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Abstract. The well-known hypervirial perturbation method (HPM), based on hypervirial relations and the Hellmann-Feynman theorem, is suitable for the calculation of perturbation corrections of large order for the non-relativistic, spinless, two-dimensional hydrogen-like atom in a uniform magnetic field. We show analytical results in terms of the quantum numbers and large-order corrections for particular states. This approach appears to be simpler and more efficient than the recently proposed one based on the Green's functions for this particular model.

1 Introduction

The two-dimensional hydrogen-like atom in a uniform magnetic field perpendicular to the atomic plane has received considerable attention as a model for excitons in thin materials, such as nano-scale multilayer semiconductor systems. The Schrödinger equation is separable in polar coordinates and has been solved approximately in many different ways [1–13]. Here we are interested in the application of perturbation theory that provides approximate solutions in terms of power series of the field strength that are suitable in the weak-field limit [3, 8, 10–13].

Several authors have obtained perturbation corrections of low order [3, 8, 10, 11, 13] but the most extended calculation was due to Szmytkowski [13] who solved the perturbation equations of first and second order by means of the Green's functions. His analytical results, which are valid for all quantum numbers, suggest that some of the earlier results [10–12] may be wrong. The Green function method is a powerful approach that requires considerable ingenuity and mastery of the technique; however, it appears to be unsuitable for the calculation of perturbation corrections of larger order because it soon becomes rather intractable.

There are other strategies for the calculation of the perturbation corrections for simple quantum-mechanical models that are more efficient [14] and the purpose of this paper is to discuss one of them. Taking into account the interest in the two-dimensional hydrogen-like atom in a magnetic field and the discrepancy between earlier perturbation calculations, the present analysis appears to be fully justified.

In sect. 2 we outline the non-relativistic, spinless model and derive a dimensionless eigenvalue equation for the radial part of the Schrödinger equation that is suitable for the application of perturbation theory. In sect. 3 we briefly develop the chosen perturbation technique and apply it to the model mentioned above. Finally, in sect. 4, we summarize the main results of the paper and draw conclusions.

2 Model

The model consists of a non-relativistic, spinless, two-dimensional hydrogen-like atom in a uniform magnetic field perpendicular to the atomic plane. It may also represent the effective-mass equation for an electron-hole pair in the presence of a uniform magnetic field [1, 2]. For concreteness, in what follows we resort to the notation of Szmytkowski [13] in order to facilitate comparison of the results. In the case of a symmetric gauge the Schrödinger equation is separable in polar coordinates ($0 \leq r < \infty$, $0 \leq \phi < 2\pi$). If we write the eigenfunctions as

$$\psi(r, \phi) = \frac{1}{\sqrt{r}} P(r) \frac{1}{\sqrt{2\pi}} e^{im_l \phi}, \quad m_l = 0, \pm 1, \pm 2, \dots, \quad (1)$$

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the radial part of the Schrödinger equation becomes [13]

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2(l^2 - 1/4)}{2mr^2} + \frac{e\hbar B}{2m} m_l - \frac{Ze^2}{4\pi\epsilon_0 r} + \frac{e^2 B^2 r^2}{8m} \right] P(r) = EP(r), \quad (2)$$

where m and $-e$ are the electron mass and charge, respectively, Ze is the charge of the spinless nucleus (clamped at the coordinate origin), $l = |m_l|$ and B is the field intensity. The bound-state solutions satisfy

$$\lim_{r \rightarrow 0} P(r) = 0, \quad \lim_{r \rightarrow \infty} P(r) = 0. \quad (3)$$

Straightforward application of perturbation theory to eq. (2) is unnecessarily cumbersome because one has to carry all the physical constants and model parameters through the whole algebraic process [13]. For this reason it is preferable to convert eq. (2) into a dimensionless eigenvalue equation. To this end, we define a dimensionless coordinate $q = r/L$, where

$$L = \frac{a_0}{Z}, \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2}, \quad (4)$$

and eq. (2) becomes

$$HP(q) = \epsilon P(q),$$

$$H = \left[-\frac{1}{2} \frac{d^2}{dq^2} + \frac{\xi}{2q^2} - \frac{1}{q} + \lambda q^2 \right], \quad (5)$$

where

$$\epsilon = \frac{mL^2}{\hbar^2} \left(E - \frac{e\hbar B}{2m} m_l \right),$$

$$\xi = l^2 - \frac{1}{4}, \quad \lambda = \frac{e^2 B^2 L^2}{8\hbar^2}. \quad (6)$$

The unit of energy is

$$\frac{\hbar^2}{mL^2} = \frac{Ze^2}{4\pi\epsilon_0 L} = \frac{Z^2 e^2}{4\pi\epsilon_0 a_0} \quad (7)$$

and

$$\frac{e\hbar B}{2m} \frac{mL^2}{\hbar^2} = \sqrt{2\lambda}. \quad (8)$$

If we define

$$B_0 = \frac{\hbar}{ea_0}, \quad (9)$$

then

$$\lambda = \frac{1}{8Z^4} \left(\frac{B}{B_0} \right)^2 \quad (10)$$

enables us to compare the present results with those of Szmytkowski [13]. By means of the perturbation theory we easily obtain the coefficients of the perturbation series

$$\epsilon(\lambda) = \sum_{p=0}^{\infty} \epsilon_p \lambda^p. \quad (11)$$

Note that when we convert the Schrödinger equation into a dimensionless eigenvalue equation, we realize that the natural perturbation parameter is λ and not B .

