The Hydrogen Atom in a strong Magnetic Field: A Quantitative Measure of Quantum Chaos

A. A. Kotzé

Department of Applied Mathematics
Rand Afrikaans University
PO Box 524
Aucklandpark 2006
South Africa

March 1993

Abstract

The coupling matrix elements of a chaotic Hamilton system play a crucial role in describing the chaotic behaviour where the coupling elements are related to the imaginary parts of the exceptional points. The relationship between the coupling matrix elements and the avoided level crossings is investigated. From this analysis a quantitative measure of the quantum chaotic behaviour for degenerate systems of the form $H_0 + \lambda H_1$ is defined. This measure is a function of the interaction strength λ, the density of exceptional points and coupling matrix elements. Its implementation is demonstrated considering the hydrogen atom in a strong magnetic field which is known to be chaotic.

1 Introduction

In a series of previous papers the connection between the occurrence of statistical properties of the spectrum ascribed to quantum chaos and the exceptional points of the Hamilton operator $H_0 + \lambda H_1$ has been discussed [1, 2, 3]. The exceptional points of the operator are the points λ for which two eigenvalues coalesce in the complex λ-plane. The exceptional points are a distinct property of the Hamilton operator where we exclude genuine degeneracies. It has been argued that quantum chaotic behaviour is expected to occur generically for those real λ-values where a high density of exceptional points is found in the complex λ-plane. Furthermore, it has been shown that the ranges of λ-values where this happens can be determined from the knowledge of the two operators H_0 and H_1 alone. The connection between the distribution of exceptional points and the emergence of quantum chaos is seen as the fundamental mechanism that produces quantum chaos as far as operators of the form $H_0 + \lambda H_1$ are concerned [3, 4]. Here λ can play the role of a perturbation parameter or it may serve to effect a phase transition or it may , under variation, steer the system from an ordered into a chaotic regime.

Guhr and *Weidenmüller* argued that there are two physical quantities that prescribe the behaviour of a system: the density of states and the coupling matrix elements [5]. The density of exceptional points is an indication of the density of states and the coupling matrix elements determine in particular the imaginary parts of the exceptional points which in turn determine the fluctuation properties of the spectrum [6]. It is the aim of this paper to investigate the relation between the coupling matrix elements and the avoided level crossings of a Hamilton system where symmetries relating to H_0 and H_1 or both impose a particular structure on the full problem $H_0 + \lambda H_1$. Taking the density of exceptional points into account leads to the definition of a quantitative measure whereby the *quantum chaotic behaviour of a degenerate system can be quantified*.

As an application the hydrogen atom in a strong magnetic field is used. In a previous paper the density of exceptional points was obtained for this system [7]. The results showed that the symmetries relating to H_0 and H_1 play an important role in the behaviour in that there are regions in the spectrum where the density of exceptional points is high but the behaviour is nonchaotic. This seems to contradict the aforementioned argument in that a high density of exceptional points is a prerequisite for the occurrence of quantum chaos [1]. This discrepancy is explained through the measure defined which sheds more light onto the intriguing behaviour of this system. We will also show that the results are in line with known quantum results for this system.

2 The Effect of the Coupling Matrix Elements

The correspondence between the exceptional points and the avoided level crossings, which determine the fluctuation properties of the spectrum, is known [6]. In order to gain insight into the behaviour of the coupling matrix elements and their effect onto the spectrum, we investigate their relationship with the avoided level crossings for a degenerate system. This problem is illuminated by first considering a simple two dimensional model.

Let the eigenvalues of H_0 be denoted by ϵ_1 and ϵ_2 where 1 and 2 can be related to a quantum number say n. Because H_0 is diagonal, it is reducible into two subspaces both of dimension one. These subspaces are characterized by the quantum number n and we term them as n-subspaces. For very small λ we use perturbation theory and the coupling between the different n-subspaces can be neglected up to a first order approximation. H_1 is then in block diagonal form and also reducible into two n-subspaces both of dimension one. The eigenvalue of H_1 in the first subspace is denoted by δ_1 and that in the second subspace by δ_2. H_1 is of the form

$$H_1 = \begin{pmatrix} \delta_1 & C \\ C & \delta_2 \end{pmatrix} \tag{1}$$

where C denotes the coupling between the eigenvalues (different n-subspaces). For problems with dimensions higher than two, a more general form of H_1 exists, namely

