveness of DPT diminishes when m is significantly reduced for a given *physical* field strength. It is shown that for many states of diamagnetic hydrogen DPT can still produce strongly convergent and accurate energy values when m is small, even when $m=0$ ($\delta=1/2$). For those regions where even Padé summation failed to converge adequately, a technique is presented based on economized rational approximants.

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I. INTRODUCTION

The diamagnetic hydrogen problem has been widely studied since it has direct applications in such fields as astrophysics, quantum chaos, and solid-state physics [1]. The energy levels of diamagnetic hydrogen have been calculated by many authors [2–8]. Starace and Webster [3] calculated rigorous upper and lower bounds for low-lying states using an adiabatic approximation for fields below 10^5 T. This work was extended to fields above 10^5 T by Liu and Starace [4]. Rösner and colleagues [5] calculated the energy values of diamagnetic hydrogen for many low-lying states below 10^8 T. Later, Shertzer, Ram-Mohan, and Dossa calculated highly accurate lower bounds on the binding energies of the ground state [6] and lowest-lying excited states [7]. More recently, Ruder and colleagues calculated, among other things, low-lying energy levels of states corresponding to magnetic quantum numbers $m\leqslant 4$, which appear to be the most accurate and extensive to date [8].

II. DIMENSIONAL PERTURBATION THEORY

Dimensional perturbation theory [9] (DPT) has recently been applied to the diamagnetic hydrogen problem [10], and has been shown to be especially effective for circular (and near-circular) Rydberg states [11,12], which are highly excited states having maximal values of m for each principal quantum number n. In a previous article, we used DPT to plot energy levels appearing in the energy spectrum as both the field strength β and magnetic quantum number m were swept independently [10]. A significant advantage of DPT is that the field strength is incorporated into the zeroth-order Hamiltonian so that the zeroth-order wave functions automatically adapt as the magnetic-field strength changes. This adaptation is sensitive to the interplay between the Coulombic and diamagnetic potentials. Therefore, DPT does not require a switch in basis as the field strength sweeps from the low-field to the high-field region.

With dimensional perturbation theory, the diamagnetic hydrogen Hamiltonian is generalized to an arbitrary dimension D and the physical parameters scaled as functions of

TABLE I. Strong convergence of partial sums S_N and Padé approximants $P_{m,k}$ for the ground state and lowest-lying $m=-2$ state ($3d_{-2}$) energies (in a.u.) of diamagnetic hydrogen at $\beta=10^{-3}$ (470 T). All four states were chosen because they are examples of circular states. The Padé approximants belong to the diagonal sequence, so $m=k=N/2$. The energy values E_{RWHG} of Ruder *et al.* [8] are tabulated at the bottom.

	m							
	0 ($1s$)		-2 ($3d$)		-4 ($5g$)		-24 ($n=25$)	
N	S_N	$P_{m,k}$	S_N	$P_{m,k}$	S_N	$P_{m,k}$	S_N	$P_{m,k}$
0	1.001 999	1.001 998	0.117 030 2	0.117 003 2	0.049 384 3	0.049 266 3	0.013 076 08	0.013 076 08
1	1.001 998		0.117 003 2		0.049 265 2		0.012 732 43	
2	1.001 998	1.001 998	0.117 003 3	0.117 003 3	0.049 266 3	0.049 266 3	0.012 743 33	0.012 743 00
3	1.001 998		0.117 003 3		0.049 266 3		0.012 742 98	
4	1.001 998	1.001 998	0.117 003 3	0.117 003 3	0.049 266 3	0.049 266 3	0.012 742 99	0.012 742 99
E_{RWHG}	1.001 998		0.117 003 3		0.049 266 3		(none given)	

TABLE II. The first six excited states of the $m=0$ manifold. Again, $\beta=10^{-3}$ (470 T). Since the partial sums diverge for these states, only the Padé approximants $P_{m,k}$ are listed.