When $B = 0$ ($\lambda = 0$) the problem is exactly solvable and the allowed energies are given by [13]

$$\epsilon_0 = -\frac{1}{2(n_r + l + 1/2)^2}, \quad (12)$$

where $n_r = 0, 1, \dots$, is the radial quantum number (number of zeroes of $P(r)$). Following previous papers we also define $n = n_r + l + 1$ that resembles the principal quantum number of the three-dimensional hydrogen atom.

The weak-field series (11) is divergent. If we define the new variable $u = \lambda^{1/4}q$ then the dimensionless operator H becomes

$$H = \sqrt{\lambda} \left(-\frac{1}{2} \frac{d^2}{du^2} + \frac{\xi}{2u^2} - \frac{\lambda^{-1/4}}{u} + u^2 \right), \tag{13}$$

which clearly shows that we can also expand the eigenvalues in the strong-field series

$$\epsilon = \sqrt{\lambda} \sum_{j=0}^{\infty} e_j \lambda^{-j/4}, \tag{14}$$

which has a finite radius of convergence.

3 Hypervirial perturbation method

One of the most efficient implementations of perturbation theory for separable problems is the hypervirial perturbation method (HPM) that combines the hypervirial relations and the Hellmann-Feynman theorem. If O is a linear operator, then

$$\langle P | [H, O] | P \rangle = 0 \tag{15}$$

is called a hypervirial relation, where $[H, O] = HO - OH$ is the commutator between such pair of operators [14]. This equation holds if O is chosen so that $\langle P | HOP \rangle = \langle HP | OP \rangle$. Another important ingredient of the method is the Hellmann-Feynman theorem that states that [14]

$$\frac{\partial \epsilon}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle. \tag{16}$$

If

$$H = -\frac{1}{2} \frac{d^2}{dq^2} + \frac{\xi}{2q^2} - \frac{1}{q} + \lambda q^K, \quad K = 1, 2, \dots, \tag{17}$$

and $O = \frac{j+1}{2}q^j - q^{j+1} \frac{d}{dq}$ [14] then eq. (15) becomes

$$2j\epsilon Q_{j-1} + (j-1) \left[\frac{j(j-2)}{4} - \xi \right] Q_{j-3} + (2j-1)Q_{j-2} - (2j+K)\lambda Q_{j+K-1} = 0, \quad j = 1, 2, \dots, \tag{18}$$

where $Q_j = \langle q^j \rangle$. On expanding the expectation values in a Taylor series

$$Q_j = \sum_{p=0}^{\infty} Q_{j,p} \lambda^p, \tag{19}$$

we obtain

$$Q_{j,i} = \frac{1}{2(j+1)\epsilon_0} \left\{ j \left[\xi - \frac{j^2-1}{4} \right] Q_{j-2,i} - (2j+1)Q_{j-1,i} - 2(j+1) \sum_{m=1}^i \epsilon_m Q_{j,i-m} + (2j+K+2)Q_{j+K,i-1} \right\}, \tag{20}$$

$j = 1, 2, \dots$

In addition to this equation we also have

$$Q_{-1,i} = -2\epsilon_i + (K+2)Q_{K,i-1}, \tag{21}$$

which comes from (18) with $j = 1$. It is assumed that $Q_0 = 1$, so that $Q_{0,i} = \delta_{i0}$ is a starting point for the recurrences.

In order to obtain the perturbation coefficients ϵ_i and $Q_{j,i}$ we need an additional equation provided by the Hellmann-Feynman theorem (16)

$$\epsilon_i = \frac{1}{i} Q_{K,i-1}, \quad i = 1, 2, \dots \tag{22}$$

The calculation is straightforward and for $K = 2$ (present case) we obtain

$$\epsilon_1 = \frac{(2n - 1)^2}{8} (-3l^2 + 3 + 5n^2 - 5n), \tag{23}$$

$$\epsilon_2 = -\frac{(2n - 1)^6}{1024} (-21l^4 - 138l^2 + 159 - 90l^2n^2 + 90l^2n + 582n^2 - 439n + 143n^4 - 286n^3), \tag{24}$$

$$\begin{aligned} \epsilon_3 = \frac{(2n - 1)^{10}}{65536} & (17967 - 65495n + 68835n^4 - 107070n^3 + 115970n^2 - 18066l^2 - 35130l^2n^2 \\ & + 29910l^2n + 231l^4 - 132l^6 - 18360n^5 + 6120n^6 + 10440l^2n^3 - 5220l^2n^4), \end{aligned} \tag{25}$$

$$\begin{aligned} \epsilon_4 = -\frac{(2n - 1)^{14}}{16777216} & (15522195 - 67825511n - 4005l^8 + 153888490n^4 - 180523168n^3 + 145662172n^2 \\ & - 17506020l^2 - 64292340l^2n^2 + 43194060l^2n + 1991850l^4 - 4020l^6 - 80558702n^5 + 33863592n^6 \\ & + 43836660l^2n^3 - 26018580l^2n^4 - 1640100l^2n^6 + 4920300l^2n^5 - 502740l^4n^3 + 2563680l^4n^2 \\ & - 2312310l^4n - 3060l^6n^2 + 3060l^6n + 251370l^4n^4 - 6009164n^7 + 1502291n^8), \end{aligned} \tag{26}$$

