Energy levels of a two-dimensional hydrogenic donor in the presence of a constant magnetic field

1996 J. Phys.: Condens. Matter 8 8067

(http://iopscience.iop.org/0953-8984/8/42/024)

J. Phys.: Condens. Matter **8** (1996) 8067–8072. Printed in the UK

COMMENT

Energy levels of a two-dimensional hydrogenic donor in the presence of a constant magnetic field

Víctor M Villalba†§ and Ramiro Pino‡‖

† Centro de Física, Instituto Venezolano de Investigaciones Científicas, IVIC, Apartado 21827, Caracas 1020-A, Venezuela

‡ Centro de Química and Centro de Física, Instituto Venezolano de Investigaciones Científicas, IVIC, Apartado 21827, Caracas 1020-A, Venezuela

Received 25 January 1996, in final form 16 April 1996

Abstract. In the present article we study the energy levels of a 2D hydrogenic atom when a constant magnetic field is applied. We compute the energy spectrum with the help of a generalization of the mesh point technique recently proposed by Schwartz. We also estimate, via a variational method, the upper energy bound for small and large values of the external magnetic field. We show that the results obtained by O Mustafa (1993 *J. Phys.: Condens. Matter* **5** 1327) have to be modified in the weak-magnetic-field regime.

The study of two-dimensional hydrogen-like atoms in magnetic fields has been the object of a series of publications during the last decade. The physical motivation for this problem lies in the study of quantum well and superlattice systems. Probably the best known superlattice configuration consists of regions of GaAs which act as wells for the conduction electrons separated by regions of $Ga_{1-x}Al_xAs$ which act as barriers.

The Hamiltonian describing the Coulomb interaction between a conduction electron and a donor impurity centre when a constant magnetic field $\boldsymbol{B}$ is applied perpendicular to the x–y plane can be written as

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

where we have chosen the vector potential

$$\boldsymbol{A} = \frac{B}{2}(-y, x, 0) = \frac{Br}{2}\hat{\boldsymbol{e}}_\varphi$$

in the symmetric gauge. The coupling constant γ, which measures the ratio between the magnetic energy and Coulomb energy, is defined as $\gamma = \epsilon^2\overline{h}^3B/(ce^3m^{*2})$ where m^* is the effective mass, and ϵ the dielectric constant of the host material. ∇^2 is the two-dimensional Laplacian, and L_z is the angular momentum operator $-\mathrm{i}\overline{h}\,\partial/\partial\phi$ with eigenvalue $\overline{h}m$. The units of energy are given in terms of the effective Rydberg constant $\mathcal{R}_0^* = m^*e^4/2\overline{h}^2\epsilon^2$ and the effective Bohr radius $a^* = \overline{h}^2\epsilon/m^*e^2$, respectively.

The substitution

$$\Psi = \frac{\mathrm{e}^{\mathrm{i}m\varphi}}{\sqrt{2\pi}}\frac{u(\rho)}{\sqrt{\rho}} \tag{2}$$

§ E-mail: villalba@dino.conicit.ve.

‖ E-mail: rpino@ivic.ivic.ve.

0953-8984/96/428067+06$19.50

reduces the Schrödinger equation $H\Psi = E\Psi$ to the following second-order ordinary differential equation:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \left(m^2 - \frac{1}{4}\right)\frac{1}{\rho^2} + \frac{\gamma^2\rho^2}{4} - \frac{2}{\rho} + m\gamma - E\right]u(\rho) = 0. \tag{3}$$

It is well known that exact solutions of equation (3) cannot be expressed in closed form in terms of special functions. There are analytical expressions for the energy for particular values of γ and m, as pointed out by Lozanskii and Firsov [1] and more recently by Taut [2, 3]. Because of the importance of the problem in question, different techniques have been used in order to obtain the eigenvalues E in equation (3). In addition to numerical and perturbation methods [4, 5], the two-point Padé approximation [6, 7] has been shown to be of help in computing the different values of the energy not only in the regimes where the magnetic field is strong or negligible, but also for intermediate magnetic field strengths. Recently, Mustafa [10] has computed the energy levels for a 2D donor impurity in the presence of a magnetic field. Using the shifted $1/N$ expansion method proposed by Imbo *et al* [8], with an N-dimensional Hamiltonian [9], he obtains the 1s, $2p^-$ and $3d^-$ energy levels, showing that his results are in good agreement with those reported by Martín *et al* [7]. There is disagreement for the $2p^-$ ($m = -1$, $n_\rho = 0$) and $3d^-$ ($m = -2$, $n_\rho = 0$) states as $\gamma \to 0$. Mustafa claims that such a disagreement could be attributed to a bad selection of the magnetic quantum number n made by Martín *et al.* In order to reinforce his thesis, he refers to the work by Whittaker and Elliot [4] which takes into account the modification of the Landau levels due to the presence of impurities. It is the purpose of the present article to show that the disagreement reported by Mustafa cannot be imputed to the choice of the quantum number n_ρ instead of n [11], nor to the presence of impurities in the model, and in fact may be due to a simple computational error. Mustafa uses expression (1) as his Hamiltonian, without the 'impurity' correction proposed by Whittaker ($[(m_h - m_e)/(m_h + m_e)]m\gamma$ instead of $m\gamma$ in the term γL_z of (1)). Therefore the Hamiltonian used by Mustafa coincides with that presented by Martín *et al.* Since neither the Martín nor the Mustafa results are accurate, we will determine the validity of these methods by means of the Schwartz [12] interpolation technique as well as the well known variational method [13].