$[m/k]$	$2s_0$	$3d_0$	$3s_0$	$4d_0$	$4s_0$	$5g_0$
[0/0]	1.001 999 0	1.001 999 0	1.001 999 0	1.001 999 00	1.001 999 00	1.001 999 00
[1/1]	0.201 991 8	0.001 994 9	0.000 989 1	−0.088 916 64	−0.088 921 33	−0.140 862 85
[2/2]	0.251 980 7	0.113 095 8	0.113 069 0	0.064 470 38	0.064 440 02	0.041 976 63
[3/3]	0.251 972 9	0.113 040 6	0.112 270 9	0.064 832 87	0.064 682 43	0.042 055 45
[4/4]	0.251 972 0	0.113 071 0	0.112 964 8	0.064 367 96	0.064 170 57	0.041 889 74
[5/5]	0.251 972 0	0.113 069 7	0.112 954 5	0.064 351 24	0.063 968 09	0.041 751 91
[6/6]	0.251 972 0	0.113 069 8	0.112 954 8	0.064 351 78	0.063 981 37	0.041 773 65
[7/7]	0.251 972 0	0.113 069 8	0.112 954 7	0.064 351 89	0.063 981 27	0.041 777 46
[8/8]	0.251 972 0	0.113 069 8	0.112 954 7	0.064 351 67	0.063 981 70	0.041 775 53
E_{RWHG}	0.251 972 0	0.113 069 8	0.112 954 7	0.064 351 66	0.063 981 70	0.041 776 04

$\delta\equiv(D+2|m|+1)^{-1}$. (See Ref. [9].) Most importantly for the purpose of this report, the physical field strength β is scaled as

$$\tilde{B}=\beta/\delta^3, \tag{1}$$

where β is expressed in units of 4.7×10^5 T. It is also important to note that $\tilde{B}$ is m dependent. The eigensolutions of the resulting Hamiltonian are then expanded in a perturbation series about the infinite-dimensional limit, with δ as the perturbation parameter. The infinite-dimensional limit is essentially a static potential problem, since in this limit the derivative terms of the kinetic energy drop out of the Hamiltonian and the electron becomes localized at the bottom of an effective potential that is symmetric about the z axis. Therefore, DPT is highly effective for circular and near-circular states because the symmetry of the wave functions and the large-dimensional effective potential about the z axis are much the same.

III. ENERGY CALCULATIONS AT LOW $|m|$

Since all m dependence for a given $\tilde{B}$ is incorporated into a perturbation parameter that varies inversely with $|m|$, it is no surprise that DPT is especially effective for large values of $|m|$ [9,13]. However, this principle applies only when comparing states having the same *scaled* field strength $\tilde{B}$. For a fixed *physical* field strength β the perturbation series coefficients corresponding to lower values of $|m|$ are, in general, smaller than those corresponding to larger values of $|m|$. Therefore, despite the fact that the perturbation parameter is increasing in value, it is not obvious whether the perturbation

TABLE III. Energy levels for $|m|=0$ at various field strengths. The energies of Ruder *et al.* [8] are given in parentheses. To the left of each value the summation method is noted, with straight summation denoted S_N, Padé summation $P_{m,k}$, and optimized economized rational approximants $C_{m,k}^{\alpha_0}$, where α_0 and the optimization method are described in the Appendix. The indices indicate the minimum order at which convergence was achieved. Padé summation was used once partial summation failed to converge to seven significant figures by 50th order (quadruple precision). Similarly, the optimization method was used once Padé summation failed to converge to seven significant figures by the same order. (For practical reasons optimization was always performed using the largest-ordered economized rational approximant available, in this case $C_{25,25}$, given the limited number of power series coefficients at hand.) For a discussion of the precision of the results found using optimized ERAs, see Sec. III.

