Analytic approximations to the energy eigenvalues of the quadratic Zeeman effect in two dimensions

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SUMMARY

Accurate energy eigenvalues for the quadratic Zeeman effect in 2D are presented using a new approximation technique. This technique is an extension of the two-point quasi-rational approximations, applied to multiple points. The calculations are carried out for the ground state 1s and the excited states $1s$, $2p^-$ and $3d^-$. The results obtained are much better than those obtained in previous works. We have also shown the advantage of our approximants with respect to other approximate methods.

Aproximaciones analíticas a los autovalores de la energía del efecto Zeeman Cuadrático en dos dimensiones

RESUMEN

En este trabajo se presenta una técnica muy precisa para el cálculo de los autovalores de la energía para el efecto Zeeman cuadráticos en 2D. Esta técnica es una extensión de las aproximaciones cuasiracionales a dos puntos, aplicada a múltiples puntos. Los cálculos se realizaron para el estado base 1s y los estados excitados $2p^-$ and $3d^-$. Los resultados obtenidos son muchos mejores que aquellos obtenidos en trabajos previos. Mostramos también las ventajas de nuestros aproximantes con respecto a otros métodos aproximados.

KEYWORDS / Quasirational approximations / Solutions of wave equations: bound states / Quadratic Zeeman effect

Introduction

In this work, hydrogenlike atoms in a magnetic field in 2-D are considered for systems where the Coulomb energy scale is about the magnetic interaction. This is the case for instance of conduction electrons in GaAS. Since neither the Coulomb energy, neither the magnetic energy can be considered small parameters, the linear approximation, denoted as Zeeman effect, is not a good approximation and the quadratic Zeeman effect should be taken in account. The characteristic parameter γ is of order one, being γ the ratio between both energies, that is, $\gamma = \left(\mu_B B / R_0^*\right) = \left(\varepsilon^2 \hbar^3 B\right) / (c e^3 m^{*2})$, where **B** is the induction magnetic field, R_0^* is the effective Rydberg constant, m^* is the effective mass of the conduction electrons, h is the Planck constant, (-e) is the electron charge, c is the speed of light and μ_B is the Bohr magneton. The Hamiltonian with energy in units of R_0^* and position in units of effective Bohr radius $a^* = m^* e^4 / 2\varepsilon^2 \hbar^2$ is

$$H = -\nabla^2 + \gamma L_z - \frac{2}{\rho} + \frac{\gamma^2}{4}\rho^2 \quad , \tag{1}$$

where ∇^2 is two-dimensional Laplacian (i.e., $a_0^* \approx 100$ $\overset{0}{\text{A}}$ for GaAs), the magnetic field is considered to be in z-direction and the symmetric gauge $\mathrm{A} = \mathrm{B}\left(-y, x, 0\right)/2$ has been used. Considering the solution of Eq.(1) as $\Psi(\rho) = R(\rho) e^{im\phi} / \sqrt{2\pi}$ then the Schrödinger equation becomes the second order differential equation

$$\left(-\frac{d^2}{d\rho^2} - \frac{1}{\rho}\frac{d}{d\rho} + \frac{m^2}{\rho^2} - \frac{2}{\rho} + m\gamma + \frac{\gamma^2 \rho^2}{4} \right) R(\rho) = E\, R(\rho) \quad . \tag{2}$$

No analytic solutions are know for Eq.(2). Several methods have been used to obtain approximate solutions, such as the two-point quasi-rational approximants TPQA (Martin P. 1992); Padé Method (McDonald and Richie 1986), 1/N shifted technique (Mustafa O. 1993) and numerical computations (Villalba and Pino 1998). An extension of the TPQA method will be used here, denoted as multipoint

quasi-rational approximants (MPQA), where power expansions in several points will be used simultaneously (Castro E. et. al.).

Multipoint quasi-rational approximants

In this method there is not need to use the asymptotic expansion, thought this can also be used mainly to define the form of the approximants. The numerical value of the functions and its derivatives of first and second order mainly have to be used and they can be determined by numerical computations. Once the form of the approximant has been decided, their parameters will be determined by equalizing its values and derivatives to those obtained by the numerical computations explained above.

In our case, the functions to approximate are the eigenvalues of equation (2). The form of the approximants will be

$$\widetilde{E}(\gamma)=\frac{\mathrm{P_L}(\gamma)}{\mathrm{Q_M}(\gamma)}=\frac{\sum_{k=0}^{L} p_k\,\gamma^k}{1+\sum_{i=0}^{M} q_i\,\gamma^i} \quad . \tag{3}$$

