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Expansion-variational studies of hydrogenlike systems in arbitrary magnetic fields

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We propose an expansion-variational calculation for the evaluation of the energy spectrum of a hydrogenlike system in an arbitrary magnetic field. A field-dependent hydrogen Landau-type basis has been used for the ground state and the lowest 13 excited states. Such a basis, expressed in parabolic coordinates, leads to analytical calculations. The numerical results have been found accurate in the case of both low- and high-field limit. The method proposed here is believed to be very tractable for more complicated problems.

I. INTRODUCTION

The problem of hydrogenlike systems in an external magnetic field is fundamental in various domains of physics, for instance, solid-state physics[1] and astrophysics.[2] In the low-field limit, both standard perturbation and variational methods have been proved to be valid,[3] while people generally use adiabatic techniques in the high-field limit.[4] In the past few years, a great deal of work has been done to obtain the energy values and the wave functions of the system in the whole range of field strength from unified calculations.

Reviewing these efforts, one needs to distinguish between two different methods. The first one refers to the variational method and was widely used by Yafet, Keyes, and Adams,[5] Larsen,[6] Pokatilov and Rusanov,[7] Aldrich and Greene,[8] Gallas,[9] Cohen and Herman,[10] and Kais.[11] Choosing some adequate trial functions, one obtained rather easily the energy values of the ground state and of some excited states. The second one named "expansion-perturbation method" was used by Cabib, Fabri, and Fiorio,[12] Praddaude,[13] Simola and Virtamo,[14] Rosner, Wanner, Herold, and Ruder.[15] Using one or two suitable expansion(s) of the wave function and numerical integrations, this method allows one to calculate the energy value of a given state accurately.

Since the accuracy of the variational methods depends on the choice of the wave function used as trial function to solve a given problem, one must select a "good" wave function. But in this case, the problem is generally to keep a right balance between simplicity and accuracy. Simple calculations give a clear physical picture, but the results are not so accurate. Increasing the number of variational parameters, one obtains better solutions for the excited states but the clear physical picture is lost. In contrast to the variational method, the expansion-perturbation approach can give accurate values of most energy levels, however, it does not provide a simple description of the system. Moreover, the extension of this method is not so easy, even for standard problems like, e.g., a real exciton in a semiconductor, and it also often involves elaborated calculations.

From the above arguments, we will try to answer the following questions in this paper.

(i) What is the best way to combine the usual variational method and the expansion-perturbation calculation?

(ii) How does one get a unified insight for the evolution of the complete energy spectrum of the system in the whole range of field strength? It will be shown that an improved expansion-variational calculation can give satisfactory answers, both for the description of the physical system and the accuracy of the energy levels.

The paper is organized in the following way: In Sec. II we present a general theory of the expansion-variational method. Taking a new expansion of a set of field-modulated and distance-scaled hydrogenic wave functions, we calculate the energy levels of the system after a two-dimensional optimization search procedure. Then, in Sec. III, we give the results obtained for the ground state and the lowest 13 excited states. This is followed by some comparisons and discussions with earlier results. All details of the calculation have been given in the Appendix.

II. THEORY

We start with the spinless Hamiltonian of a hydrogenic system in a magnetic field. Using the effective rydberg ($R_0^* = \mu e^4/2\hbar^2\epsilon^2$) as a unit of energy, the effective Bohr radius ($a_0^* = \epsilon\hbar^2/\mu e^2$) as a unit of length, this can be expressed as

$$\mathscr{H} = -\nabla^2 - \frac{2}{r} + \gamma L_z + \frac{\gamma^2}{4}(x^2+y^2) , \tag{1}$$

where $L_z = -i\,\partial/\partial\varphi$ is the z component of the angular momentum operator and the dimensionless parameter γ is the reduced field strength ($\gamma = e\hbar H/2c\mu R_0^*$), where ϵ is the static dielectric constant and μ is the reduced mass of the system. $\gamma = 1$ for $H = 2.35\times10^5$ T in the case of the hydrogen atom in vacuum and for $H = 23.5$ T in the case of a real exciton in a model semiconductor with $\mu = 0.1m_0$ and $\epsilon = 10\epsilon_0$.[16]

All eigenstates of the system can be classified according to the symmetry of the Hamiltonian. Here, $\mathscr{H}$ commutes with L_z and has cylindrical symmetry for all γ, so L_z is a momentum constant and the eigenstates must have a definite parity.

