Detecting level crossings without solving the Hamiltonian. I. Mathematical background

M. Bhattacharya and C. Raman
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA
(Received 21 December 2006; published 15 March 2007)

When the parameters of a physical system are varied, the eigenvalues of observables can undergo crossings and avoided crossings among themselves. It is relevant to be aware of such points since important physical processes often occur there. In a recent paper [M. Bhattacharya and C. Raman, Phys. Rev. Lett. **97**, 140405 (2006)] we introduced a powerful algebraic solution to the problem of finding (avoided) crossings in atomic and molecular spectra. This was done via a mapping to the problem of locating the roots of a polynomial in the parameters of interest. In this article we describe our method in detail. Given a physical system that can be represented by a matrix, we show how to find a bound on the number of (avoided) crossings in its spectrum, the scaling of this bound with the size of the Hilbert space and the parametric dependencies of the Hamiltonian, the interval in which the (avoided) crossings all lie in parameter space, the number of crossings at any given parameter value, and the minimum separation between the (avoided) crossings. We also show how the crossings can reveal the symmetries of the physical system, how (avoided) crossings can always be found without solving for the eigenvalues, how they may sometimes be found even in case the Hamiltonian is not fully known, and how crossings may be visualized in a more direct way than displayed by the spectrum. In the accompanying paper [M. Bhattacharya and C. Raman, Phys. Rev. A **75**, 033406 (2007)] we detail the application of these techniques to atoms and molecules.

DOI: 10.1103/PhysRevA.75.033405 PACS number(s): 32.60.+i, 31.50.Gh, 31.15.−p, 33.55.Be

I. INTRODUCTION

Level crossing is a ubiquitous phenomenon with examples in many disciplines of physics. Possibly the first effect to be associated with degenerate eigenvalues was conical refraction in optics, identified by Hamilton in 1833 [1]. In quantum physics the celebrated work of von Neumann and Wigner [2] related level crossing to symmetry, while the analysis of avoided crossings was pioneered by Landau [3] and Zener [4]. Since then a variety of interesting phenomena have been associated with quantum level crossings. Examples include Berry's phase in adiabatic quantum mechanics [5], Fermi resonances in molecular physics [6], and the production of entanglement in quantum information [7]. A more extensive list of crossing phenomena in atoms and molecules is provided in the accompanying paper [8].

In this article we present the details of a versatile theoretical technique introduced earlier [9] for detecting the presence of level crossings in physical systems. We consider systems where the underlying Hamiltonian (or other physical quantity) can be represented as a matrix depending on several parameters. We remind the reader that the values of the parameters for which (avoided) crossings occur among the eigenvalues of this matrix correspond to the roots of a certain polynomial in the same parameters. The power of this approach derives from the well known fact that the Hamiltonian does not need to be solved in order to generate this polynomial and therefore to find its roots, i.e., to find the (avoided) crossings. We go further and show that even if the Hamiltonian is not completely known (avoided) crossings can still sometimes be located.

Very powerful polynomial root-finding techniques already exist, in a branch of mathematics known as *algebraic geometry* [10]. We have demonstrated how these techniques may be exploited to yield quite remarkable results regarding crossing phenomena in physical systems of interest [9]. In the case of atoms for example, they enabled us to derive a new class of invariants of the Breit-Rabi Hamiltonian of magnetic resonance, without solving the Hamiltonian. These invariants turn out to be complete catalogs of the parametric symmetries of the problem, and encode information about (avoided) crossings in a manner more compact and easier to visualize than allowed by the spectrum. In the case of molecules the techniques allowed us to determine magnetic fields at which the electronic curves crossed, i.e., the Born-Oppenheimer approximation broke down, for a diatomic molecule. Remarkably we could do this without using any information about the corresponding complicated Born-Oppenheimer potentials other than the fact that they are real.