As in Padé method, $\mathrm{P_L}(\gamma)$ and $\mathrm{Q_M}(\gamma)$ are polynomials in γ of degrees L and M, respectively. The coefficients p_k and q_i of the approximant are determined by imposing that $\widetilde{E}(\gamma)$ and $E(\gamma)$, and its first and second derivatives $\left(d\,E(\gamma)/d\gamma,\, d^2\,E(\gamma)/d\gamma^2\right)$ should coincide in some chosen points γ_r (r = 1, 2, 3, …n)

$$\mathrm{Q_M}(\gamma_r)\;\widetilde{E}(\gamma_r)-P_{\mathrm{L}}(\gamma_r)\;=0\,, \tag{4}$$

$$\left.\frac{\mathrm{dQ_M}(\gamma)}{\mathrm{d}\gamma}\right|_{\gamma=\gamma_r}\widetilde{\mathrm{E}}(\gamma_r)\;+\;Q_M(\gamma_r)\left.\frac{d\widetilde{\mathrm{E}}(\gamma)}{d\gamma}\right|_{\gamma=\gamma_r}-\left.\frac{dP_{M+1}(\gamma)}{d\gamma}\right|_{\gamma=\gamma_r}=0 \quad , \tag{5}$$

$$\left.\frac{\mathrm{d}^2Q_M(\gamma)}{\mathrm{d}\gamma^2}\right|_{\gamma=\gamma_r}\widetilde{E}(\gamma_r)+2\left.\frac{dQ_M(\gamma)}{d\gamma}\right|_{\gamma=\gamma_r}\left.\frac{d\widetilde{E}(\gamma)}{d\gamma}\right|_{\gamma=\gamma_r}+Q_M(\gamma_r)\left.\frac{\mathrm{d}^2\widetilde{E}(\gamma)}{\mathrm{d}\gamma^2}\right|_{\gamma=\gamma_r}-\left.\frac{\mathrm{d}^2\mathrm{P_L}(\gamma)}{\mathrm{d}\gamma^2}\right|_{\gamma=\gamma_r}=0. \tag{6}$$

The number of equations must be equal to the number of parameters to be determined. First the relation between L and M must be determined in order to produce the largest accuracy with the same number of parameters. Several cases were tested and the best results were obtained when $L = M + 1$. Now, increasing the degree of the polynomials the accuracy increases. Sometimes as in our case, it is better to leave a free parameter, by using a number of equations one unit lesser than the unknowns, and determining the free parameter by minimizing the error between the approximant and the numerical solutions. In the present work the free parameter was q_M .

Coefficients	$\tilde{E}_{1s}$	$\tilde{E}_{2p^-}$	$\tilde{E}_{3d^-}$
p_0	0.16000	-0.444450	-4.000002
p_1	59.9455	-6.58034	-3.069952
p_2	1882.11	-32.3552	-1.254528
p_3	6363.85	-33.2901	-0.1089466
p_4	-3991.15	16.0552	0.02184713
p_5	-4641.90	6.63643	0.0008673304
q_0	1	1	1
q_1	-390.215	-12.5657	0.7674965
q_2	-6438.80	50.4000	0.3370093
q_3	-16263.9	50.1129	0.04541116
q_4	-5648.44	7.94572	0.000987723

Tabla I : Values of the coefficients of the parameters p's and q's for the MPQA (L = 5, M = 4) for the $1s$, $2p^-$ y $3d^-$ states.

Results and Conclusions

The accuracy of the MPQA depends first on the accuracy with which the eigenenergies and its derivatives were determined by numerical computation.. The numerical calculations of the eigenvalues

was performed with the shooting method using Eq.(2). The derivatives were determined by central differences. The calculated values for the coefficients of the MPQA, for the $1s$, $2p^-$ and $3d^-$ states, are shown in Table I. The number of parameters to determine were equal to those used in Martin P et. al. (1992), using the TPQA method. This was necessary in order to obtain an adequate comparison.

States	TPQA			MPQA		
	$\varepsilon_{máx}$	$\varepsilon\%$	γ'_ε	$\varepsilon_{máx}$	$\varepsilon\%$	γ'_ε
1s	4.7×10^{-6}	1.2×10^{-4}	0.5	1.7×10^{-4}	2.7×10^{-3}	0.95
$2p^-$	5.6×10^{-6}	1.3×10^{-3}	0	4.2×10^{-5}	1.0×10^{-2}	0.5
$3d^-$	3.8×10^{-6}	1.9×10^{-3}	0.35	1.2×10^{-5}	8.6×10^{-3}	0.05

Tabla II: Maximum errors for the MPQA and TPQA of higher order for the three electron states considered.

In Table II, the MPQA and TPQA method are compared. The best way to do it is by looking at the maximum errors for the parameters to be determined. The accuracy of the MPQA is high and better than those previously published by Martín P et. al., showing better results and arround one or two orders of magnitude lower error than the TPQA method.

The MPQA technique looks like a worthwhile technique to obtain approximate eigenvalues for some potentials in Quantum Mechanics. The application range of applications seems ampler than that of other approximation techniques and the accuracy obtained is better for the same number of parameters to determine. An additional advantage is that the form of the approximants can be simpler than that of the TPQA method.

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