In order to apply the variational method to our problem, we look for a trial wave function. Since equation (3) reduces to the hydrogen atom equation when $\gamma = 0$, we can consider as a basis for $\gamma \ll 1$ the hydrogen wave funtions Ψ_H. Since $\langle \Psi_H | H | \Psi_H \rangle < E$, we obtain an upper bound of the energy for small values of the parameter γ. The solution of equation (3) when $\gamma = 0$ is

$$u_H(\rho) = D_{m,n}\mathrm{e}^{-\rho/(1/2+n_\rho+|m|)}\rho^{(|m|+1/2)}L\left(n_\rho, 2|m|, \frac{2\rho}{(1/2+n_\rho+|m|)}\right) \tag{4}$$

where $D_{m,n}$ is a normalization constant, and $L(a, b, x)$ are the Laguerre polynomials [14]. Consequently the energy spectrum in the zero-field limit takes the form

$$E_H = -\frac{1}{(1/2+n_\rho+|m|)^2}. \tag{5}$$

Conversely, for large values of γ, a good trial basis is that of the spherical oscillator. In this case the solution of equation (3) has the form

$$u_{osc}(r) = C_{m,n}\mathrm{e}^{-\gamma\rho^2/4}\rho^{(|m|+1/2)}L\left(n_\rho, |m|, \frac{\gamma}{2}\rho^2\right) \tag{6}$$

and, in the high-field limit, the energy levels are

$$E_{osc} = \gamma(2n_\rho + |m| + m + 1). \tag{7}$$

Then, for the state 1s ($m = 0$, $n_\rho = 0$) the two trial functions to be used for small and large values of γ are respectively

$$u_{H(1s)} = 4\mathrm{e}^{-2\rho}\rho^{1/2} \qquad u_{osc(1s)} = \sqrt{\gamma}\mathrm{e}^{-(1/4)\gamma\rho^2}\rho^{1/2}. \tag{8}$$

Substituting (8) into the expression

$$\langle u_{H,osc}\,|H|\,u_{H,osc}\rangle = \tilde{E}_{H,osc} \tag{9}$$

where the tilde indicates that the energy is obtained via the variational method, we readily obtain

$$\tilde{E}_{H(1s)} = -4 + \frac{3}{32}\gamma^2 \qquad \tilde{E}_{osc(1s)} = -\sqrt{2\pi\gamma} + \gamma. \tag{10}$$

Analogously, we have for the $2p^-$ level ($m = -1$, $n_\rho = 0$)

$$u_{H(2p^-)} = 2^{7/2}3^{-5/2}\mathrm{e}^{-2\rho/3}\rho^{3/2} \qquad u_{osc(2p^-)} = \sqrt{\frac{\gamma}{2}}\mathrm{e}^{-(\gamma/4)\rho^2}\rho^{3/2} \tag{11}$$

which, after substituting into (9), gives as the result

$$\tilde{E}_{H(2p^-)} = -\frac{4}{9} + \frac{45}{16}\gamma^2 - \gamma \qquad \tilde{E}_{osc(2p^-)} = -\frac{1}{2}\sqrt{2\pi\gamma} + \gamma. \tag{12}$$

Finally, we proceed to compute the energy spectrum for the $3d^-$ level ($m = -2$, $n_\rho = 0$). In this case the trial wave function takes the form

$$u_{H(3d^-)} = 2^{9/2}5^{-7/2}3^{-1/2}\mathrm{e}^{-2\rho/5}\rho^{5/2} \qquad u_{osc(3d^-)} = 2^{-3/2}\gamma^{3/2}\mathrm{e}^{-(1/4)\gamma\rho^2}\rho^{5/2} \tag{13}$$

and substituting (13) into (9) we obtain

$$\tilde{E}_{H(3d^-)} = -\frac{4}{25} - 2\gamma + \frac{525}{32}\gamma^2 \qquad \tilde{E}_{osc(3d^-)} = -\frac{3}{8}\sqrt{2\pi\gamma} + \gamma. \tag{14}$$