The use of algebraic techniques to find (avoided) crossings is not unknown in physics. For example, they have been used to track singularities in optical polarization [11], to establish the link between level crossing in a quantum system and integrability of its classical analog [12], to examine the local behavior of the complex (Riemann) eigenvalue surface of Hamiltonian matrices [13], and to design magnetic traps for ultracold atoms [14]. However, some of the more powerful algebraic techniques have not been exposed in the work just mentioned. For instance we do not know of a case where it has been shown that the (avoided) crossings can also be found even if the Hamiltonian is not fully known. Also, to the best of our knowledge, there has been no application to matrices that describe realistic atomic and molecular spectra. Further we have not seen the use of algebraic quantities to visualize crossings. Last, we have not come across any systematic exposition of algebraic technique explicitly geared to the analysis of level crossing in a generic physical system representable by a matrix.

Thus in this and the accompanying article [8] our intention is to introduce algebraic technique somewhat systematically, generalize it to matrices of arbitrary but finite dimen-

sion, apply it to matrices that describe atoms and molecules realistically, and exhibit some its more powerful aspects by adapting methods already developed in mathematics. We hope these results and techniques will be added to the existing calculus of level crossing, which presently contains useful tools such as Landau-Zener transition theory among others. Since algebraic geometry is a very well developed branch of mathematics and parameter-dependent matrices are rife in physics, we have not made an effort at either rigor or completeness. Our intention in this article will be to rationalize the relevant theorems and present working tools. Part of the material in this article is a review of well-known methods, part nontrivial adaptation of existing mathematics to questions of physical importance, and part derivation of original results regarding the mathematics of curve crossing. The original results obtained in this paper have been specifically pointed out in one of the concluding sections.

A word as to our intention in presenting two accompanying but distinct papers. In writing the papers we found that the mathematics and the physics separated naturally enough for us to effectively decouple the theoretical background from the physical applications. Therefore, the present article is intended to stand on its own as a small manual on the algebraics of level crossing. The accompanying article [8] contains fully developed examples involving atoms and molecules, and provides detailed guidelines for applications to such physical systems.

The paper is organized as follows. In Sec. II we discuss briefly the motivation behind analyzing (avoided) crossings algebraically, contrasting it in particular to numerical methods; in Sec. III we introduce the simplest nontrivial example of algebraic technique using a 2×2 matrix; in Sec. IV we treat the general case of (avoided) crossings in the spectrum of an n-dimensional matrix; in Sec. V we examine the principal mathematical tool in the investigation of (avoided) crossings, the discriminant; in Sec. VI we provide the details of some properties of polynomials that are crucial to (avoided) crossing analysis; in Sec. VII we make contact with the Wigner–von Neumann noncrossing theorem; Sec. VIII contains a list of the original results presented in this work, a critique of algebraic technique and a discussion of some specific questions that would be interesting to answer in future research; Sec. IX contains the Conclusion.

II. MOTIVATION

Much effort has gone into developing numerical as well as analytical techniques to detect and analyze level (avoided) crossings ([15] and references therein). Numerical analytic continuation of eigenvalues [16,17], constrained energy minimization [15], adiabatic transport of eigenstates [5,18–20], dimensional perturbation theory [6], symmetry-based calculations [21] and tracing the Shannon entropy across crossings [22] are some of the methods previously used. However the use of algebraic techniques does not seem to have been explored in too much detail. Our motivation for studying (avoided) crossings algebraically is threefold.

First, it turns out that numerically calculating the spectrum is not enough to distinguish crossings from fine anticrossings [16,18]. One solution is to examine the topological changes in the eigenstates during an adiabatic circuit of the crossing point [5,23,24] to see if the states pick up a Berry's phase. However constructing and transporting eigenstates can quickly become inefficient. Algebraic technique provides a rigorous and efficient alternative to such numerical methods.

Beyond the issue of resolution lies an inherent advantage with algebraic methods. Typically in order to establish the existence of an (avoided) crossing numerically one has to find the parameter values for which it actually occurs. However if the (avoided) crossings correspond to the roots of some polynomial in those very parameters, algebra allows us to ask if those roots exist in some given parameter interval. It can be seen readily that this leads to an efficient search technique which allows us to quickly discard large parameter regimes where "nothing interesting" is happening.

