How to detect level crossings without looking at the spectrum

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It is possible to tell if two or more eigenvalues of a matrix are equal without calculating the eigenvalues. We use this property to detect (avoided) crossings in the spectra of 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 that is sometimes superior to that provided by the spectrum directly. 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. © 2007 American Association of Physics Teachers. [DOI: 10.1119/1.2757622]

I. INTRODUCTION

When two eigenvalues in a spectrum intersect, a crossing is said to occur; when they approach each other but diverge without meeting, an avoided crossing is said to happen. Crossings and avoided crossings occur in the spectra of many systems such as atoms, molecules, semiconductors, and microwave cavities. For instance, they can occur as a result of tuning an external field, or as the consequence of varying an internal coordinate. Several interesting physical phenomena are associated with crossings and 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 spite of their 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 include the following. Is there a way to predict the total number of (avoided) crossings in the spectrum? Is there a systematic way to locate all the (avoided) crossings in the spectrum? Is there a way to identify the physical mechanisms responsible for the occurrence of (avoided) crossings in the spectrum? Can the degeneracies, if any, in the spectrum be thought of as crossings? If the crossings are difficult 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 somewhat neglected mathematical tool, the discriminant. In a series of articles we have demonstrated how the use of algebraic techniques is a powerful way to locate (avoided) crossings in the spectra of quantum-mechanical systems. We have shown that these techniques 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, but they can also find (avoided) crossings when the Hamiltonian is not completely determined.

For 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. The use of algebraic methods also allows us to detect the breakdown of the Born-Oppenheimer approximation for molecules, assuming only that the complicated molecular potentials are real.

The rest of the paper is arranged as follows. Section II contains a simple mathematical introduction using a 2 × 2 matrix. Section III generalizes this introduction to the case of an n × n matrix. In Sec. IV we apply these techniques to the ground-state hydrogen atom in a uniform magnetic field. Section V suggests some exercises for the reader, and Sec. VI discusses our results.

II. A 2 × 2 MATRIX

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 λ₁,₂. The notation implies that all the matrix elements depend on some tunable parameter P. E₁,₂ could be the bare energies of a two-level quantum system, which are mixed by the perturbation V. To find λ₁,₂ we usually solve the equation

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

(2)

where λ is a parameter. Equations (1) and (2) yield

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

(3)

where C₀ = E₁E₂ − V² and C₁ = −(E₁ + E₂). The eigenvalues λ₁,₂ also satisfy the relation

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

(4)

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

$$C_0 = \lambda_1 \lambda_2,$$

(5a)

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

(5b)

We are interested in crossings in the spectrum of H(P) and therefore consider the discriminant defined by
\[ \Delta = (\lambda_1 - \lambda_2)^2. \]  

A little tinkering with Eq. (5) shows that the discriminant can be rewritten solely in terms of the coefficients of Eq. (3),

\[ \Delta = C_1^2 - 4C_0. \]  

Note that we did not actually calculate \( \lambda_{1,2} \) 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 result 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 for 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

\[
[H(P) - \lambda] = \sum_{m=0}^{n} C_m \lambda^m, \tag{8}
\]

where the coefficients \( C_m \) are all real. The discriminant is defined as \(^{17}\)

\[
D[H(P)] = \prod_{i<j} (\lambda_i - \lambda_j)^2, \tag{9}
\]

in terms of the \( n \) eigenvalues \( \lambda_i \). It can also be expressed only in terms of the \( n+1 \) coefficients \( C_m \), \(^{18}\)

\[
D[H(P)] = (-1)^{n(n-1)/2} C_n \begin{vmatrix}
C_n & C_{n-1} & \cdots & C_0 \\
C_{n-1} & \cdots & \cdots & \cdots \\
\vdots & \ddots & \ddots & \ddots \\
nC_n & \cdots & \cdots & 2C_2 \\
nC_n & \cdots & \cdots & C_1 \\
\cdots & \cdots & \cdots & \cdots \\
nC_n & \cdots & \cdots & C_1 \\
2C_2 & C_1 & \cdots & \cdots
\end{vmatrix} \tag{10}
\]

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:

1. The real roots of \( D[H(P)] \) correspond, as in Sec. II, to crossings in the spectrum of \( H(P) \).
2. The real parts of the 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 Sec. II, a factor quadratic in \( P \) to \( D[H(P)] \). See Ref. 15 for a proof.
5. Because \( H(P) \) is real symmetric, the eigenvalues \( \lambda_i \) are all real. It follows from Eq. (9) 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 the 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.\(^{20}\) Such an atom is accurately described by the Breit-Rabi Hamiltonian,\(^{21}\)

\[
H_{BR} = A I \cdot S + B (a S_z + b I_z), \tag{11}
\]

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

\[
\begin{pmatrix}
1 \\
2 \\
2
\end{pmatrix}, \quad \begin{pmatrix}
-1 \\
1 \\
2
\end{pmatrix}, \quad \begin{pmatrix}
1 \\
-1 \\
2
\end{pmatrix}, \quad \begin{pmatrix}
-1 \\
-1 \\
2
\end{pmatrix}. \tag{12}
\]

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

\[
H_{BR} = \frac{1}{4} \begin{pmatrix}
A - 2(a + b)B & -A + 2(a - b)B & 2A \\
-A + 2(a - b)B & 2A & -A - 2(a - b)B \\
2A & -A - 2(a - b)B & A + 2(a + b)B
\end{pmatrix}. \tag{13}
\]
points to the only crossings in the spectrum characteristic polynomial, and find the discriminant to be.

If we consider

sive than the electron.22 We set

0.0473 cm−1 and

the eigenvalues.

of Eq. 9 gives

cases at

b

0 case

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 \(\binom{1}{3} = 3\) crossings. Further, each crossing contributes a factor quadratic in \(B\) to the discriminant in Eq. (14), which therefore contains a factor of \(B^6\). Thus, we see that the spectral degeneracies of the Hamiltonian show up as algebraic degeneracies in the discriminant. More specifically, the discriminant accounts for the (hyperfine) degeneracies of the Breit-Rabi spectrum by counting them as crossings.

An avoided crossing occurs at \(B=0\) between the states drawn with dotted lines. In Fig. 1(b) a logarithmic representation of \(D[H_{\text{BR}}]\) shows a dip corresponding to the degeneracies at \(B=0\).

B. The \(b \neq 0\) case

If \(b \neq 0\), we find from Eq. (13) that

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

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

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

Switching \(b\) off and on 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

\[
B = \pm \frac{A}{a - b} i,
\]

and imply an avoided crossing at \(B=0\) as in Eq. (15).

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

(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. (16) show that there are crossings but no avoided crossings in the spectrum of $H_{BR}$.

(4) Plot $D[H_{BR}]$ as a function of $B$ and identify the zeros that correspond to crossings. This problem is designed to show that the highly nonlinear nature of the discriminant implies that each of its terms dominates in a different regime of $B$. Therefore, it is 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 noncrossing rule\(^6\) says that states of the same symmetry (that is, quantum number) do not cross, except accidentally. Verify this rule for the $M_F$ states in Figs. 1(a) and 2(c). That is, show that states that (avoid) crossing possess (same) different $M_F$’s.

VI. DISCUSSION

The examples we have presented illustrate that the discriminant is an elegant and simple method for locating and counting (avoided) crossings. It also is an effective tool for investigating the physical mechanisms behind the occurrence of (avoided) crossings. Visualization of the discriminant offers an alternative to locating crossings in the spectrum. We note 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 crossings, which give rise to strong features in the discriminant. For all such information the spectrum has to be calculated.

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 (the archetypal two-level system) and the hydrogen atom in an electric field (usually presented as an example of degenerate perturbation theory). The method can also yield insight into physical systems whose Hamiltonians are usually truncated at a finite dimension for practical calculations such as the nucleus modeled as a triaxial rotor and a polar molecule in an electric field. Another interesting application is the calculation of critical parameters of quantum systems, because 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. 15.

We believe that the exposition in this article could be included in the physics curriculum for (under)graduates as a way to enhance student understanding of quantum mechanics as well as linear algebra.

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21 In MATHEMATICA the Discriminant is defined in terms of the Resultant function.

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