The numerical computations of the energy spectra associated with equation (3) will be carried out with the help of the Schwartz method [12] which is a generalization of the mesh point technique for numerical approximation of functions. This method gives highly accurate results given a thoughtful choice of the reference function. For equation (3) we chose as the interpolation function

$$f(\rho) = \sum_m f_m \frac{u(\rho)}{(\rho - r_m)a_m} \tag{15}$$

where

$$u(\rho) = \sin[\pi(\rho/h)^{1/2}]. \tag{16}$$

r_m is a zero of $u(\rho)$, a_m is a zero of its derivative, and h is the step of the quadratic mesh. The use of this scheme for equation (3) leads to an algebraic eigenvalue problem, giving as a result a non-symmetric matrix to be diagonalized in order to obtain the energy values. The accuracy of this technique has been verified using the analytic results obtained by Taut [2] for the excited states. The calculations were performed using up to 500 mesh points and a step of 10^{-5}, obtaining in this way an accuracy of at least eight digits. It is worth mentioning that a finite-difference scheme with a linear mesh of up to 2000 points failed to provide a good estimation of the ground state for the 2D hydrogen atom, probably because of the strong singularity at the origin.

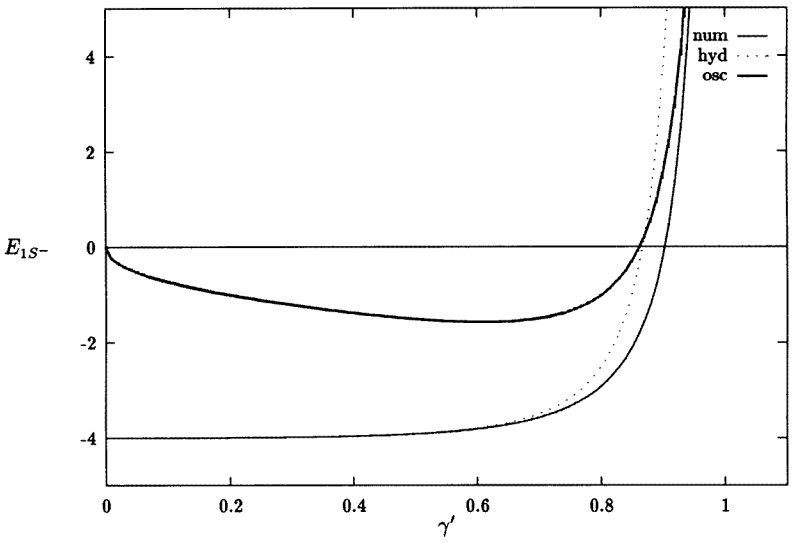

Figure 1. The energy of the 1s state as a function of γ'. The thin solid line was obtained by numerical methods; the dotted line corresponds to the hydrogen basis; and the thick solid line was obtained by using the oscillator as the wave function.

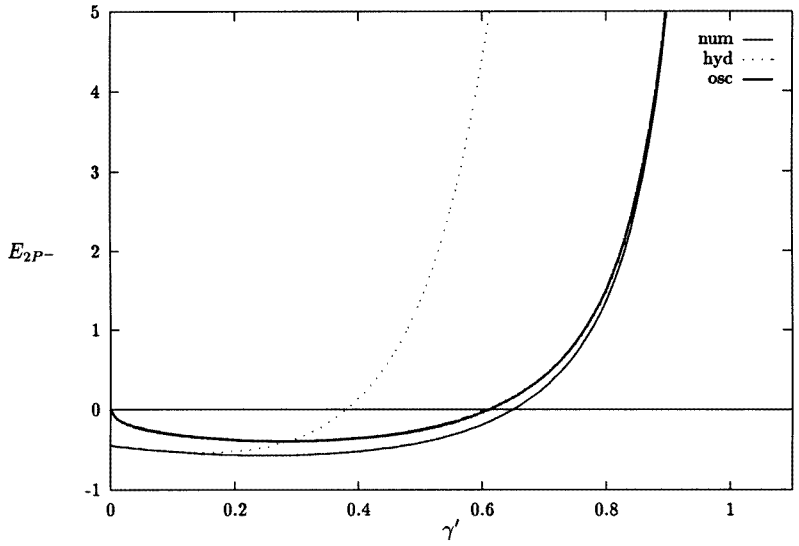

Figure 2. The energy of the $2p^-$ state as a function of the magnetic parameter γ'.