β	$1s_0/\|000\rangle$[a]		$2s_0/\|002\rangle$		$3d_0/\|004\rangle$[b]	
5×10^{-4}	S_1	1.001 000 (1.000 999)	$P_{4,4}$	0.250 993 0 (0.250 993 0)	$P_{5,5}$	0.112 100 8 (0.112 100 8)
5×10^{-3}	S_2	1.009 950 (1.009 950)	$P_{6,6}$	0.259 303 1 (0.259 303 1)	$P_{9,9}$	0.120 095 8 (0.120 095 8)
5×10^{-2}	S_5	1.095 053 (1.095 053)	$P_{12,12}$	0.296 149 4 (0.296 178 3)	$C_{25,25}^{(0.0407)}$	0.150 098 3 (0.149 876 0)
5×10^{-1}	$P_{4,4}$	1.662 338 (1.662 338)		Not found[c] (0.320 937 9)		Not found[c] (0.132 02)
5	$P_{10,10}$	3.495 594 (3.495 594)	$C_{25,25}^{(0.059)}$	0.417 897 9 (0.417 77)		Not found[c] (0.154 286)
50	$P_{16,16}$	7.579 610 (7.578 1)	$C_{25,25}^{(0.051)}$	0.512 045 7 (0.512 339)	$C_{25,25}^{(0.0387)}$	0.174 946 1 (0.173 767 9)
500	$P_{21,21}$	15.324 82 (15.324 1)	$C_{25,25}^{(0.041)}$	0.577 280 0 (0.591 709 9)	$C_{25,25}^{(0.0498)}$	0.197 533 5 (0.188 704 7)

[a]The asymptotic large-field state has the form $|nm\nu\rangle$, where n and m are the principal and magnetic quantum numbers and ν counts the number of nodes along the field axis. See Ref. [8], Sec. 3.1.2.

[b]For this state, Ruder *et al.* used a linear combination of the $3d_0$ and $3s_0$ states as their initial state. On the other hand, all initial states in this research were pure states.

[c]At this field strength neither Padé approximants nor optimized ERAs successfully converge. This does not appear to be due to a limitation of optimized ERAs, but rather to a limitation of the nondegenerate perturbation series evaluated at a finite number of decimal places. We think that the method of almost-degenerate perturbation theory will greatly improve the results. This is an avenue of future investigation.

