How to detect level crossings without looking at the spectrum

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We remind the reader that it is possible to tell if two or more eigenvalues of a matrix are equal, without calculating the eigenvalues. We then use this property to detect (avoided) crossings in the spectra of quantum Hamiltonians representable by matrices. This approach provides a pedagogical introduction to (avoided) crossings, is capable of handling realistic Hamiltonians analytically, and offers a way to visualize crossings which is sometimes superior to that provided by the spectrum. We illustrate the method using the Breit-Rabi Hamiltonian to describe the hyperfine-Zeeman structure of the ground state hydrogen atom in a uniform magnetic field.

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I. INTRODUCTION

Crossings and avoided crossings occur in the spectra of many physical systems such as atoms, molecules, semiconductors, and microwave cavities. They can occur as a result of tuning an external (e.g. electric) field or as the consequence of varying an internal (e.g. internuclear) coordinate. A number of interesting physical phenomena have been associated with such (avoided) crossings. For example an eigenstate transported in a closed circuit around a crossing in the spectrum picks up a Berry phase. As another example, points in the spectrum where a large number of eigenvalues cross correspond to ‘hidden’ symmetries of the physical system. These symmetries are hidden in the sense that they are not evident a priori as observables that commute with the Hamiltonian. As a third example eigenvalue avoidance in the spectrum signals the emergence of quantum chaos in a physical system.

Inspite of its importance as a basic phenomenon ubiquitous in physics, few introductory texts treat (avoided) crossings in any detail. Some questions that arise in the context of simple physical systems, and that could be considered at the (under)graduate level, are:

1. Is there a way to predict the total number of (avoided) crossings in the spectrum?
2. Is there a systematic way to locate all the (avoided) crossings in the spectrum?
3. Is there a way to identify the physical mechanisms responsible for the occurrence of (avoided) crossings in the spectrum?
4. Can the degeneracies - if any - in the spectrum be thought of as crossings?
5. Sometimes the crossings are hard to discern in the spectrum - can they be visualized in a clearer way?

In this article we employ an algebraic method that addresses these basic questions as well as some others. It allows for a simple but systematic approach to (avoided) crossings. In describing this approach we reintroduce to the study of (avoided) crossings a very useful but perhaps neglected mathematical tool, the discriminant. In a series of articles we have demonstrated in detail how use of algebraic techniques is a powerful way to locate (avoided) crossings in the spectra of quantum mechanical systems. We have shown that they are not only capable of locating (avoided) crossings without requiring solution of the Hamiltonian - a fact well known to mathematicians and not unknown to physicists - they can also find (avoided) crossings when the Hamiltonian is not completely determined. As one example, algebraic techniques allow us to derive a new class of invariants of the Breit-Rabi Hamiltonian. These invariants encode complete information about the parametric symmetries of the Hamiltonian. As another example, the use of algebraic methods allows us to detect the breakdown of the Born-Oppenheimer approximation for molecules assuming only that the complicated molecular potentials are real.

Although in the work just mentioned algebraic techniques were used in the context of advanced research, namely Feshbach resonances, we show below that they also form an effective pedagogical tool. Indeed we believe the exposition in this article could easily be included in the physics curriculum for (under)graduates as a striking demonstration that enhances their understanding of quantum mechanics as well as linear algebra.

The rest of the paper is arranged as follows. Section II contains a simple mathematical introduction using a $2 \times 2$ matrix. Section III generalizes this to the case of an $n \times n$ matrix. Section IV demonstrates the technique developed so far on the ground state hydrogen atom in a uniform magnetic field. Section V suggests some exercises for the reader; Section VI supplies a discussion.
II. A 2 × 2 MATRIX

In order to motivate the general case we first consider a real-symmetric 2×2 matrix

$$H(P) = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix},$$

(1)

with (unknown) eigenvalues $\lambda_{1,2}$. The notation implies that all the matrix elements depend on some tunable parameter $P$. Also $E_{1,2}$ could be the bare energies of a two-level quantum system, which are mixed by the perturbation $V$. Usually to find $\lambda_{1,2}$ we solve the equation

$$|H(P) - \lambda| = 0,$$

(2)

where $\lambda$ is a parameter. Eqs. (1) and (2) yield

$$\lambda^2 + C_1 \lambda + C_0 = 0,$$

(3)

where $C_0 = E_1 E_2 - V^2$ and $C_1 = -(E_1 + E_2)$. However $\lambda_{1,2}$ also satisfy Eq. (2), i.e.

$$(\lambda - \lambda_1)(\lambda - \lambda_2) = 0.$$

(4)

Comparing the coefficients of Eqs. (3) and (4), we find

$$C_0 = \lambda_1 \lambda_2,$$
$$C_1 = -(\lambda_1 + \lambda_2).$$

(5)