$$\begin{pmatrix} \begin{bmatrix} \delta_1^s & & & \mathbf{0} \\ & \delta_2^s & & \\ & & \ddots & \\ \mathbf{0} & & & \delta_u^s \end{bmatrix} & \begin{bmatrix} C & \cdots & \cdots & C \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ C & \cdots & \cdots & C \end{bmatrix} \\ \begin{bmatrix} C & \cdots & \cdots & C \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ C & \cdots & \cdots & C \end{bmatrix} & \begin{bmatrix} \delta_1^t & & & \mathbf{0} \\ & \delta_2^t & & \\ & & \ddots & \\ \mathbf{0} & & & \delta_v^t \end{bmatrix} \end{pmatrix}$$

where s and t are adjacent subspaces. This matrix is equivalent to (1) if $u = v = 1$. This specific form of H_1 will later be used to define an appropriate measure for the coupling strength.

Returning to the two dimensional case, the matrix representation of H is

$$H(\lambda) = \begin{pmatrix} (\epsilon_1 + \lambda\delta_1) & \lambda C \\ \lambda C & (\epsilon_2 + \lambda\delta_2) \end{pmatrix} \tag{2}$$

with eigenvalues ξ given by

$$\xi_{1,2} = \frac{1}{2}[(\epsilon_1 + \epsilon_2) + \lambda(\delta_1 + \delta_2)] \pm \frac{1}{2}\sqrt{[(\epsilon_2 - \epsilon_1) + \lambda(\delta_2 - \delta_1)]^2 + 4\lambda^2 C^2}.$$

The exceptional point for this two dimensional matrix H is given at the λ-value where the discriminant vanishes [3] and

$$\lambda_c = \frac{\epsilon_2 - \epsilon_1}{\delta_1 - \delta_2 \pm 2iC} = -\Delta\epsilon \frac{\Delta\delta \pm 2iC}{\Delta\delta^2 + 4C} \tag{3}$$

where $\Delta\epsilon = \epsilon_2 - \epsilon_1$ and $\Delta\delta = \delta_2 - \delta_1$. If $C \ll \Delta\delta$ we have from Eq.(3)

$$\Re\lambda_c = -\frac{\Delta\epsilon}{\Delta\delta}; \quad \Im\lambda_c = \pm 2C; \quad \tan\varphi = \frac{2C}{\Delta\delta} \tag{4}$$

with $\Re\lambda_c$ denoting the real and $\Im\lambda_c$ the imaginary part of λ_c. It is known that to evoke chaos, the imaginary part of the exceptional point has to be appreciable in size [3]. Eq.(4) shows that small coupling will give a small $\Im\lambda_c$ and a small angle φ. The exceptional point thus lies close to the real axis and the avoided crossing is not appreciable. The two levels are too close to one another and the avoided level crossing is nearly an exact crossing which can not lead to chaotic behaviour.

To determine the effect of the coupling C on the avoided crossing we determine the minimum of the spacing between the two levels which is given by

$$\Delta\xi = \xi_2 - \xi_1 = \sqrt{(\Delta\epsilon + \lambda\Delta\delta)^2 + 4\lambda^2 C^2}; \quad \text{at } \lambda = \Re\lambda_c.$$

By eliminating $\Delta\delta$ we obtain

$$\Delta\xi = \left[\frac{\Delta\epsilon^2}{2} - \frac{\Delta\epsilon}{2}\sqrt{\Delta\epsilon^2 - (4\Re\lambda_c C)^2}\right]^{\frac{1}{2}}. \tag{5}$$

Eq.(5) shows that if $\Delta\epsilon$ and C are both fixed, the spacing between the levels $\Delta\xi$ widens the larger $\Re\lambda_c$. Also, $\Re\lambda_c$ is fixed, the spacing can be enlarged by enlarging C. From these findings and the form of Eq.(5) we now conclude that the relevant parameter in determining the minimum spacing $\Delta\xi$ (of the avoided level crossing) is given by $\mathcal{B}$ *viz.*

$$\mathcal{B} \propto \lambda \cdot C. \tag{6}$$

If $\mathcal{B}$ is small we expect the avoided crossing to have a small gap (the levels nearly cross actually) and, if this happens on a large scale, to be outside the chaotic regime; in turn, for a larger value of $\mathcal{B}$ the gap size increases and the behaviour tends to be chaotic. These arguments are general and can also be applied to higher dimensions.