Second, it is often desirable to know the dependence of the location and existence of crossings on various parameters. Such a situation can arise, for instance, when investigating the physical mechanisms underlying the crossings. These mechanisms can be "switched off" by setting the relevant parameters to zero, for example. The process of calculating and inspecting the entire spectrum anew for each numerical value taken on by the parameter set is quite inefficient and is always restricted by resolution. In our experience crossings which result from the delicate balance of two physical mechanisms may move around by orders of magnitude on the various axes in the spectrum as the balance is tweaked. As we show in this article algebraic technique provides a much more direct and efficient way of tracking the functional dependence of the crossings on the parameters.

A related issue is that of *hidden symmetries* [25] of which a relevant example will be made in the accompanying article [8]. These are symmetries of a physical system which do not manifest themselves *a priori*, i.e., as observables which obviously commute with the Hamiltonian. Rather, they reveal themselves in the form of (large) degeneracies that occur in the spectrum at special values of the parameters in the Hamiltonian. Once these degeneracies are identified, the corresponding symmetries can be constructed [25]. Algebraic technique furnishes a systematic and explicit way of uncovering such parameter-dependent degeneracies. This removes the need to discover these symmetries by numerical exploration of the spectrum.

Third, the method of numerically searching the spectrum for crossings fails completely if the Hamiltonian of the physical system is not known fully since in this case it is not possible to solve for the spectrum. Remarkably, as we will show, the algebraic method can yield information about level crossings even when only partial knowledge about the physical system is available.

An obvious shortcoming of algebraic technique is the fact that it does not yield any information about eigenvalues or eigenvectors. For instance, it cannot tell which eigenvalues are intersecting at a crossing, nor what the value of the physical observable is at that point. We point out that it is not our intention to prescribe algebraic technique as a complete substitute to consulting the spectrum. It just happens to be better

than the spectrum at finding (avoided) crossings in a useful variety of cases. Once these points have been found, the spectrum of course may be consulted freely. Only in this way can complete knowledge about the problem be achieved.

The most pressing deficiencies of the algebraic method actually have to do with practice rather than principle. It relies on symbolic computation which is much more expensive than numerical computation. For larger systems such as polyatomic molecules, where the number of parameters as well as the Hilbert space is sizable, algebraic techniques quickly become computationally inefficient and numerical methods have to be resorted to [15].

III. SIMPLE EXAMPLE

We will now introduce algebraic technique using a simple matrix that depends on a single parameter. The only condition for our algebraic method to work is that the matrix should be diagonalizable [26]. However we will be concerned with observables of physical systems, which are usually represented by matrices which are Hermitian. This allows us to work with a smaller class of matrices. In fact with no loss of generality we can operate with real symmetric matrices; the simplest nontrivial example of algebraic technique can thus be made using a 2×2 real symmetric matrix,

$$M(P) = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix}. \tag{1}$$

Equation (1) can be used to model the Hamiltonian of a two-state quantum system in which the "bare" energies of the two levels are E_1 and E_2 and V is a "perturbation" via which the two levels interact. The notation of Eq. (1) implies all the matrix elements may be functions of the tunable real parameter P, which could be an external field in which the two-state system has been placed.

To find eigenvalues E of $M(P)$, labeled λ_1 and λ_2, we consider the characteristic polynomial

$$\Gamma(E) = |M(P) - E| = E^2 + C_1 E + C_0, \tag{2}$$

where $C_0 = E_1E_2 - V^2$ and $C_1 = -(E_1 + E_2)$. However, the eigenvalues $\lambda_{1,2}$ are also roots of the polynomial $\Gamma(E)$, i.e.,

$$(E - \lambda_1)(E - \lambda_2) = 0. \tag{3}$$

Comparing Eqs. (2) and (3) the coefficients may equivalently be written in terms of the eigenvalues: $C_0 = \lambda_1\lambda_2$ and $C_1 = -(\lambda_1 + \lambda_2)$. It is important to note that we did not explicitly calculate the eigenvalues $\lambda_{1,2}$ in order to arrive at this conclusion.

