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Application of 2-point Padé approximants to the ground state of the 2-dimensional hydrogen atom in an external magnetic field*

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The 2-dimensional hydrogen atom in an external field λr^2 is important in certain problems of solid-state physics. The exact results for the ground state are obtained from the numerical solution of the radial Schrödinger equation and are compared with various 2-point Padé approximants. Terms to order λ^4 in the low-field RS expansion are combined with 5 terms in the high-field expansion in order to obtain the Padé approximants. The results indicate that the best approximants have relative errors in the range 10^{-8} to 10^{-5} throughout the interval $\lambda = 0 \cdots 4$.

Key words: Padé approximants — Lie algebras — Hydrogen atom

1. Introduction

The 2-dimensional hydrogen atom in a strong magnetic field is of interest in quantum chemistry and solid-state physics. In the latter context it is a model for the study of shallow donor levels for semiconductor impurities near the center of a well. The physics of the problem is discussed in a paper by MacDonald and Ritchie [1].

The low-field RS perturbation expansion has recently been obtained by Čížek and Vinette [2] using symbolic computation and the so(2,1) Lie algebraic approach. The advantage of the algebraic approach to perturbation theory is well

* Dedicated to Professor J. Koutecký on the occasion of his 65th birthday

known [3–7]. The difficulty of the continuum states of the hydrogen atom is circumvented and the low-field perturbation coefficients can be obtained to high order using only finite summations rather than the complicated integrations involved in the conventional approach. Thus, MacDonald and Ritchie in their comprehensive study [1] were only able to obtain the low-field expansion to order γ^2 in the magnetic field strength γ.

On the other hand, the high-field expansion must be treated by conventional perturbation theory since the unperturbed states are harmonic oscillator states which interact with an infinite number of excited states. Thus, the perturbation coefficients are expressed as infinite sums over the so-called Landau levels. It is rather paradoxical that MacDonald and Ritchie were able to obtain coefficients to fourth order in the perturbation theory for the high-field limit through a complex extrapolation scheme for the slowly convergent infinite sums, but they were only able to obtain one term beyond the linear field term for the low-field expansion using conventional perturbation theory. This underlines the difficulty in applying high-order perturbation theory when continuum states are involved and points to the power of the so(2, 1) algebraic methods.

In the present paper we first discuss the numerical solution of the radial Schrödinger equation. This gives exact results for the ground state energy which are used to assess the accuracy of the 2-point Padé approximants. Then the low and high-field expansions are discussed and the results for the ground state are presented. These expansions have also been extended to several excited states and a more detailed analysis of the 2-point Padé approximants for excited states will be presented in a forthcoming paper.

Finally a brief discussion of 2-point Padé approximants is presented and a comparison with the exact numerical results is given for several approximants differing in how much information from the low-field expansion is used. In each case the complete information from the high-field expansion is used. It is clear from the results presented that the 2-point Padé approximants provide high accuracy over a wide range of effective field strengths.

2. Numerical solution of the Schrödinger equation

In order to obtain the Schrödinger equation for an N-dimensional hydrogen atom it is necessary to use the following expressions for the square of the momentum and radial momentum [6, 8, 9].

$$p^2 = p_r^2 + \frac{1}{r^2}\left[\frac{(N-1)(N-3)}{4} + L^2\right] \tag{1}$$

$$p_r^2 = -\frac{\partial^2}{\partial r^2} - \frac{N-1}{r}\frac{\partial}{\partial r} - \frac{(N-1)(N-3)}{4r^2} \tag{2}$$

where N is the dimension and the eigenvalues of L^2 for $N \geq 2$ are $l(l+N-2)$.

The $N=2$ case with an r^2 perturbation and a magnetic field perpendicular to the x-y plane gives the Schrödinger equation

$$\left[\frac{1}{2}p^2-\frac{i\gamma}{2}\frac{\partial}{\partial\phi}-\frac{1}{r}+\frac{\gamma^2}{8}r^2-E\right]\psi(r,\phi)=0 \tag{3}$$

where γ is the effective magnetic field strength. For solutions of the form $\psi_{n,m}(r,\phi)=e^{im\phi}R_{n,m}(r)$ appropriate in the low-field case we obtain the radial equation

$$\left[\frac{1}{2}p_r^2+\frac{1}{2r^2}\left(-\frac{1}{4}+l^2\right)+\frac{1}{r}+\frac{\gamma^2r^2}{8}-E_{n,m}\right]R_{n,m}(r)=0 \tag{4}$$

where $l=|m|$, m is the magnetic quantum number, $n=1,2,3,\ldots$ and $l=0,1,\ldots,n-1$ as usual. Here we have absorbed the linear field term $m\gamma/2$ into the energy eigenvalue.

