Two-dimensional hydrogenlike atoms in the presence of a magnetic field: Quasifractional approximations

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Two-point quasifractional approximations have been used to study the energy levels for a hydrogenic atom when a magnetic field is applied perpendicular to the x-y plane. Perturbation theory gives power-series expansions for weak magnetic fields and asymptotic expansions for very high magnetic fields. Using appropriate forms of the two-point quasifractional approximants, we recover both expansions and have found a better interpolation between the two limiting situations for the ground- and excited-state energies than those previously published.

I. INTRODUCTION

In a recent paper, MacDonald and Ritchie[1] have used a two-point Padé approximant for the eigenvalue spectrum of a two-dimensional hydrogenic atom in the presence of a uniform magnetic field of arbitrary strength. As they point out, this problem is very relevant in several areas of physics.

A perturbation analysis for the weak-field limit gives the energy levels in terms of a power expansion where the parameter of expansion is the coupling constant γ, which measures the ratio between the magnetic energy and the Coulomb energy.[2] On the other hand, in the strong-field regime, the Coulomb potential is considered as the perturbative potential and the expansion is given in terms of the parameter $x=(\pi/2\gamma)^{1/2}$. The parameter γ is defined as

$$\gamma=(\epsilon^2\hbar^3B)/(ce^3m^{*2}) , \tag{1}$$

where m^* is the effective mass, ϵ the dielectric constant of the host material, e the electron charge, $\hbar$ the Planck constant divided by 2π, and c the speed of light in vacuum.

A straightforward application of the two-point Padé method has to be done in terms of the x variable. The power expansion is made in terms of the γ variable, which is x^2, and the efficiency of the procedure is low since the odd powers have to be chosen equal to zero, and they do not carry additional information. On the other hand, the curves obtained from different Padé approximants are very different. No regular pattern appears and the results become unreliable. Also, the lowest-order approximant curve has unphysical characteristics, such as negative derivative at the origin for the $1S$ state. However, recently a method[3,4] has been published to interpolate between zero and infinity where they use fractional approximations combined with other functions such as exponentials, fractional powers, trigonometric functions, etc., in such a way that the approximant has the same singularities as the exact functions in all the region of interest, including the boundaries ($x\rightarrow\infty$ in our case).

The two-point Padé method uses both the power and the asymptotic expansions. Once one has the correct form of the approximation, all the equations for the parameters are obtained uniquely from the significant terms of both expansions. Irrelevant zero odd-power terms as sometimes may occur in the Padé method do not appear here.

Using this method, we have postulated five two-point quasifractional approximants. These approximants do not show unphysical curves. Furthermore, all the approximants are really close to one another and to the numerical solutions. Also, they agree very well with the potential and asymptotic expansions in the appropriate regimes of magnetic field (γ).

The energy levels are classified with respect to the angular-momentum quantum number L_z, which depends on the azimuthal angle for a given magnetic field. In Sec. II we consider the theoretical background which leads to the expansion for weak and strong magnetic fields. In Sec. III we propose our two-point quasifractional approximants which interpolate between these two limits. We conclude in Sec. IV.

II. PERTURBATION EXPANSIONS

The Hamiltonian H which describes the physical system is composed to two contributions: (1) the Coulomb energy, which represents the interaction between a conduction electron and a donor atom; (2) the "kinetic" energy $(1/2m^*)[\mathbf{p}+(e/c)\mathbf{A}]^2$, where $\mathbf{A}$ is the magnetic vector potential. If we adopt the symmetric gauge $\mathbf{A}=(B/2)(-y,x,0)$, the Hamiltonian can be expressed

TABLE I. Coefficients of five two-point quasifractional approximants for $E_{k,m}$ [Eq. (8)].