We are interested in crossings in the spectrum of $H(P)$ and therefore consider the discriminant[^17] defined by

$$\Delta \equiv (\lambda_1 - \lambda_2)^2.$$  

(6)

A little tinkering with Eqs. (5) shows that the discriminant can be re-written solely in terms of the coefficients of Eq. (3):

$$\Delta = C_1^2 - 4C_0.$$  

(7)

It is important to note that we did not actually calculate $\lambda_{1,2}$ at any point in the discussion so far. Clearly, $\Delta = 0$ whenever a level crossing occurs in the spectrum of $H(P)$. For example, if $E_1 = E_2 = P$, and $V = 2P$, then $\Delta = 4P^2$, and there is a level crossing at $P = 0$. This may be verified by calculating the eigenvalues $\lambda_{1,2} = P, 3P$. Note that a single crossing in the spectrum corresponds to a double root of the discriminant.

We see from this example that use of the discriminant transforms the problem of finding crossings in the spectrum to a polynomial root-finding problem. Further, it enables us to avoid calculating the eigenvalues. Lastly, it provides the locations of all the crossings in the spectrum. In the next section we generalize these statements to the case of an $n \times n$ matrix.

III. AN $n \times n$ MATRIX

For a real symmetric $n \times n$ matrix $H(P)$ all of whose entries are polynomials in $P$ the characteristic polynomial is

$$|H(P) - \lambda| = \sum_{m=0}^{n} C_m \lambda^m,$$

(8)

where the coefficients $C_m$ are all real. The discriminant is defined as[^17]

$$D[H(P)] = \prod_{i<j} (\lambda_i - \lambda_j)^2,$$

(9)

in terms of the $n$ eigenvalues $\lambda_i$. It can also be written purely in terms of the $n+1$ coefficients $C_m$[^18].

$$D[H(P)] = \left\{ \begin{array}{c} C_n & C_{n-1} \ldots & C_0 \\ C_n & \ldots & C_0 \\ \vdots & \ddots & \vdots \\ C_n & \ldots & C_1 \\ \ldots & \ldots & 2C_2 \end{array} \right\} nC_n \ldots C_1,$$

(10)

In practice we will calculate discriminants of characteristic polynomials using the built-in Discriminant function in Mathematica[^19] or Maple. In addition we will use the following ‘toolbox’ of general results in our discussion of (avoided) crossings below:

1. The real roots of $D[H(P)]$ correspond, as in Section II, to crossings in the spectrum of $H(P)$.

2. The real parts of complex roots of $D[H(P)]$ correspond to avoided crossings in the spectrum of $H(P)$. For a proof, see Ref.10.

3. A crossing is defined as the intersection of two eigenvalues. Hence the simultaneous intersection of $m$ eigenvalues gives rise to $\binom{m}{2} = m(m-1)/2$ crossings.

4. Every (avoided) crossing contributes, as in Section II, a factor quadratic in $P$ to $D[H(P)]$. For a full proof, see Ref.10.

5. Since $H(P)$ is real symmetric, the eigenvalues $\lambda_i$ are all real. It follows from Eq. (10) that $D[H(P)] \geq 0$. Hence $\log[D[H(P)]] + 1 \geq 0$ and goes to zero at every crossing. We will plot this function in order to visualize crossings.
IV. THE HYDROGEN ATOM

A simple but real example of a physical system whose spectrum exhibits both crossings and avoided crossings is a ground state hydrogen atom in a uniform magnetic field. Such an atom is accurately described by the Breit-Rabi Hamiltonian.

\[ H_{BR} = AI \cdot S + B(aS_z + bI_z), \]  

(11)

where \( I \) and \( S \) indicate the proton and electron spin respectively, and \( B \) is the magnetic field along the \( z \)-axis. \( A \) equals the hyperfine splitting and \( a = g_e \mu_B \) and \( b = g_p \mu_B \), where \( g_e(p) \) are the electron(proton) gyromagnetic ratios and \( \mu_B/N \) are the Bohr (nuclear) magnetons respectively. The numerical values for these constants were obtained from Ref.22 and are to be found in the figure captions in this article. In the basis \( |M_F, M_S\rangle \) which denotes the projections of \( I \) and \( S \) along \( B \), the states are

\[ \left\{ \frac{1}{2} \left\{ \begin{array}{c} 1 \\ 1 \\ -1 \\ -1 \end{array} \right\}, \frac{1}{2} \left\{ \begin{array}{c} 1 \\ 1 \\ -1 \\ -1 \end{array} \right\} \right\}. \]  

(12)