Thus, we obtain an equation suitable for numerical integration

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{1}{2r}\frac{d}{dr}+\frac{l^2}{2r^2}-\frac{1}{r}+\lambda r^2-E_{n,m}\right]R_{n,m}(r)=0 \tag{5}$$

where $\lambda=\gamma^2/8$. Note that we are using atomic units rather than Rydbergs for the energy scale.

We have integrated this equation numerically by converting it into a system of two first order differential equations. For the ground state the boundary conditions are $R(0)=1$, $R'(0)=-2$, $R(\infty)=0$. The IMSL routine DVERK [10] was used to integrate outwards. This routine is a variable step Runge-Kutta-Verner fifth and sixth order method with prescribed error tolerance developed by Hull et al. [11]. Shanada and Tanaka [12] have also considered the numerical integration of Eq. (5) although no values of the energy were reported.

Since trial values of the energy eigenvalue produce solutions which ultimately diverge to $\pm\infty$ the integration was performed for each value of λ until a narrow eigenvalue interval was obtained such that the solution diverged to $+\infty$ at one end and $-\infty$ at the other. It was possible to obtain eigenvalues having from 6 to 10 significant figures throughout the range $\lambda=0\cdots4$. The results are given in the first column Table 1 for selected values of λ.

3. The low-field expansion

The low-field expansion for the eigenvalues of Eq. (5) has the form

$$E_{n,m}=E_n^0+\frac{m}{2}\gamma+\sum_{i=1}^{\infty}E_{n,l}^{(i)}\lambda^i. \tag{6}$$

It is more convenient to use the perturbation parameter $z=\gamma^{1/2}$ so that (dropping the subscripts n, l, m)

$$E(z)=\sum_{i=0}^{\infty}c_iz^i \tag{7}$$

where the non-zero coefficients are given by

$$c_0 = -\tfrac{1}{2}(n-\tfrac{1}{2})^{-2} \tag{8}$$

$$c_2 = m/2 \tag{9}$$

$$c_{4i} = E_{n,l}^{(i)}/8^i \tag{10}$$

As mentioned in the introduction the results in Eq. (10) for $i > 1$ would be virtually impossible to obtain using conventional perturbation theory due to the presence of continuum states. However, the algebraic approach, which removes the continuum by a scaling transformation, gives them as finite sums in terms of the simple matrix elements of the generator T_3 of the so(2, 1) Lie algebra. The exact rational results for the coefficients c_{4i} have been obtained from this formalism by Čížek and Vinette [2] using the Maple symbolic manipulation language. For the ground state which we are considering the energy is given by ($n = 1$, $l = 0$)

$$E = -2 + \frac{3}{8}\delta z^4 - \frac{159}{1024}\delta^2 z^8 + \frac{17\,967}{65\,536}\delta^3 z^{12} - \frac{15\,522\,195}{16\,777\,216}\delta^4 z^{16} + \cdots \tag{11}$$

where $\delta = \frac{1}{8}$.

4. The high-field expansion

In the high-field limit the Coulomb term in Eq. (3) is the perturbation and the unperturbed problem is just the 2-dimensional harmonic oscillator. Thus, the high-field expansion of the energy eigenvalues has the form

$$\varepsilon_{N,M} = z^2\left[N + \tfrac{1}{2} + \sum_{i=1}^{\infty} \varepsilon_{N,M}^{(i)} z^{-i}\right] \tag{12}$$

where N, $M = 0, 1, 2, \ldots$ and $m = N - M$ is the eigenvalue of the z component L_z of the angular momentum. The harmonic oscillator quantum numbers N and M are also called the Landau level numbers.