A level crossing occurs in the spectrum of the Hamiltonian (1), if the two eigenvalues become degenerate ($\lambda_1 = \lambda_2$) at some value of the parameter P. To locate the crossing, we introduce the *discriminant*

$$\Delta \equiv (\lambda_1 - \lambda_2)^2 \tag{4}$$

of the characteristic polynomial $\Gamma(E)$ [Eq. (2)] of $M(P)$. The discriminant however can be rewritten purely in terms of the coefficients of $\Gamma(E)$:

$$\Delta = C_1^2 - 4C_0. \tag{5}$$

We now choose a simple parametrization for $M(P)$ in Eq. (1), say $E_{1,2} = 2P$ and $V = P$. Equation (5) then yields $\Delta = 4P^2$, a polynomial in P. The root of this polynomial, $P = 0$, corresponds to the only crossing in the spectrum of $M(P)$, as may be verified by explicitly calculating the eigenvalues $\lambda_{1,2} = P, 3P$. Note that a single crossing in the spectrum corresponds to a double root of the discriminant at $P = 0$.

This simple example illustrates several key features of algebraic technique. First, it shows how the discriminant provides a mapping from the problem of finding crossings in the spectrum to one of locating roots of a polynomial. Second, it demonstrates how the need to find eigenvalues can be bypassed in the search for level crossings. Last, it provides a complete catalog of crossings for all possible values of the parameter P. In the next section we will show how these statements can be powerfully generalized for the case of an n-dimensional matrix representing a physical variable.

IV. GENERAL CASE

An extension of the simple example [Eq. (1)] of Sec. III to larger matrices and more than one parameter leads to the study of multivariate polynomials, a topic in algebraic geometry [10]. From this branch of mathematics we will now introduce techniques which are very useful in finding (avoided) crossings in the spectrum of an n-dimensional matrix.

Let $H(P)$ denote an n-dimensional Hermitian matrix, not trivially diagonal, and dependent polynomially on the set of parameters $P = \{P_1, \ldots, P_N\}$. The characteristic polynomial of $H(P)$ is therefore of degree n in the eigenvalue E:

$$G(E) = |H(P) - E| = \sum_{i=0}^{n} C_i(P)E^i, \tag{6}$$

and has $n+1$ coefficients, C_i. The reader should prove to herself that the C_i are all polynomials in P, and also that $C_n = 1$. The roots $\lambda_{1,2,\ldots,n}$ of the polynomial Eq. (6) are used to define its discriminant [10]

$$D[H(P)] \equiv \prod_{i<j}^{n} (\lambda_i - \lambda_j)^2. \tag{7}$$

The discriminant of a polynomial is therefore defined to be the product of the squares of the pairwise differences of its roots. There are $\binom{n}{2} = n(n-1)/2$ factors in the product in Eq. (7).

As in the case of Δ in Sec. III [Eq. (5)], $D[H(P)]$ can also be calculated purely from the coefficients C_i of the characteristic polynomial without recourse to the roots λ_i. This is a remarkable fact, but not a coincidence. Its existence is guaranteed by the fundamental theorem of symmetric functions [27], which states that a polynomial (such as $D[H(P)]$) symmetric in n variables (such as $\lambda_{1,\ldots,n}$) can always be expressed in terms of the n elementary symmetric polynomials

$$f_1 = \lambda_1 + \cdots \lambda_n,$$

$$f_2 = \lambda_1\lambda_2 + \cdots + \lambda_{n-1}\lambda_n,$$

$$f_3 = \lambda_1\lambda_2\lambda_3 + \cdots + \lambda_{n-2}\lambda_{n-1}\lambda_n,$$

$$\cdots$$

$$f_n = \lambda_1\lambda_2 \ldots \lambda_n. \tag{8}$$

However the polynomials in Eq. (8) are simply related to the coefficients in Eq. (6): $f_i=(-1)^i C_{n-i}, i=1,2,3\ldots$. Hence $D[H(P)]$ can be written exclusively in terms of the C_i for $H(P)$ of any size; a compact way of doing this is in terms of the determinant of the Sylvester matrix of the characteristic polynomial $G(E)$ [Eq. (6)] [10]:

$$D[H(P)] = (-1)^{n(n-1)/2} C_n^{-1} \begin{vmatrix} C_n & C_{n-1} & \cdots & \cdots & & & C_1 & C_0 & & & \\ & C_n & C_{n-1} & \cdots & \cdots & \cdots & \cdots & C_1 & C_0 & & \\ & & & & & & \cdots & & & & \\ & & & & C_n & \cdots & & \cdots & \cdots & C_1 & C_0 \\ nC_n & (n-1)C_{n-1} & \cdots & \cdots & \cdots & 2C_2 & C_1 & & & & \\ & nC_n & (n-1)C_{n-1} & \cdots & \cdots & \cdots & 2C_2 & C_1 & & & \\ & & & & & & \cdots & & & & \\ & & & & & nC_n & \cdots & & \cdots & 2C_2 & C_1 \end{vmatrix}. \tag{9}$$