We first write down the trial functions in the parabolic coordinates (ξ,η,φ),

$$\Psi=\frac{1}{\sqrt{2\pi}}e^{im\varphi}\psi(\xi,\eta)\ , \tag{2}$$

where $\psi(\xi,\eta)$ has the appropriate parity given an eigenvalue m for L_z. Next, we expand $\psi(\xi,\eta)$ in terms of a set of hydrogenic states $|\chi_j\rangle$ which are all assumed to be distance scaled and modulated by a field-dependent exponential factor

$$|\psi\rangle=\sum_j c_j\,|\chi_j\rangle\ , \tag{3}$$

$$\chi_j=e^{-\alpha\xi\eta}\phi_j(\beta\xi,\beta\eta)\ . \tag{4}$$

Here, $\phi_j(\beta\xi,\beta\eta)$ are the field-free distance-scaled (by β) hydrogenic eigenfunctions. The summation on j extends over all hydrogenic states having identical parity. The two positive variational parameters α and β vary with the field strength. It is expected that $\alpha\rightarrow 0$ and $\beta\rightarrow 1$ when $\gamma\rightarrow 0$. Some discussion about these parameters will be found in Sec. III.

Now the Schrödinger equation of the physical system can be transformed into the following form:

$$\frac{1}{\sqrt{2\pi}}e^{im\varphi}\sum_j c_j e^{-\alpha\xi\eta}[\beta^2\mathscr{H}_0+\mathscr{H}'-E]\phi_j(\beta\xi,\beta\eta)=0\ , \tag{5}$$

where $\mathscr{H}_0$ is the well-known hydrogenic Hamiltonian, and $\mathscr{H}'$ depends on the field strength. Under parabolic coordinates[17]

$$\mathscr{H}_0=-\frac{4}{u+v}\left[\frac{\partial}{\partial u}\left(u\frac{\partial}{\partial \mu}\right)+\frac{\partial}{\partial v}\left(v\frac{\partial}{\partial v}\right)+1-\frac{m^2}{4}\left(\frac{1}{u}+\frac{1}{v}\right)\right]\ , \tag{6}$$

with

$$(\mathscr{H}_0+n_j^{-2})\phi_j(u,v)=0\ , \tag{7}$$

n_j is the principal quantum number, $u=\beta\xi$, and $v=\beta\eta$,

$$\mathscr{H}'=4\left[\left(\alpha+\frac{\gamma}{4}m\right)+\left(\frac{\gamma^2}{16}-\alpha^2\right)\xi\eta+(\beta-1)\frac{1}{\xi+\eta}+\frac{2\alpha\xi\eta}{\xi+\eta}\left(\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}\right)\right]\ . \tag{8}$$

Let us consider the matrix form of Eq. (5) in the representation $|\chi_j\rangle$; we have to calculate two kinds of matrix elements,

$$H_{ij}=\langle\phi_i\,|\,e^{-2\alpha\xi\eta}(\beta^2\mathscr{H}_0+\mathscr{H}')\,|\,\phi_j\rangle\ , \tag{9}$$

$$U_{ij}=\langle\phi_i\,|\,e^{-2\alpha\xi\eta}\,|\,\phi_j\rangle\ . \tag{10}$$

Some useful expressions and relations concerning the wave functions $|\phi_j\rangle$ and these elements are given in the Appendix.

The eigenvalues of Eq. (5) can then be found by solving the secular equation

$$HC=EUC\ , \tag{11}$$

where H and U are the Hamiltonian and overlap matrix, respectively, and C is the eigenvector.

Let us remember that we will have to minimize the energy E from Eq. (11). Given a quantum number m and a parity π, the eigenvalues of interest can be minimized by varying the parameters α and β in a two-dimensional optimization search. In principle, the complete spectrum of eigenvalues and eigenfunctions can be obtained by evaluating the infinite determinant (11) in that way.

III. RESULTS AND DISCUSSION

Before presenting numerical results, let us consider two special cases which are interesting tests.