For the ground state ($N = M = 0$) we obtain the perturbation expansion of the form

$$\varepsilon = z^2(d_0 + d_1 z^{-1} + d_2 z^{-2} + d_3 z^{-3} + d_4 z^{-4} + \cdots) \tag{13}$$

where the following results are known

$$d_0 = \tfrac{1}{2} \tag{14}$$

$$d_1 = \beta(-1) \tag{15}$$

$$d_2 = \beta^2(-0.440\,101\,489\,993\,231) \tag{16}$$

$$d_3 = \beta^3(-0.233\,116\,7) \tag{17}$$

$$d_4 = \beta^4(-0.072\,674\,51) \tag{18}$$

and $\beta = (\pi/2)^{1/2}$. The coefficients d_0 and d_1 are exact and the others are accurate to the number of significant figures given. To obtain these results conventional perturbation theory must be used. The matrix elements of the $1/r$ perturbation can be expressed in closed form in terms of the ${}_3F_2$ hypergeometric function which reduces to a polynomial in all cases [2, 13]. However, the ground state level interacts with an infinite number of excited levels so the coefficients d_i, $i = 2, 3, \ldots$, are given in general by slowly convergent infinite summations over the Landau levels. Thus, an extrapolation scheme for the partial sums is needed to obtain accurate values for the coefficients. We have used a Neville polynomial interpolation scheme [14] to fit several partial sums and extrapolate the results to the infinite summation limit.

5. 2-Point Padé approximants

The usual approach to obtaining higher accuracy for the low-field expansion in Eq. (11) over a range of z values is to use the 1-point Padé approximants [15]. However, the range can be significantly extended using information from the high-field expansion and 2-point approximants. Thus, noting the z^2 leading behavior (linearity in the magnetic field strength) fo the expansion in Eq. (13) we can consider the $[K+2/K]$ approximants for the form

$$R_K(z) = \left[\sum_{i=0}^{K+2} p_i z^i\right] \Big/ \left[\sum_{j=0}^{K} q_j z^j\right] \tag{19}$$

$$= z^2 \left[\sum_{i=0}^{K+2} p_{K+2-i} z^{-i}\right] \Big/ \left[\sum_{j=0}^{K} q_{K-j} z^{-j}\right] \tag{20}$$

where the first expression is appropriate for the low-field expansion and the latter is appropriate for the high-field expansion. The usual normalization condition $q_0 = 1$ is assumed.

Except for a re-ordering of the coefficients p_i and q_j and the use of $1/z$ instead of z as the variable, Eq. (20) has an identical form to Eq. (19). Thus, the fitting of Eq. (11) to Eq. (19) is formally the same as the fitting of Eq. (13) to Eq. (20). In either case we can obtain a linear system of equations which can be solved for the coefficients q_j [2, 16]. The remaining equations give linear expressions for the coefficients p_i. We can take some equations from the low-field group and the remaining ones from the high-field group to obtain a variety of 2-point approximants. There are usually several choices for a given order K depending on how the equations chosen from each group are combined. In our study of the ground state we shall use all available information from the high-field expansion in Eq. (13) combined with various orders of the low-field expansion in Eq. (11).

6. Results and discussion

The results for the ground state for several 2-point Padé approximants are given in Table 1. The first column gives selected values of the perturbation parameter

Table 1. Comparison of selected 2-point Padé approximants with the exact numerical results for the ground state of the hydrogen atom in a λr^2 external magnetic field. The exact results from numerical integration are shown in column 1 and the approximants shown use all information in Eq. (13) for the high-field expansion. The order 5 approximant in column 3 is essentially the result of MacDonald and Ritchie [1], using low-field coefficients in Eq. (11) to order λ. The range of λ considered is equivalent to the range considered by these authors in terms of the parameter $\gamma' = \gamma/(1+\gamma)$. The final three approximants use low-field coefficients to orders λ^2, λ^3 and λ^4, respectively. Beneath each energy value is the relative error compared to the exact result using the notation $a(b)$ to denote $a \times 10^b$