(N,J,M)	Asymptotic γ^{-1}	Asymptotic $\gamma^{-1/2}$	γ^0	$\gamma^{1/2}$	γ^1
(1,1,0)				$B_0\sqrt{\lambda}=p_1$	$b_0=t_1$
(2,1,1)		$B_1q_1+\sqrt{\lambda}+B_0\sqrt{\lambda}+B_0q_1/2\sqrt{\lambda}=p_1$	$b_1q_1+b_0=t_1$	$B_0q_1=p_1\sqrt{\lambda}$	$b_0q_1=t_2$
(2,2,1)		$B_1q_1\sqrt{\lambda}+B_0\sqrt{\lambda}+B_0q_1/2\sqrt{\lambda}=p_1$	$b_1q_1+b_0=t_1$	$B_0q_1\sqrt{\lambda}=p_2$	$b_0q_1=t_2$
(3,2,1)	$b_2q_1\lambda+b_1q_1+\lambda b_1+b_0=t_1$	$B_1q_1\sqrt{\lambda}+B_0\sqrt{\lambda}+B_0q_1/2\sqrt{\lambda}=p_1$	$\lambda b_1q_1+b_0q_1+\lambda b_0=t_2$	$B_0q_1\sqrt{\lambda}=p_2$	$\lambda b_0q_1=t_3$
(3,2,2)	$b_2q_2+b_1q_1+b_0=t_1$	$B_1q_2+B_0q_1=\sqrt{\lambda}(p_1+p_2/2\lambda)$	$b_1q_2+b_0q_1=t_2$	$B_0q_2=p_2\sqrt{\lambda}$	$b_0q_2=t_3$

as

$$H=-\nabla^2+\gamma L_z-2/\rho+\gamma^2\rho^2/4\ , \tag{2}$$

where ∇^2 is the two-dimensional Laplacian, L_z is the angular-momentum operator, $-i\hbar\partial/\partial\phi$, and the units of energy and length are the effective rydberg constant and modified Bohr radius, respectively, $\mathcal{R}_0^*$ and a_0^*. a_0^* is given by $\epsilon\hbar^2/m^*e^2$ and $\mathcal{R}_0^*$ by $m^*e^4/2\epsilon^2\hbar^2$.

Using perturbation theory for $\gamma\ll 1$, MacDonald and Ritchie[1] have obtained the weak-field expansion for the energy levels $E_{n,l}$, up to third order in γ, as follows:

$$E_{n,l}=-(n-\tfrac{1}{2})^{-2}+m\gamma+\gamma^2\langle\rho^2\rangle_{n,l}/4+O(\gamma^4)\ . \tag{3}$$

Values of $\langle\rho^2\rangle_{n,l}$ for $n=1,2,3,4$ have been taken from Ref. 1.

For the case of $\gamma\gg 1$, our unperturbed Hamiltonian does not include the Coulomb term. In this case, the solutions of Eq. (3) are of the form $\psi\cong e^{im\phi}R(\rho)$, where $R(\rho)$ satisfies the radial Schrödinger equation. This radial equation may be solved by using the confluent hypergeometric function. The results are

$$E_{N,m}=\hbar\omega_c[N+(|m|+m)/2] \tag{4}$$

and

$$\begin{aligned}R_{N,m}(\rho)=&[(|m|+N)!]^{1/2}e^{-\rho^2/4a_B^2}\rho^{|m|}\\&\times F(-N,|m|+1,\rho^2/2a_B^2)\\&\times(a_B^{|m|+1}|m|2^{|m|}N!)^{-1}\ ,\end{aligned} \tag{5}$$

where $a_B=(h/m^*\omega_c)^{1/2}$, $F(\alpha,\beta;x)$ is the confluent hypergeometric function, and $\omega_c=eB/m^*c$. There exists a close connection between the confluent hypergeometric function and the Laguerre polynomials.[5] Using perturbation theory for the Coulomb potential, MacDonald and Ritchie[1] have obtained and expression for the energy levels as follows:

$$\begin{aligned}E_{n,m}=&2\gamma(n+\tfrac{1}{2}+\alpha_{n,m}^{(1)}x+\alpha_{n,m}^{(2)}x^2\\&+\alpha_{n,m}^{(3)}x^3+\alpha_{n,m}^{(4)}x^4+\cdots)\ ,\end{aligned} \tag{6}$$

where $x=(\pi/2\gamma)^{1/2}$ and the numerical constants $\alpha_{n,m}^{(i)}$'s are taken from MacDonald and Ritchie's work.