The Sylvester matrix is of dimensions $(2n-1)\times(2n-1)$ and hence implies, for the full analytical expression for $D[H(P)]$, the presence of $(2n-1)!$ terms. This estimate turns out to be naive but nonetheless points out a major practical obstacle to the use of algebraic technique: To be algebraically useful the discriminant has to be calculated symbolically, which is typically more intensive to do than a numerical computation. For example, in the case of atoms provided in the accompanying paper [8] $H(P)$ is an 8×8 matrix and the discriminant can have as many as $15! = 1\,307\,674\,368\,000$ terms, not accounting for the internal structure of the C_i's themselves (each may consist of more than one term). However, a large number of the elements of the Sylvester matrix are identically zero as can be seen from Eq. (9); also cancellations occur due to the physical symmetries of $H(P)$. These two reasons result in the $D[H(P)]$ for atoms actually possessing far fewer terms than estimated above; it finally contains only four terms. As a contrast, in the case of molecules $H(P)$ turns out to be a 4×4 matrix but the discriminant contains 13 430 terms. This is more than the $7! = 5040$ terms estimated without accounting for the complexity of the C_i's. Thus the symmetries of $H(P)$ and the complexity of the matrix elements of its representation play a major role in shaping the form of the discriminant $D[H(P)]$.

The reader should prove to himself that the C_i in Eq. (9) are all real since they are the coefficients of the characteristic polynomial [Eq. (6)] of a Hermitian matrix. In Eq. (9) the sequence of coefficients $(C_n \ldots C_0)$ occupies the first $n-1$ rows of the determinant of the Sylvester matrix and is shifted by one column to the right in every successive row. Likewise the sequence $(nC_n \ldots C_1)$ appears in the next n rows, also shifted similarly. It is not a coincidence that the second sequence consists of the coefficients of the derivative of $G(E)$ [Eq. (6)]. The discriminant is a special instance of a more general mathematical object, the *resultant*, a function of two polynomials which vanishes whenever they have a root in common [10]. The discriminant is obtained by applying the resultant to a polynomial and its derivative. It follows that if the polynomial has a repeated root, its discriminant vanishes.

We note here that since the C_i are all always polynomials in P so is $D[H(P)]$, since a determinant is a polynomial in its matrix elements. Thus Eq. (9) provides an analytical mapping between the level-crossing and polynomial root finding problems for the Hamiltonian $H(P)$. This mapping exists for any n, i.e., we can always obtain an analytical expression for $D[H(P)]$ independent of the analytical solvability of $H(P)$.

It is worth mentioning that in standard symbolic computation applications such as *Mathematica* and *Maple*—both of which have been used in this work—resultants and discriminants are defined functions. In this connection it is interesting to note that some of the machinery of root finding in algebraic geometry described in this article has been developed in the context of computer algebra [10].

V. PROPERTIES OF DISCRIMINANTS

We now list some properties of discriminants that are important to the problem of finding (avoided) crossings.

A. Independence from spectrum

The fact that $D[H(P)]$ can be calculated directly from the coefficients of the characteristic polynomial has three important implications. First, in general the roots of $H(P)$ cannot be calculated analytically (i.e., using radicals and the operations of addition, subtraction, division, and multiplication) for $n>4$. However, Eq. (9) implies that $D[H(P)]$ can be

calculated analytically (as a polynomial) for any n. This means that the discriminant supplies an analytical mapping—between the level-crossing and polynomial root-finding problems—for all n. Hence algebraic techniques can be applied to $D[H(P)]$ for any n, without regard to the analytical solvability of the Hamiltonian, or of course of $D[H(P)]$ itself.

The ability to detect level crossings without solving for the spectrum has a second implication. It allows, as will be shown below as well as in the accompanying paper, for the existence of powerful algebraic alternatives to numerically intensive spectral searches for crossings.