(i) Simple approximation for the ground state. If we have only the first term in the trial function (3), e.g.,

$$\psi(\xi,\eta)=c_1e^{-\alpha\xi\eta-\beta(\xi+\eta)} \tag{12}$$

we have exactly the trial function used by Pokatilov and Rusanov[7] and Gallas.[18] Using this trial function, the ordinary variational calculation leads to the good approximate energy values of the ground state which are tabulated in column 4 of Table I.

(ii) Calculation without optimization. Let us now restrict the variation of the two parameters in the expansion of the trial function (3): Let $\alpha=\gamma/4$ and $\beta=1$. In this case, we find in Ref. 16 that such an expansion of the wave function can describe a hydrogenlike system in an arbitrary magnetic field. One gets simultaneously the energy levels and the wave functions for both ground and excited states. Clearly, this improved calculation gives more reasonable solutions than that of the one-term perturbation calculation.[19] This can be seen from the comparison of the energy values of the ground state gathered in the second and third columns of Table I. The results in column 2 have been obtained after restriction of the j summation to the first hydrogenic state, we find again the results of Ekardt.[19] The extension of the j summation to the lowest 20 states with identical m and π quantum numbers leads to the values of column 3 in Table I.

Since the trial functions (3) are always based on the hydrogenic functions and have a Landau levellike exponential dependence in a magnetic field, they have the freedom to converge to hydrogenic states at low field and display a continuous evolution in the whole range of fields. From the above two special cases, we see that the dependence of the trial function in the magnetic field is driven by two variational parameters α and β. The α parameter accounts for anisotropic changes of each individual orbital; it varies almost linearly versus field strength in a large range of reduced field parameter. The scaling parameter β, in the hydrogenic functions, accounts for some isotropic changes of the orbitals. In addition to this, Eq. (11) gives rise to coupling between various orbitals so it is expected that our expansion-variational calculation should give accurate values of hydrogen atom levels.

In practice we have limited the j summation in expan-

TABLE I. Comparison of the binding energies (in units of R_0^*) of the ground state in the magnetic field, obtained by various methods.

γ	E_{PT} Ref. 19	E_{EPT} Ref. 16	E_{VAR}[a] Ref. 18	E_{EV} This work	E_{CFF}[a] Ref. 12	E_{RWHR}[a] Ref. 15
0.2	1.200	1.179	1.181	1.181	1.181	1.181
0.5	1.362	1.388	1.394	1.394	1.394	
1.0	1.605	1.649	1.659	1.661	1.662	1.662
2.0	1.995	2.013	2.035	2.041	2.045	2.044
3.0	2.213	2.282	2.314	2.324	2.329	2.329
4.0	2.428	2.502	2.541	2.554	2.562	2.562
5.0	2.608	2.690	2.735	2.751	2.761	
10.0	3.259	3.377	3.448	3.476	3.496[b,a]	3.496
20.0	4.046	4.220	4.351	4.397		4.431
50.0	5.283	5.556	5.892	5.975		
100.0	6.348	6.767	7.367	7.477		7.578

[a] Rounded to three decimals.

[b] Reference 13.

sion (3) to a few terms. We can enlarge the expansion if we need to calculate the energy levels with a greater accuracy. We can also choose a better basis which has eigenvalues and eigenstates closer to the real ones.

For a given state, the minimization is obtained after the following "step-by-step" computational procedure: First, we minimize the corresponding eigenvalues of Eq. (11) by taking $\alpha=\gamma/4$ and $\beta=1$ as initial values in the case of only one term for the trial function (3). Then, the found values of α and β are used as initial values to minimize the energy in the case of a two-term expansion of the trial function (3) and so on. We extend the summation in the trial function in order to obtain better accuracy.

The numerical results, obtained for the ground state with this expansion-variational method, are given in Table I, column 5. We have used an expansion of the trial function (3) up to the lowest six $m=0$ even-parity hydrogen-like basis function. The lowest Landau level has been taken as energy origin. Let us first compare this calculation with the previous one[16] given in column 3, clearly the present calculation gives better results. Remember that 20 $m=0$ even-parity states have been used in order to get the numerical results of column 3 and only 6 for the present calculation. Now, let us compare the data of columns 4 and 5; our expansion-variational method gives high-order corrections to the results obtained by the usual variational method of Ref. 18.

As a final comparison are shown in columns 6 and 7 the corresponding results of Cabib *et al.*,[12] Praddaude,[13] and of a recent most accurate calculation by Rosner *et al.*[15] Despite the simplicity of the present approach, a satisfactory agreement is found between our results and those obtained after more elaborate computations.