III. TWO-POINT QUASIFRACTIONAL APPROXIMANTS

For the two-point quasifractional approximation it is useful to rewrite Eqs. (3) and (6) in the following manner:

$$E_{k,m}=\begin{cases}\displaystyle\sum_{n=0}^{\infty}a_n\gamma^n, & \gamma\ll 1\\ \displaystyle\gamma\sum_{n=0}^{\infty}b_n/\gamma^n+\gamma^{1/2}\sum_{n=0}^{\infty}B_n/\gamma^n, & \gamma\gg 1\ ,\end{cases} \tag{7}$$

where $b_n=\tilde{\alpha}^{(2n)}$; $B_n=\tilde{\alpha}^{(2n+1)}$; the a_n's are given by Eq. (3) in Ref. 1 and $\tilde{\alpha}_{k,m}^{(i)}=2(\pi/2)^{i/2}\alpha_{k,m}^{(i)}$.[1]

The strategy of this approach using the two-point quasifractional approximation is to reproduce the singularity of the exact function introducing additional nonfractional as well as fractional powers, exponentials, etc. In this case, we want to recover the ramification point at infinity defined by the $\gamma^{1/2}$ factor. We must keep in mind that the ramification points come in pairs. So we have to introduce a function in such a way that the second ramification point is outside the region of interest, that is, the negative axis. For this reason we use as a factor the function $(1+\lambda\gamma)^{1/2}$, $\lambda>0$. Now one of the ramification points is at infinity and the second one is at $\gamma=-1/\lambda$. Since $\gamma\geq 0$, the second ramification point is outside the region of interest. λ is fixed by a minimization procedure for the two-point quasifractional approximant with respect to the numerical solution of the eigenvalues of the Schrödinger equation.

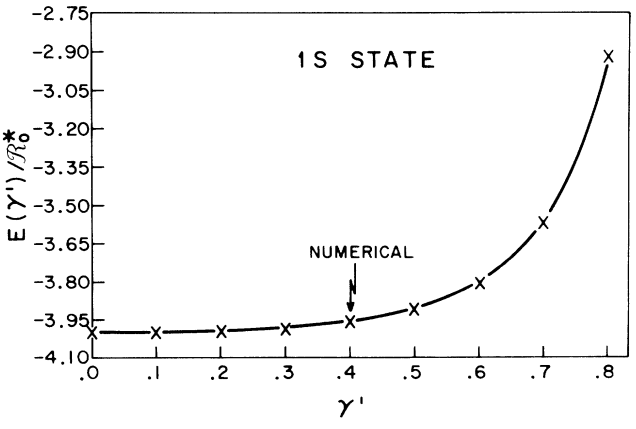

FIG. 1. Our lowest two-point quasifractional approximant for the ground state (1S). The continuous line represents the approximant and the crosses refer to the numerical solution of the eigenvalues. The energy scale is in $\mathcal{R}_0^*$ and we have used $\gamma'=\gamma/(1+\gamma)$ as the horizontal scale. The same is valid for Figs. 2 and 3. $\lambda=0.28$.

TABLE I. (*Continued*).

	Potential			
(N,J,M)	γ^0	γ^1	γ^2	γ^3
(1,1,0)	$a_0=p_0+t_0$	$t_1+p_1-\lambda p_0/2=a_1$		
(2,1,1)	$a_0=p_0+t_0$	$t_1+p_1+\lambda p_0/2=a_0q_1+a_1$		
(2,2,1)	$a_0=p_0+t_0$	$t_1+p_1-\lambda p_0/2=a_0q_1+a_1$	$a_1q_1+a_2=t_2+p_2-\lambda p_1/2+3\lambda^2p_0/8$	
(3,2,1)	$a_0=p_0+t_0$	$t_1+p_1+\lambda p_0/2=a_0(\lambda+q_1)+a_1$	$\lambda(a_1+a_0q_1)+a_1q_1+a_2=t_2+p_2+\lambda p_1/2-\lambda^2p_0/8$ $-\lambda^2p_0/8$	
(3,2,2)	$a_0=p_0+t_0$	$a_0q_1+a_1=t_1+p_1+\lambda p_0/2$	$a_0q_2+a_1q_1+a_2=t_2+p_2+\lambda p_1/2$	$a_2q_1+a_1q_2=t_3+\lambda p_2/2-\lambda^2p_1/8$ $+\lambda^3p_0/16$