The first two perturbation corrections agree with those of Szmytkowski [13] to which we added ϵ_3 and ϵ_4 that were not reported before as far as we know. We can obtain as many perturbation corrections as desired by means of the recurrence relations (20), (21) and (22) and available computer algebra software. However, the perturbation corrections in terms of the quantum numbers may probably be too long for any practical use. If one is interested in weak-field expansions of large order it appears to be preferable to obtain them for particular values of n and l by means of those recurrence relations. For example, when $n = 1$ and $l = 0$, we have

$$\begin{aligned} \epsilon_1 = 3/8, \quad \epsilon_2 = -\frac{159}{1024}, \quad \epsilon_3 = \frac{17967}{65536}, \quad \epsilon_4 = -\frac{15522195}{16777216}, \quad \epsilon_5 = \frac{5189052801}{1073741824} \\ \epsilon_6 = -\frac{4896676641339}{137438953472}, \quad \epsilon_7 = \frac{3094900497137871}{8796093022208}, \quad \epsilon_8 = -\frac{20233178231139761499}{4503599627370496}, \\ \epsilon_9 = \frac{20808558827825859998445}{288230376151711744}, \quad \epsilon_{10} = -\frac{52693485465369543566065089}{36893488147419103232}, \\ \epsilon_{11} = \frac{80639435078901048406195920633}{2361183241434822606848}, \quad \epsilon_{12} = -\frac{587353055515797037508553136130823}{604462909807314587353088}, \\ \epsilon_{13} = \frac{1255613239147236284205667622925365349}{38685626227668133590597632} \\ \epsilon_{14} = -\frac{622966805761998001055555519950165544755}{4951760157141521099596496896} \\ \epsilon_{15} = \frac{17753264589549239693872523415436400485638255}{316912650057057350374175801344} \\ \epsilon_{16} = -\frac{921721759137179716887942948086717222595277533675}{324518553658426726783156020576256} \\ \epsilon_{17} = \frac{3379056665253674076167201632469154672196055608756005}{20769187434139310514121985316880384} \\ \epsilon_{18} = -\frac{27797116247667972439940810526714208588100705850127986405}{2658455991569831745807614120560689152} \\ \epsilon_{19} = \frac{127484555261829518463134910686385252583016203699835125715445}{170141183460469231731687303715884105728} \\ \epsilon_{20} = -\frac{2593203450314371618931792865686398116783507010792581025252777725}{43556142965880123323311949751266331066368}. \end{aligned} \tag{27}$$

The only purpose of showing these expressions here is just to provide a benchmark for anybody interested in the application of present approach. All the perturbation corrections can be easily and straightforwardly calculated by means of the recurrence relations (20), (21) and (22) [14].

It is worth noting that the HPM cannot be applied to the operator (13) for the calculation of the strong-field series (14). The reason is that the unperturbed operator $H_0 = \lim_{\lambda \rightarrow \infty} \lambda^{-1/2} H$ is an even function of the coordinate u and therefore the recurrence relations do not yield the expectation values $U_j = \langle u^j \rangle$ for odd and even j necessary for the application of the technique and the calculation of U_{-1} .

4 Conclusions

The calculation of perturbation corrections of large order by means of the Green's functions does not appear to be practicable. On the other hand, the HPM yields simple straightforward recurrence relations for the systematic calculation of the perturbation corrections to the energy and expectation values of powers of the coordinate. These recurrence relations are suitable for programming in available computer algebra systems which greatly facilitates the systematic calculation of those perturbation corrections to any desired order. It is worth mentioning that the HPM applies to the Schrödinger equation that is suitable for deriving the necessary hypervirial relations. It is not, at present, clear whether this approach (or a suitable variant) can be successfully applied to the relativistic Dirac equation recently treated by means of perturbation theory [15]. In this case the author resorted to the Sturmian expansion of the two-dimensional generalized radial Dirac-Coulomb Green function.

Present results agree with those of Szmytkowski [13] and not with those derived by other authors by means of the Levi-Civita transformation of the coordinates and the expression of the resulting two-dimensional Hamiltonian operator in terms of suitable creation-annihilation operators [10–12]. We have no doubt that their weak-field expansions do not agree with the actual ones. For example, the weak-field expansions derived by Hoang *et al.* [12] are not correct because they come from approximate variational expressions for the energies. However, it is worth mentioning that for sufficiently large field intensities they fit the actual eigenvalues more accurately than the exact weak-field expansions that are strongly divergent.

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