Table II displays a comparison of the field dependence of the lowest 13 states above the ground state. These excited states are labeled in column 1 by the asymptotic

TABLE II. Comparison of the energy values (in units of R_0^*) of the 13 lowest states above the ground state in the magnetic field, obtained by various methods.

	$\gamma=0.2$		$\gamma=1$		$\gamma=10$	
State	This work	Ref. 15[a]	This work	Ref. 15[a]	This work	Ref. 15[a]
$2s_0$ (1^+00)	0.296	0.298	0.314	0.321	0.411	0.418
$2p_{-1}$ $(0^-0\bar{1})$	0.500	0.501	0.911	0.913	2.235	2.251
$2p_0$ (1^-00)	0.370	0.370	0.519	0.520	0.760	0.765
$2p_{+1}$ (0^-01)	0.100	0.101	−1.089	−1.087	−17.765	−17.749
$3s_0'$ (1^+10)	0.079	0.083[b]	0.066	0.071	0.076	0.079
$3p_{-1}$ $(1^-0\bar{1})$	0.176	0.182	0.245	0.251	0.358	0.365
$3p_0$ (2^-00)	0.148	0.150	0.178	0.180	0.217	0.220
$3p_{+1}$ (1^-01)	−0.224	−0.218	−1.755	−1.748	−19.642	−19.636
$3d_{-2}$ $(0^+0\bar{2})$	0.362	0.363	0.703	0.706	1.805	1.816
$3d_{-1}$ $(1^+0\bar{1})$	0.263	0.264	0.412	0.413	0.673	0.678
$3d_0'$ (2^+00)	0.144	0.145	0.129	0.132	0.150	0.154
$3d_{+1}$ (1^+01)	−0.137	−0.136	−1.588	−1.587	−19.327	−19.322
$3d_{+2}$ (0^+02)	−0.438	−0.437	−3.297	−3.294	−38.195	−38.184

[a] Rounded to three decimals.

[b] Reference 8.

quantum number corresponding to the zero field case $n_i l_i m(N_1^{\pi} N_2 m)$. The results in columns 3, 5, and 7 are taken in the work of Rosner *et al.*[15] and of Aldrich and Greene.[8] The variational expansion used for $2s_0$, $3s'_0$, and $3d'_0$ states are up to the lowest six (identical parity and m component) hydrogeniclike basis functions. Concerning the remaining levels, we have restricted our expansion to the lowest four corresponding states. Again, a fair agreement is obtained when compared with previous data.

IV. CONCLUSION

We have proposed a two-parameter expansion-variational method in order to treat the problem of hydrogenlike systems in an arbitrary magnetic field. This has been shown to give results in satisfactory agreement with earlier propositions without variational treatment. Moreover, by using only two variational parameters, the present results are the best ones. Furthermore, if we enlarge the expansion terms, the exact solution of the problem should be approached. As a consequence of the choice of the basis states, both wave functions and transition probabilities can be obtained immediately. Finally, this algorithm is expected to be very useful for solving other problems when we have to consider variational calculations.

APPENDIX

Let us write the eigenstates of $\mathscr{H}_0$ in the parabolic coordinates (φ dependence dropped, $u=\beta\xi$, and $v=\beta\eta$) as

$$\phi_i = A_i \exp\left[-\frac{1}{2n_i}(u+v)\right]\left[\frac{uv}{n_i^2}\right]^{|m|/2} \times \mathscr{L}_{N_1+|m|}^{|m|}(u/n_i)\mathscr{L}_{N_2+|m|}^{|m|}(v/n_i) , \tag{A1}$$

where $\mathscr{L}_{N_1+|m|}^{|m|}$ is the Laguerre associated polynomial and A_i is the normalization constant. $n_i = N_1 + N_2 + |m| + 1$ is the principal quantum number and $N_1, N_2 = 0, 1, 2, \ldots$.