In order to recover the behavior of the energy levels around $\gamma=0$ and $\gamma\to\infty$, we must use two-point quasifractional approximants whose forms are chosen as follows:

$$T_N(\gamma)/Q_M(\gamma)(1+\alpha\gamma)^{N-M-1} + P_J(\gamma)/Q_M(\gamma)(1+\alpha\gamma)^{J-M-1/2} . \quad (8)$$

The denominator $Q_M(\gamma)$, with $q_0=1$, can be determined at the same time as $T_N(\gamma)$ and $P_J(\gamma)$. However, as it also happens in the Padé method, the zeros of $Q_M(\gamma)$ sometimes appear in the physical region, that is, the interval $(0,\infty)$. In order to avoid these problems, we choose only $\gamma>0$ and $q_i>0$. To get the same accuracy with this method, one should go to higher degrees of the polynomials.

Figures 1–3 show all the five two-point quasifractional approximants obtained by using the power series [Eq. (4)] and asymptotic expansion [Eq. (7)] for the ground state $1S$ and the excited states $2P^-$ and $3D^-$. We observe that all our approximants are very close to one another. We also compare them with the numerical solution of the Schrödinger equation. Table I gives the hierarchy of equations obtained for the five two-point quasifractional approximants.

Practically all five approximants [Eq. (8)] give almost the same accuracy, which is always better than the accuracy of the best MacDonald-Ritchie approximants. Also, we must note that from the very beginning we supply two asymptotic expansion terms to our approximants throughout, b_0 and $B_0\gamma^{1/2}$.

We have chosen λ by requiring that the maximum absolute error be minimum. This approach is valid when we know the exact numerical value of $E(\gamma)$ for a given state. We have solved numerically the eigenvalues of the Schrödinger equation with a precision of four digits and a step of $\Delta\gamma'=0.1$, where $\gamma'=\gamma/(\gamma+1)$. The value of λ is different for each state and each approximant.

The values of λ obtained are 0.28, 30, and 133 for the lowest-degree approximants for the states $1S$, $2P^-$, and $3D^-$, respectively. Their coefficients are presented in Table II.

In Table III we present the largest errors of our best approximants, ε_B, and our lowest approximants, ε_L, with respect to the numerical solution to the Schrödinger equation. We also show the maximum error, ε_{MR}, for the best MacDonald and Ritchie interpolation formulas with respect to the numerical solution. λ_B and λ_L correspond to the λ's which make the maximum error a minimum for our highest- and lowest-order approximants, respectively.

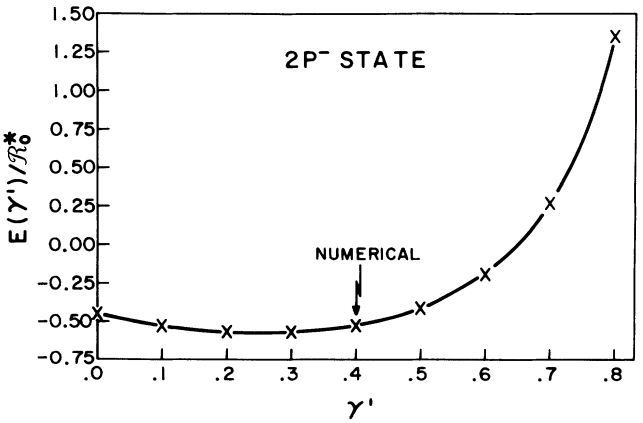

FIG. 2. Our lowest two-point quasifractional approximant for the excited state ($2P^-$). The continuous line represents the approximant and the crosses refer to the numerical solution of the eigenvalues. $\lambda=30$.