In this basis, the representation of Eq.(11) is

\[ H_{BR} = \frac{1}{4} \left( \begin{array}{cccc} A - 2(a + b)B & A + 2(a - b)B & A - 2(A - a - b)B & A + 2(b + a)B \\ A + 2(a - b)B & -A + 2(a + b)B & -A - 2(b + a)B & A + 2(a + b)B \\ A - 2(a - b)B & -A + 2(a + b)B & -A - 2(b + a)B & A + 2(b + a)B \\ A + 2(b + a)B & A + 2(a + b)B & A + 2(b + a)B & A + 2(a + b)B \end{array} \right). \]  

(13)

We now systematically locate all the (avoided) crossings in the spectrum. There is a 6-fold real root at \( B = 0 \), which points to the only crossings in the spectrum (Section III 1.). Conventionally these ‘zero-field’ crossings are called degeneracies and are not considered to be crossings. Hence we will maintain that there are no crossings in the spectrum of \( H_{BR}^{b=0} \). Eq.(14) has two complex roots:

\[ B = \pm \frac{A}{a}. \]  

(15)

This conjugate pair corresponds to a single avoided crossing at \( B = 0 \) (Section III 2. and 4.). From Eq.(15) we can see that \( A \), the hyperfine coupling of the two spins, is the physical mechanism responsible for the avoided crossing. Setting \( A = 0 \) turns the avoided crossing into a zero-field degeneracy.

We can confirm the predictions of the discriminant (Eq.14) by looking at Fig.1(a). At \( B = 0 \), three states in the upper manifold coincide, giving rise to \( \left( \begin{array}{c} 3 \\ 2 \end{array} \right) = 3 \) crossings (Section III 3.). Further, each crossing contributes a factor quadratic in \( B \) (Section III 4.) to the discriminant (Eq.14), which therefore should - and does - contain a factor of \( B^6 \). This shows that the discriminant accounts for the (hyperfine) degeneracies of the spectrum by counting them as crossings.

If we now add to our system a magnetic field \( B \), the 6-fold real root at \( B = 0 \) persists from the ‘zero-field’ crossings (Section III 4.) to the magnetic field \( M_F \) of the states \( |F, M_F\rangle \) to label the eigenstates of \( H_{BR} \). Here \( F = I + S \) is the total angular momentum and \( M_F \) its projection along the magnetic field. This labelling is loose as strictly speaking in the presence of a magnetic field \( M_F \) is a good quantum number but \( F \) is not.

A. The \( b = 0 \) case

To begin we recollect that \( |b| \ll |a| \), since the proton is more massive than the electron. We set \( b = 0 \) in Eq.(16), calculate its characteristic polynomial, and find the discriminant to be

\[ D[H_{BR}^{b=0}] = \frac{1}{16} A^4 a^6 B^6 \left( A^2 + a^2 B^2 \right). \]  

(14)

Considering \( D[H_{BR}^{b=0}] \) as a polynomial in \( B \), the total number of its roots equals its degree, namely 8. Using the results 1., 2., and 4. from Section III we can then say that the total number of the avoided crossings plus the number of crossings in the spectrum of \( H_{BR}^{b=0} \) is exactly \( 8/2 = 4 \), a fact verified below. Thus the discriminant allows us to predict the number of (avoided) crossings before they are actually found.

\[ D[H_{BR}^{b=0}] = \frac{1}{16} (a + b)^2 B^6 \left( A^2 + (a - b)^2 B^2 \right)^2 \times [(a + b)A + 2abB]^2 [(a + b)A - 2abB]^2. \]  

(16)

The 6-fold real root at \( B = 0 \) persists from the \( b = 0 \) case (Eq.14), but now there are (‘authentic’) crossings for \( B \neq 0 \) at

\[ B = \pm \frac{(a + b)A}{2ab}. \]  

(17)

‘Switching’ \( b \) off and on therefore reveals the physical mechanism behind the appearance of crossings in the Breit-Rabi spectrum : it is the interaction of the proton spin with the external magnetic field \( B \).

The complex roots of Eq.16 are

\[ B = \pm \frac{A}{a - b}(i). \]  

(18)
and imply an avoided crossing at $B = 0$ as in Section IV.A (Eq.15).

We can confirm the predictions of the discriminant (16) by looking at Fig.2. The crossings which occur at $±16.6$ T (from Eq.17) for actual values of the hydrogenic parameters $a$, $b$, and $A$ cannot be seen in the spectrum [Fig.2(a)] as the energy level pairs are separated by less than the width of the lines used to plot them, a point made earlier in this journal (see Fig.2 in Ref.20). However the logarithmic representation [Fig.2(b)] of the discriminant on the same scale clearly shows dips at all the crossings. A scaled spectrum has been shown in Fig.2(c) using a much larger relative value of $b$ in order to display the crossings clearly. This example illustrates how the discriminant can sometimes prove superior to the spectrum in displaying crossings. For another example see Ref.16.