3 A Quantitative Measure for Quantum Chaos

For Eq.(6) to be used as a meaningful measure for the spectral behaviour of a high dimensional system we have to find a suitable measure of the coupling strength C. This is achieved by transforming H_1 to H_1' having a similar form than (1). This is done through the following transformation

$$H_1' = U_{n_{\max}}^{-1} \cdots U_2^{-1} \cdot U_1^{-1} \cdot H_1 \cdot U_1 \cdot U_2 \cdots U_{n_{\max}} \tag{7}$$

where the different U matrices commute with one another and $n_{\max}$ is the maximum quantum number n considered. U_k is an orthogonal matrix such that

$$U_k = \begin{pmatrix} 1 & 0 & \cdots & & & & & \cdots & 0 \\ 0 & \ddots & 0 & & & & & & \vdots \\ \vdots & 0 & 1 & & & & & \cdots & 0 \\ & & & u_1^1 & u_1^2 & \cdots & u_1^{M_k} & & \\ & & & u_2^1 & u_2^2 & \cdots & u_2^{M_k} & & \\ & & & \vdots & \vdots & \ddots & \vdots & & \\ & & & u_{M_k}^1 & u_{M_k}^2 & \cdots & u_{M_k}^{M_k} & & \\ 0 & \cdots & & & & & & 1 & 0 \\ \vdots & & & & & & & \ddots & \vdots \\ 0 & \cdots & & & & & & 0 \;\; \cdots & 1 \end{pmatrix} \tag{8}$$

which is a unit matrix except for the matrix in place of the k-th block and M_k denotes the dimension of the k-th subspace. The k-th block in (8) is the orthogonal matrix that diagonalizes the k-th block of H_1 with no n coupling and H_1 rotated to the basis of diagonal H_0. We stress the fact here that H_1' can only be obtained if H_0 is diagonal and degenerate.

A quantitative measure for the strength of the coupling can be obtained if we assume that the n-coupling between individual elements of different blocks are small. H_1' is also in semiblock form and we only have to consider the coupling between the diagonal blocks as a whole. As a reasonable measure of the coupling between nearest neighbour diagonal blocks of H_1' we use the norm of the off-diagonal block matrices *viz.*

$$\bar{C}^{(i)} = \frac{1}{sr} \sum_{k=1}^{s} \sum_{l=1}^{r} |C_{kl}^{(i)}|; \quad i = 1, 2, \ldots, n_{\max} - 1. \tag{9}$$

Here, C_{kl} denotes the elements of the off-diagonal block matrices of H_1' with s the number of rows and r the number of columns of the i-th block.

The density of states also plays a crucial role and has to be incorporated into any measure of the behaviour [5]. We now propose the following quantity to be taken as a measure for the chaotic behaviour

$$\mathcal{B} \propto \lambda \cdot \bar{C} \cdot d \tag{10}$$

where d denotes the density of states and $\bar{C}$ the coupling as defined in Eq.(9). Eq.(10) measures the average gap between levels that cross in the complex E-plane i.e., *the amount by which the levels repel one another*. $\mathcal{B}$ is dimensionless in the sense that the unit of $\bar{C}$ is energy and that of d is number of states per unit energy interval. We expect regular behaviour if $\mathcal{B}$ is small and chaotic behaviour if $\mathcal{B}$ has an appreciable value.

Because of the physical relevance of the exceptional points in describing chaotic behaviour, we prefer to use the density of exceptional points rather than the density of states. A precise theoretical relation between the density of states and the density of exceptional points has not yet been established but it can be determined for a particular system under investigation. The measure defined in Eq.(10) will now be tested on a system that is known to chaotic, classically and quantally.

4 The Hydrogen Atom in a Strong Magnetic Field

As an application to the arguments above we investigate the behaviour of the hydrogen atom in a strong magnetic field by implementing the measure defined in Eq.(10).

4.1 The System and Matrix Representation

In the subspace for positive parity with $m = 0$, the Hamiltonian is given by (using atomic units, spherical coordinates and a field in the z-direction) [7, 8]

$$H = H_0 + \lambda H_1 \tag{11}$$

with (scaled by a factor 2)

$$\begin{aligned} H_0 &= p^2 - \frac{2}{r} \\ H_1 &= \frac{1}{4} r^2 \sin^2\theta \end{aligned} \tag{12}$$

with λ a dimensionless parameter depicting the field strength. In Eq.(12) H_0 is just the expression for the ordinary Hydrogen atom and H_1 describes the quadratic Zeeman effect. *Wintgen* and *Friedrich* showed that the quantum behaviour of the system is only dependent on a scaled energy ε (similar to the classical behaviour) [9] where

$$\lambda = \left(\frac{\varepsilon}{E}\right)^{-3} = (\varepsilon n^2)^{-3} \tag{13}$$

with E the energy. The system is nonchaotic for $\varepsilon = -0.8$ but shows a transition to chaotic behaviour at $\varepsilon \approx -0.35$ and is fully chaotic at $\varepsilon = -0.1$.