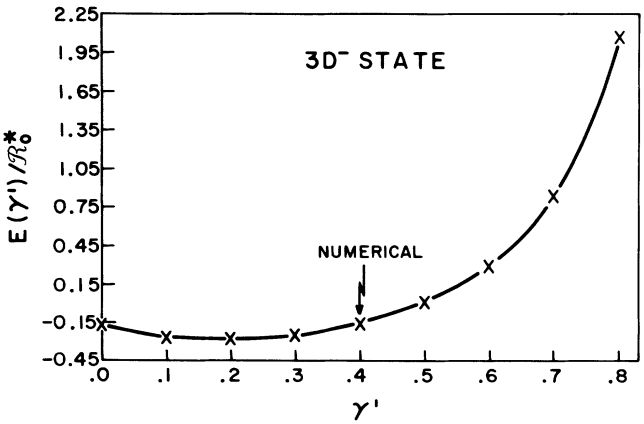

FIG. 3. Our lowest two-point quasifractional approximant for the excited state ($3D^-$). The continuous line represents the approximant and the crosses refer to the numerical solution of the eigenvalues. $\lambda=133$.

TABLE II. Coefficient values for the lowest approximant with $N=1$, $J=1$, and $M=0$.

State	λ	t_0	t_1	P_0	P_1
$1S$	0.28	−1.668 690	1.000 000	−2.331 310	−1.326 380
$2P^-$	30	−0.120 132	1.000 000	−0.324 312	−6.864 680
$3D^-$	133	−0.042 098 6	1.000 000	−0.117 901	−10.840 40

TABLE III. Comparison of the largest errors of the best approximants, ε_B; of the lowest approximants, ε_L; and of the MacDonald-Ritchie interpolation formulas, ε_{MR}.

State	λ_B	ε_B	ε_{MR}	ε_L	λ_L
$1S$	0.7	0.0003	0.021	0.032	0.28
$2P^-$	10.8	0.0001	0.004	0.007	30.0
$3D^-$	34.0	0.0001	0.001	0.003	133.00

IV. CONCLUSIONS

We have proposed two-point quasifractional approximants for the energy levels of a two-dimensional hydrogenlike atom in the presence of an external magnetic field. We have obtained an interpolation between the low magnetic-field and the high-field limit for the states $1S$, $2S$, $3P^-$, $3S$, $3D^-$, and $4S$. The values of the optimum λ for these states are 0.28, 84, 30, 11.2, 133, and 27, respectively. It is important to mention that these values of λ correspond to the lowest approximant.

The advantage of our method is that our approximants show a clear pattern and they stay close together for any value of the approximants. Unphysical curves do not appear here. The efficiency of the method is higher with polynomials of lower degree than those of MacDonald and Ritchie due to the fact that irrelevant zero odd-power terms do not appear here. At the same time, we recover the values of the energy levels for both extreme field regimes where perturbation theory works perfectly for the two-dimensional case. This feature is particularly attractive since perturbation theory does not work in the three-dimensional case. The results obtained should be useful for the study of shallow donor impurities near the center of a quantum well under appropriate conditions.[6,7]

We see that our approximants have achieved better accuracy than those of MacDonald and Ritchie and they are much simpler. The polynomials presented in this paper contain only four unknown coefficients, while the expressions of MacDonald and Ritchie have thirteen unknown coefficients.

We would like to point out that we have not included higher-order approximants since the lowest-degree approximant ($N=1$, $J=1$, $M=0$) reproduces the numerical solution of the energy eigenvalues. However, our approximant with nine coefficients is undistinguishable from the numerical solution. The highest error is 0.0003 for the nine-coefficient approximant while the highest error for the lowest approximant ($N=J=1$, $M=0$) is 0.03, both with respect to the numerical solution of the eigenvalue problem.

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[1]A. N. MacDonald and D. S. Ritchie, Phys. Rev. B **33**, 8336 (1986).

[2]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1977), pp. 458 and 459.

[3]P. Martín and G. Baker, J. Math. Phys. **32**, 1470 (1991).

[4]P. Martín and A. L. Guerrero, J. Math. Phys. **26**, 705 (1986).

[5]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1977), pp. 665–659.

[6]G. Bastard, Phys. Rev. B **24**, 4714 (1981).

[7]L. E. Oliveira and L. M. Falicov, Phys. Rev. B **34**, 8676 (1986).