FIG. 1: (a) The spectrum of $H_{BR}^{R0}$ for atomic hydrogen ($S = 1/2, I = 1/2$) with states labelled using the $|F, M_F\rangle$ basis. The parameters used were $A = 0.0473\text{cm}^{-1}$ and $a = 9.35 \times 10^{-5}\text{cm}^{-1}\text{G}^{-1}$. The spectrum was calculated by analytically diagonalizing the matrix in Eq.(13) and numerically plotting the eigenvalues. (b) $\log[N_0 D[H_{BR}^{R0}] + 1]$ plotted using the same parameters as in (a) and the scaling factor $N_0 = 10^{35}$ used to optimize visibility. The overall logarithmic trend is clearly visible.

FIG. 2: (a) The spectrum of $H_{BR}$ for atomic hydrogen ($S = 1/2, I = 1/2$). The parameters used were $A = 0.0473\text{cm}^{-1}$, $a = 9.35 \times 10^{-5}\text{cm}^{-1}\text{G}^{-1}$ and $b = -1.4202 \times 10^{-7}\text{cm}^{-1}\text{G}^{-1}$. The spectrum was calculated by analytically diagonalizing the matrix in Eq.(15) and numerically plotting the eigenvalues. The crossings at $B = ±16.6$ T cannot be resolved on this scale. (b) $\log[N_0 D[H_{BR}] + 1]$ plotted using the same parameters as in (a) and the scaling factor $N_0 = 10^{10}$. All three crossings are distinctly indicated by the minima of the discriminant; those corresponding to crossings at $B = ±16\text{T}$ actually do reach zero, but appear shorter here due to the resolution of the graphics. The overall logarithmic trend of the plot is evident. (c) The same spectrum as in (a) but redrawn using the parameters $A = 0.1, a = 0.01$, and $b = -0.1$. The larger relative value of $b$ ensures that the crossings at $B \neq 0$ can be seen in the plot.
V. SUGGESTED EXERCISES

1. Prove that the product in Eq. (9) contains \( n(n - 1)/2 \) factors.
2. Justify the presence of \( A^4 \) in Eq. (14).
3. For the parametric symmetry \( a = b \) in Eq. (10) show that there are crossings but no avoided crossings in the spectrum of \( H_{BB} \).
4. Plot \( D[H_{BB}] \) as a function of \( B \) and try to identify the zeros that correspond to crossings. This is an exercise designed to show that the highly nonlinear nature of the discriminant implies that each of its terms dominates in a different regime of \( B \). This makes it difficult to include all the features of the discriminant on a single scale unless a smoother representation - such as a logarithmic one - is adopted.
5. The Wigner von-Neumann non-crossing rule\(^6\) says “States of the same symmetry (i.e. quantum number) do not cross, except accidentally.” Verify the rule for the \( |MF⟩ \) states in Figs. 1(a) and 2(c). That is, show that states which (avoid) cross possess (same) different \( MF \)'s.

VI. DISCUSSION

The examples presented above illustrate that the discriminant is an elegant but simple device for locating and counting (avoided) crossings. Further, it is an effective tool for investigating the physical mechanisms behind the occurrence of (avoided) crossings. Lastly, visualization of the discriminant offers an alternative to locating crossings in the spectrum. It must be noted however that the discriminant yields no information about which eigenvalues avoid or intersect, or about the eigenvectors. Also shallow avoided crossings do not show up in the logarithmic representation, especially if they are near to crossings, which give rise to strong features in the discriminant. For all such information the spectrum has to be consulted.

The technique we have presented can be used algorithmically on Hamiltonians which are polynomial in some parameter \( P \), and which can be represented by finite dimensional matrices. Examples are a spin 1/2 particle in a magnetic field\(^23\) (the archetypal two-level system) and the hydrogen atom in an electric field\(^23\) (usually presented as an example of degenerate perturbation theory). However the method can also yield insight into physical systems whose Hamiltonians are usually truncated to a finite dimension for practical calculations such as the nucleus modeled as a triaxial rotor\(^23\) and a polar molecule in an electric field\(^23\). Another interesting application is the calculation of critical parameters of quantum systems\(^26\) since the critical point occurs at a crossing. An example using the Yukawa Hamiltonian has been treated in Ref.\(^27\). A list of physical systems in atomic and molecular physics to which algebraic methods can be applied is provided in Ref.\(^14\).

To conclude we have presented an algebraic technique for systematically analysing (avoided) crossings in the spectra of physical systems and pointed out its usefulness as a pedagogical device. It is a pleasure to thank P. Meystre for support. This work is supported in part by the US Army Research Office, NASA, the National Science Foundation and the US Office of Naval Research.

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