In order to determine the density of exceptional points and coupling matrix elements, we need a matrix representation of this system [1]. This is achieved through using Sturmian functions of the form [7, 10]

$$G_{nl}^{(\zeta)}(r) = \zeta^{\frac{3}{2}} \sqrt{\frac{(n-l-1)!}{(n+l+1)!}}\; e^{-\zeta r/2} [\zeta r]^l L_{n-l-1}^{2l+2}(\zeta r) \tag{14}$$

as radial eigenfunctions with n the principle quantum number. We have $n = 1, 2, \ldots, n_{\max}$ with $n_{\max}$ the maximum quantum number n considered in our truncated matrix space and $l = 0, 2, \ldots, n-1$. Here $L_{n-l-1}^{2l+2}(\zeta r)$ denote the generalised Laguerre polynomials with ζ a positive real parameter which is used to increase convergence and accuracy. Choosing $\zeta = 2/n^*$ results in accurate eigenvalues in the vicinity of n^* where $n^* \leq n$ [11]. Using the basis (14) leads to an H_0 which is not diagonal. We, however, need a representation with H_0 diagonal [1]. The diagonalization and corresponding rotation of H_1 is done numerically.

4.2 Implementation of the Measure

In implementing $\mathcal{B}$ in Eq.(10) we have to determine the n behaviour of d and $\bar{C}$. The coupling matrix elements as given by Eq.(9) are illustrated in Fig.(1). Here $\bar{C}$ is drawn as a function of n where $n_{\max} = 90$ and $n^* = 40$ ensuring very accurate eigenvalues in the vicinity of $n = 40$. In Fig.(1) $\bar{C}$ is fitted numerically by

$$\bar{C}_1'(n) = -0.0624n - 0.4889n^2 + 0.2821n^3 \tag{15}$$

and the leading term is cubic in n. Also plotted are the coupling due to the second off-diagonal blocks. The fitted relation is

$$\bar{C}_2'(n) = 1.1938n - 0.3585n^2 + 0.0776n^3.$$

This shows that they are much smaller than $\bar{C}$ (the larger n the more so) and can thus be neglected. It is evident that the smaller n the smaller the coupling. In using the definition given in (9) we also calculated the coupling between next nearest blocks on the diagonal. This coupling was found to be appreciably smaller than the nearest neighbour coupling justifying the assumption to neglect it.

Eq.(15) shows that when n is small, the coupling is so small that it can suppress the chaotic behaviour as characterized by $\mathcal{B}$ in (6). When n is larger though, the coupling is larger but λ can be smaller and the chaotic behaviour is also suppressed.

The n-behaviour of d is determined by considering its inverse, the mean level spacing. The leading term of the mean level spacing is $1/n^3$ and hence the leading term for d is n^3. The n-behaviour of $\mathcal{B}$ is now obtained as follows: if ε is kept fixed, $\lambda \sim n^{-6}$, $d \sim n^3$, $\bar{C} \sim n^3$ and the n-behaviour of $\mathcal{B}$ is constant in n. We can thus put

$$\mathcal{B} = \lambda \cdot \bar{C} \cdot d \tag{16}$$

which can now be taken as the appropriate measure for the behaviour of the system because of the previous arguments.

Kotzé and *Heiss* described an approximate method to determine the density of exceptional points P for this system [7]. They found the density to be only dependent on the scaled energy ε where the leading term is cubic in n *viz.*

$$P = an + bn^2 + cn^3.$$

Now, by putting $d = P$ in Eq.(16) we have

$$\mathcal{B}' = \lambda \cdot \bar{C} \cdot P = \varepsilon^{-3} \cdot n^{-6} \cdot \bar{C} \cdot P \tag{17}$$

which is also constant in n if ε is fixed. This is also reflected in the numerical analysis and the corresponding graph drawn in Fig.(2) which is a plot of $\mathcal{B}'$ versus n where we used a logarithmic scale on the vertical axis. We stress the fact that $\mathcal{B}'$ is easily obtainable from H_0 and H_1 alone.