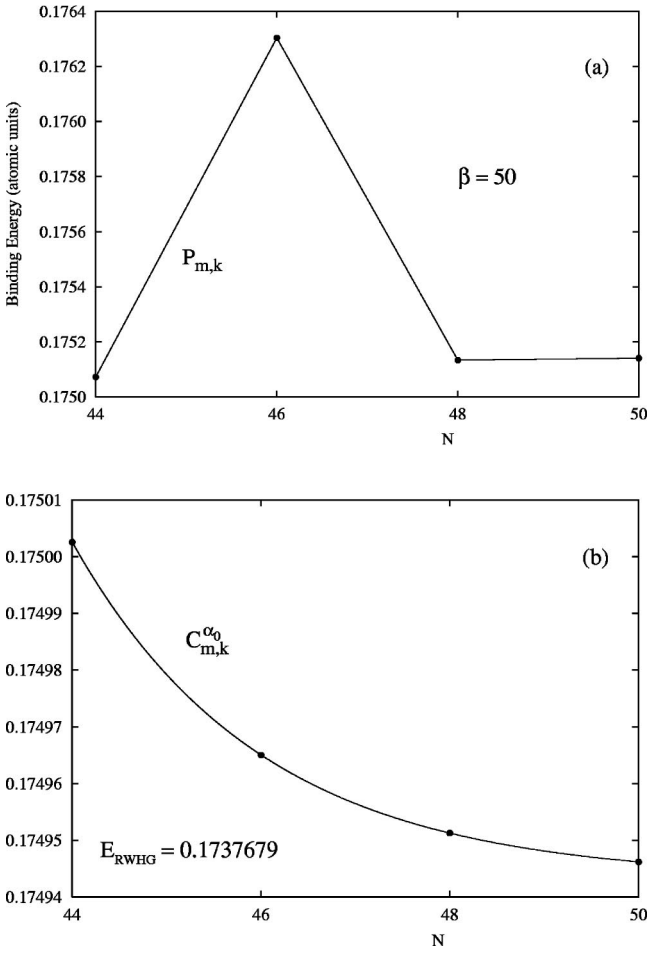

FIG. 1. One of the more dramatic improvements in convergence between (a) Padé approximants $P_{m,k}$ and (b) optimized ERAs $C_{m,k}^{\alpha_0}(\alpha=0.0387)$ for the $|004\rangle$ diamagnetic hydrogen state at $\beta=50$. Note the change in vertical scaling between the two figures. The erratic behavior in the $P_{23,23}$ Padé approximant is caused by a pole and zero that appear on the complex δ plane near the summation point $\delta=1/2$. Optimization appears to spread the poles and zeros out so that they are, on average, a maximum distance away from the summation point. For the optimized ERAs the fit between the exponential line and the ERA sequence is given by $R^2=0.999\,999\,999\,5$, where R is the coefficient of determination and $R=1$ corresponds to a perfect fit. (See Ref. [18].) The energy value of Ruder *et al.* [8] is $E_{\mathrm{RWHG}}=0.173\,767\,9$.

series would sum more effectively at lower $|m|$ [14].

Although circular Rydberg states are useful because they provide insight into the theoretical framework of Rydberg atoms at laboratory-accessible values of β, they are difficult to prepare experimentally because they require multiphotonic excitations in the dipole approximation [12]. Therefore it is necessary to determine whether the effectiveness of DPT extends to the more accessible low-$|m|$ states. In Table I we show that not only does DPT remain effective as m is reduced for fixed β, *but that its effectiveness slightly improves*. For example, at this field strength the partial sums and Padé approximants for the $1s_0$ and $3d_{-2}$ states actually converge to 12 significant figures by second order. For the same field strength the convergence at $|m|=24$ was roughly seven digits by fourth order.

Excited states (in terms of their principal quantum number n) are ''more elliptical'' when m is small, so we would expect DPT to be effective for a smaller number of states at low values of $|m|$. However, in Table II we show that, even for $|m|=0$, at sufficiently low field strengths DPT remains effective for highly noncircular states. Note from Fig. A1.2a in Ref. [8] that the field strength represented in the table is just below the region of significant n mixing of states.

In Table III we show that the DPT perturbation series for diamagnetic hydrogen can be summed quite effectively for $m=0$ for most values of β, especially for smaller field strengths [15]. (Note that all energy calculations in this research are evaluated at $D=3$.) In the large-field region, the perturbation series often fails to converge even using Padé approximants [16]. However, the sequence of Padé approximants can be economized [17,18] into a new sequence of approximants (economized rational approximants, hereafter denoted ERAs) which can be *optimized* by adjusting a variable parameter to minimize the error for particular values of the physical parameters β and $|m|$. As seen in Table III, the values of these optimized ERAs provide reasonably accurate energy values, even when the original Padé approximants fail to converge. (See the Appendix and Ref. [19].)

Finally, we note that the precision of the Padé approximants in Table III is defined by the number of digits that agree with the next-lowest-ordered approximant, whereas the precision of the optimized ERAs depends largely on the fit of the ERA sequence to an exponential line (as explained in the Appendix). It is difficult, therefore, to compare the precision of these two methods, so the results found using optimized ERAs were expressed using seven significant figures in all cases.

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APPENDIX

In this research there are instances where Padé approximants fail to sufficiently converge. In this case we can economize [17,18] the sequence of Padé approximants to create a new sequence of approximants called economized rational approximants (ERAs). The ERAs, in turn, can often be optimized to reduce the error at a particular value of the independent variable, in this case β [19]. This is done by taking advantage of the variable parameter α provided by the economization process and adjusting it until the ERA sequence converges locally along an exponential line. The optimal value of α is determined by examining the least-squares fit of the last four elements of the sequence of approximants to the exponential line $\mathcal{F}(N)=A(1+Be^{-sN})$, where $N=m+k$ is the order of the $[m/k]$ approximant and A, B, and s are variable fitting parameters [20,19]. The value of α that maximizes the fit between $\mathcal{F}(N)$ and the local ERA sequence is considered the optimal value for α, which we denote α_0. When $\alpha=\alpha_0$ the highest-ordered ERA (now

called the *optimized ERA*) provides a better representation of the perturbation series than the original Padé approximant. As an example, in Fig. 1 we illustrate the convergence of the perturbation series when summed using Padé approximants and optimized ERAs. In separate research [19] we tested this technique on well-known functions, and in all cases produced better results (in terms of accuracy and convergence) than with the original Padé approximants.

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