In order to establish a better comparison between the results (10), (12), and (14), and the energy spectra computed with the help of the Schwartz method [12] with those exhibited by Mustafa [10], we plot the energy against $\gamma' = \gamma/(\gamma + 1)$ as the horizontal scale.

As we can see from figure 1, figure 2 and figure 3, no anomalous behaviour in the vicinity of $\gamma = 0$ is observed. Since the energy levels (10), (12), and (14) were obtained

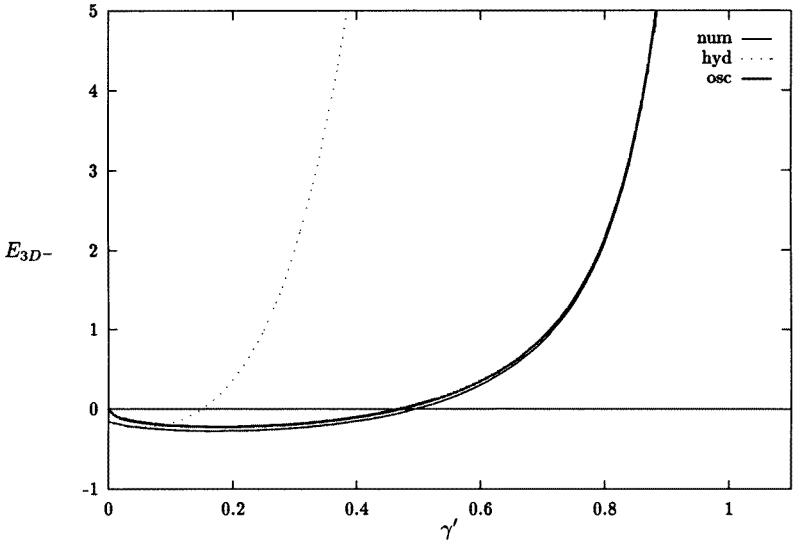

Figure 3. The energy of the $3d^-$ state as a function of γ'.

with the help of the variational method, we have that in the three cases $\tilde{E}_{H,Osc} > E$. It is straightforward to see that the solutions presented by Mustafa [10] satisfy $E_{\text{Mustafa}} > \tilde{E} > E$ as $\gamma \to 0$, and therefore they are ill-behaved for small values of the magnetic field. The variational solution obtained using the hydrogen basis is in good agreement with the results obtained by Martín *et al* and those computed with the help of the Schwartz interpolation technique, which has been shown to be very powerful in obtaining accurate numerical results. It is worth mentioning that the bizarre behaviour reported by Mustafa [10] for the $2p^-$ and $3d^-$ states cannot be imputed to a breakdown of the shifted $1/N$ expansion in the weak-field limit. In fact, using the equations presented by Mustafa [10] based on the results reported by Imbo *et al* [8], with the right quantum numbers for the $2p^-$ ($m = -1$, $n_\rho = 0$) and $3d^-$ ($m = -2$, $n_\rho = 0$) levels, one finds that the shifted $1/N$ method is in good agreement with the results presented in this article and by Martín *et al*.

It would be interesting to analyse the 2D hydrogen problem when the spin and relativistic effects are not negligible. This will be the object of a forthcoming publication.

Acknowledgments

We thank Dr Juan Rivero for helpful discussions. We also want to express our gratitude to an anonymous referee for critical comments.

References

[1] Lozanskii E D and Firsov O B 1974 *Izv. Vyssh. Ucheb. Zav. Fiz.* **6** 52
[2] Taut M 1995 *J. Phys. A: Math. Gen.* **28** 2081
[3] Taut M 1993 *Phys. Rev.* A **48** 3561
[4] Whittaker D M and Elliot R J 1988 *Solid State Commun.* **68** 1
[5] Duggan G 1988 *Phys. Rev.* B **37** 2759
[6] MacDonald A H and Ritchie D S 1986 *Phys. Rev.* B **33** 8336

[7] Martín P, Rodríguez J J and Márquez J L 1992 *Phys. Rev.* B **45** 8359
[8] Imbo T, Pagnamenta A and Sukhatme 1984 *Phys. Rev.* D **29** 1669
[9] Nieto M M 1979 *Am. J. Phys.* **47** 1067
[10] Mustafa O 1993 *J. Phys.: Condens. Matter* **5** 1327
[11] Boyle W S and Howard R E 1961 *J. Phys. Chem. Solids* **19** 181
[12] Schwartz C 1985 *J. Math. Phys.* **26** 411
[13] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)
[14] Lebedev N N 1972 *Special Functions and Their Applications* (New York: Dover)