Each line is obtained for a different value of ε and is constant in n. The larger ε the more chaotically the system behaves which is reflected in the higher $\mathcal{B}'$-values. The scaling has been chosen such that $\mathcal{B}' \approx 1.0$ at $\varepsilon \approx -0.35$ which is the known scaled energy value where chaos sets in [8]. $\mathcal{B}'$ is thus a useful qualitative measure for the behaviour of this system which clearly shows that even though the density of exceptional points is high for certain small values of ε, the system does not behave chaotically. The reason is that the chaotic behaviour is suppressed by both small λ and small coupling. From this we conclude that the quantum mechanical behaviour as depicted by $\mathcal{B}'$ is only a

function of ε. This conclusion is consistent with results given by *Wintgen* and *Friedrich* showing that the system is only dependent on the scaled energy [9].

5 Summary and Discussion

The hydrogen atom in a strong uniform magnetic field is known to be a quantum chaotic system. This has been reexamined by investigating the coupling matrix elements. We have defined a measure which quantifies the spectral behaviour of a system. This measure is easily obtainable from the two operators H_0 and H_1 alone. Further we have demonstrated that the results in using this measure are in line with known results in that $\mathcal{B}'$ has an appreciable value where chaos sets in and it is only a function of the scaled energy ε. This shows that $\mathcal{B}'$ is a useful measure for describing the chaotic behaviour of this system.

The study of the hydrogen atom in a strong magnetic field is used as a test case of the universally valid fact that all properties of the spectrum of an operator of the form $H_0 + \lambda H_1$ must reside in the exceptional points. The degeneracy of this problem adds a new dimension to it in that the coupling matrix elements play a crucial role in the behaviour. This has been incorporated into our analysis showing that a system can be chaotic even if the density of exceptional points is small.

From the form of the measure we conclude that there is a delicate relationship between the coupling matrix elements, the interaction strength and the density of exceptional points. All three quantities are important in understanding the spectral behaviour of any chaotic system of the form $H_0 + \lambda H_1$. While this is obvious from a mathematical point of view, we have demonstrated that it can be used in practical terms in a nontrivial situation.

References

[1] W. D. Heiss and A. A. Kotzé, Phys. Rev. A, **44**, 2403 (1991)

[2] W. D. Heiss and A. L. Sanino, Phys. Rev. A, **43**, 4159 (1991)

[3] W. D. Heiss and A. L. Sanino, J. Phys. A, **23**, 1167 (1990)

[4] A. A. Kotzé, Doctoral Thesis, University of the Witwatersrand, Johannesburg, South Africa (1992)

[5] T. Guhr and H. A. Weidenmüller, Ann. Phys. (NY), **199**, 412 (1990)

[6] W. D. Heiss and W.-H. Steeb, J. Math. Phys. **32**, 3003 (1991)

[7] A. A. Kotzé and W. D. Heiss, *submitted to Phys. Rev. A*

[8] H. Friedrich and D. Wintgen, Phys. Rep. **183**, 37 (1989)

[9] D. Wintgen and H. Friedrich, Phys. Rev. A **36**, 131 (1987)

[10] G. Wunner, M. Kost and H. Ruder, Phys. Rev. A **33**, 1444 (1986)

[11] C. W. Clark and K. T. Taylor, J. Phys. B **15**, 1175 (1982)

Figure 1: The coupling $\bar{C}$ as a function of n. The circles are the coupling due to the off-diagonal blocks and the diamonds due to the second off-diagonal blocks. The lines are numerical fits given by $\bar{C}_1'$ and $\bar{C}_2'$ (see text for the relations).

Figure 2: The behaviour denoted by $\mathcal{B}'$ as a function of n with a logarithmic scale on the vertical axis. Each line corresponds to a different value of ε as indicated with the corresponding $\mathcal{B}'$ values listed on the right.

Figure 1: The coupling $\bar{C}$ as a function of n. The circles are the coupling due to the off-diagonal blocks and the diamonds due to the second off-diagonal blocks. The lines are numerical fits given by $\bar{C}_1'$ and $\bar{C}_2'$ (see text for the relations).

Figure 2: The behaviour denoted by $\mathcal{B}'$ as a function of n with a logarithmic scale on the vertical axis. Each line corresponds to a different value of ε as indicated with the corresponding $\mathcal{B}'$ values listed on the right.