If we denote this wave function as $|N_1 N_2 m\rangle$, it can be seen that when $N_1 \neq N_2$ the state $|N_1 N_2 m\rangle$ is doubly degenerate, the states with definite parity are then a linear combination of $|N_1, N_2 m\rangle$ and $|N_2 N_1 m\rangle$ states,

$$|\phi_i\rangle = \frac{1}{\sqrt{2}}(1+\hat{P}_{uv})|N_1 N_2 m\rangle , \tag{A2}$$

where $\hat{P}_{uv}$ is the permutation operator on the variables u and v, with $\hat{P}_{uv}|N_1 N_2 m\rangle = \pm |N_2 N_1 m\rangle$. Let $\hat{\pi} = C_2 \hat{P}_{uv}$ be the parity operator of the system, where $C_2 f(\varphi) = f(\varphi+\pi)$ and it can be verified that (φ-dependence included)

$$\hat{\pi}|\phi_i\rangle = \pi|\phi_i\rangle , \tag{A3}$$

with $\pi = \pm 1$. Here i represents the assembly of the quantum numbers N_1, N_2, π, and m. So we can rename the basic functions $|\chi_i\rangle$ in the expansion (3) as follows:

$$|\chi_i\rangle = |N_1^{\pi} N_2 m\rangle . \tag{A4}$$

Now the symbolical state $|N_1^{\pi} N_2 m\rangle$ represents the hydrogenic function (A2) factorized by a Landau-type exponential factor $e^{-\alpha\xi\eta}$.

From the Hamiltonian $\mathscr{H}_0$, $\mathscr{H}'$, and the equations (5), (7), and (8), we express the matrix elements H_{ij} and U_{ij} in the following form:

$$H_{ij} = 4\left[\left[\alpha + \frac{\gamma}{4}m - \beta^2/4n_j^2\right]S_0 + (\gamma^2/16 - \alpha^2)S_1 + (\beta-1)S_2 + 2\alpha S_3\right] , \tag{A5}$$

$$U_{ij} = S_0 , \tag{A6}$$

with

$$S_0 = \langle\chi_i|\chi_j\rangle , \tag{A7}$$

$$S_1 = \langle\chi_i|\xi\eta|\chi_j\rangle , \tag{A8}$$

$$S_2 = \left\langle\chi_i\left|\frac{1}{\xi+\eta}\right|\chi_j\right\rangle , \tag{A9}$$

$$S_3 = \left\langle\phi_i\left|e^{-2\alpha\xi\eta}\frac{\xi\eta}{\xi+\eta}\left[\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}\right]\right|\phi_j\right\rangle . \tag{A10}$$

Now let us assume

$$\chi_i(\xi,\eta) = A_i \frac{1}{\sqrt{2\pi}} e^{im\varphi} e^{-\alpha\xi\eta - \beta(\xi+\eta)/2n_i} \times P_{N_1 N_2 m}(\beta\xi, \beta\eta) , \tag{A11}$$

where $P_{N_1 N_2 m}(\beta\xi,\beta\eta)$ is a polynomial of ξ and η. It is then a straightforward exercise the reduction of the above integrals into the following forms:

$$J_l^k(a,b) = \int_0^\infty \int_0^\infty \xi^l \eta^k e^{-a\xi\eta - b(\xi+\eta)} d\xi\, d\eta , \tag{A12}$$

with $a=2\alpha$ and $b=\beta(n_i^{-1}+n_j^{-1})/2$ and clearly

$$J_k^l(a,b) = J_l^k(a,b) . \tag{A13}$$

These two-dimensional integrals can be easily transformed into one-dimensional ones,

$$J_l^k(a,b) = l! e^q a^{-(l+1)} b^{l-k} I_l^k(q) , \tag{A14}$$

with

$$I_l^k(q) = \int_q^\infty (y-q)^k y^{-(l+1)} e^{-y} dy \tag{A15}$$

and

$$q = b^2/a .$$

All these integrals can be calculated from the following relations and depend only on the exponential integral $E_i(-q)$.[17]

$$I_l^k(q) = \sum_{i=0}^{k} C_k^{k-i}(-q)^i I_{l-k+i}^0(q) , \tag{A16}$$

$$I_l^0(q) = [1 - q^l e^q I_{l-1}^0(q)]/(l q^l e^q) , \tag{A17}$$

and

$$I_0^0(q) = -E_i(-q) , \tag{A18}$$

$$E_i(-q) = -\int_q^\infty y^{-1} e^{-y} dy . \tag{A19}$$

Initial values of this final integral can be obtained numerically.

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