λ	Exact results	[7/5]	[9/7]	[10/8]	[11/9]
0.1	−1.963842	−1.964258	−1.963520	−1.963837	−1.963842
		−2.1 (−4)	1.6 (−4)	2.5 (−6)	−1.0 (−8)
0.2	−1.929807	−1.930819	−1.929310	−1.929791	−1.929809
		−5.2 (−4)	2.6 (−4)	8.3 (−6)	−1.0 (−6)
0.3	−1.897379	−1.898977	−1.896781	−1.897352	−1.897384
		−8.4 (−4)	3.2 (−4)	1.4 (−5)	−2.6 (−6)
0.4	−1.866249	−1.868393	−1.865589	−1.866214	−1.866257
		−1.1 (−3)	3.5 (−4)	1.9 (−5)	−4.3 (−6)
0.5	−1.836207	−1.838855	−1.835511	−1.836169	−1.836220
		−1.4 (−3)	3.8 (−4)	2.1 (−5)	−7.1 (−6)
0.6	−1.807104	−1.810212	−1.806385	−1.807064	−1.807120
		−1.7 (−3)	4.0 (−4)	2.2 (−5)	−8.9 (−6)
0.7	−1.778822	−1.782353	−1.778092	−1.778784	−1.778842
		−2.0 (−3)	4.1 (−4)	2.1 (−5)	−1.1 (−5)
0.8	−1.751273	−1.755190	−1.750537	−1.751237	−1.751296
		−2.2 (−3)	4.2 (−4)	2.1 (−5)	−1.3 (−5)
0.9	−1.724381	−1.728656	−1.723645	−1.724351	−1.724407
		−2.5 (−3)	4.3 (−4)	1.7 (−5)	−1.5 (−5)
1.0	−1.69809	−1.70269	−1.697351	−1.69806	−1.69812
		−2.7 (−3)	4.4 (−4)	1.8 (−5)	−1.8 (−5)
2.0	−1.45959	−1.46648	−1.45895	−1.45967	−1.45964
		−4.7 (−3)	4.4 (−4)	−5.5 (−5)	−3.4 (−5)
4.0	−1.06155	−1.07050	−1.06109	−1.06185	−1.06162
		−8.4 (−3)	4.3 (−4)	−2.8 (−4)	−6.6 (−5)

λ introduced in Eq. (5) which is related to z by $\lambda = z^4/8$. The second column gives the exact results from the numerical integration of Eq. (5). The remaining columns give the results for four approximants of orders $K = 5, 7, 8, 9$, respectively, chosen to show how the accuracy improves as more coefficients from the low-field expansion are used.

The order 5 approximant in column 3 is essentially one of the results of MacDonald and Ritchie [2] which uses all information from the high-field expansion in Eqs. (13–18) but only coefficients to first order in λ ($c_0, \ldots, c_7$) in Eqs. (7–10). These authors provide extensive results for the ground state and several excited states, comparing them with experiment rather than with exact numerical results. The remaining approximants which we have calculated also use all high-field information. The order 7 approximant in column 4 uses low-field coefficients to second order in λ ($c_0, \ldots, c_8$), the order 8 approximant uses low-field coefficients

to third order in λ $(c_0, \ldots, c_{12})$ and the order 9 approximant uses low-field coefficients to fourth order in λ $(c_0, \ldots, c_{16})$. The relative error of each approximant compared to the exact result in column 2 is given beneath each energy value using the notation $a(b)$ to denote $a \times 10^b$.

It is clear from the results for a given value of λ that the accuracy increases by approximately one order of magnitude throughout the range $\lambda = 0$ to 0.6 as more low-field coefficients are used. Somewhat smaller increases are obtained for $\lambda = 0.7$ to 4. The [11/9] approximant is consistently two orders of magnitude better than the [7/5] approximant. The best results, for the [11/9] approximant, indicate that high accuracy in the range 10^{-8} to 10^{-5} can be obtained over a wide range of λ values using 2-point Padé approximants.

It is also interesting to compare the 2-point results with the 1-point results using only the low-field expansion and Eq. (19) with $K+2$ replaced by M (it is not possible to obtain $[K+2/K]$ approximants using only the low-field expansion). The best result is the [8/8] approximant. It has a relative error of $-2.5\,(-6)$ at $\lambda = 0.1$, increasing to $-6.4\,(-3)$ at $\lambda = 1$ and to $-2.0\,(-1)$ at $\lambda = 4$. The low-field expansion itself (the [16/0] approximant) has a relative error of $-1.5\,(-5)$ at $\lambda = 0.1$ which increases rapidly to $-4.3\,(-1)$ at $\lambda = 1$ and to $-221\,(0)$ at $\lambda = 4$.

In conclusion it is apparent that if information is available at both the low and high-field limits of a perturbation parameter λ then 2-point Padé approximants can provide high accuracy eigenvalues over a wide range of the perturbation parameter compared to the 1-point approximants.

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