Third, although complete knowledge of the Hamiltonian is required to calculate the spectrum, the discriminant is capable of finding level crossings even in case some information is missing. This will be demonstrated below using a specific example.

B. Unitary invariance

From Eq. (7) it follows that $D[H(P)]$ is an invariant of $H(P)$. This property allows us to choose any representation of $H(P)$ to calculate $D[H(P)]$. However, there is a particular representation of $H(P)$ which lets us arrive at the characteristic polynomial with the least computation and in the most algebraically transparent way. Typically such a representation is made in the direct product ("uncoupled") basis of the constituent particles of the physical system. This retains the polynomial form of the parametric Hamiltonian in the matrix elements. For example, if the Hamiltonian is of degree k in some parameter, then in this representation every matrix element is of degree k or less in the same parameter. In another basis, such as the basis that diagonalizes the Hamiltonian, the elements could be quadratic (in the parameter of interest) under radicals, for instance. Such forms are not readily amenable to algebraic arguments, and are not preferred.

C. Translational invariance

From Eq. (7) it follows that $D[H(P)]$ does not change if the same quantity is added to every eigenvalue λ_i. The reader should verify for herself that $D[H(P)]$ actually remains unchanged if the same quantity is added to each diagonal term of $H(P)$, since this merely indicates a shift in the scale of the entire spectrum. It is also important to note that the quantity being added need not necessarily be a constant; it could be an arbitrary function of any variable. $D[H(P)]$ remains unchanged as long as the *same* function is added to every diagonal element of $H(P)$. This property will prove crucial while investigating curve crossings in a molecule [8].

D. Nonnegativity

Since $H(P)$ corresponds to a physical observable it is Hermitian, and its eigenvalues λ_i are all real. Equation (7) therefore implies that $D[H(P)]$ is real and non-negative: $D[H(P)] \geq 0$. The property of non-negativity will prove useful when we consider visual representations of the discriminant below.

We have discussed above some general properties of discriminants which are of use in the study of level crossings. To learn more about the location of (avoided) crossings we now introduce some properties of polynomials.

VI. POLYNOMIALS AND (AVOIDED) CROSSINGS

We describe here how to extract information about level crossings from some algebraic properties of polynomials. We will always assume real coefficients for the polynomials. This holds true for the characteristic polynomials of Hermitian matrices, and also for the discriminants of such polynomials. Although the properties described below can be ascribed to any real-valued polynomial, we will persist in using the discriminant, typically written as $D[H(P)]$, for purposes of illustration as well as consistency.

A. Crossings and avoided crossings

As in the case of $\Delta = 4P^2$ in Sec. III the real roots of Eq. (7) correspond to crossings in the spectrum of $H(P)$. Do the complex roots correspond to anything? It can be shown that the real parts of the complex roots of Eq. (7) correspond to avoided crossings [13]. We leave the general proof to [13], and treat the 2×2 case [Eq. (1)]. Solving for the eigenvalues of the matrix $M(P)$ in Eq. (1) yields

$$\lambda_{\pm} = \frac{1}{2}[E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4V^2}]. \tag{10}$$

The difference between the two eigenvalues is given by

$$\lambda_+ - \lambda_- = \sqrt{(E_1 - E_2)^2 + 4V^2}. \tag{11}$$

By definition (7) the quantity under the radical sign in Eq. (11) is the discriminant $D[M(P)]$. If we choose the parametrization $E_{1,2} = 4P_r, 3P_r$ (where P_r is an arbitrary but real non-zero constant) and $V = P/2$ (where P is a tunable parameter), we obtain

$$\lambda_+ - \lambda_- = \sqrt{P_r^2 + P^2}. \tag{12}$$

Clearly the two eigenvalues cannot be degenerate for real values of P. However the discriminant

$$D[M(P)] = P_r^2 + P^2, \tag{13}$$

has complex roots $P_c = iP_r$ and $\bar{P}_c = -iP_r$, and it can be shown that the gap between the two eigenvalues goes through a minimum as the real parameter P is tuned through $\mathrm{Re}[P_c] = 0$. To this end we rewrite Eq. (12)

$$\lambda_+ - \lambda_- = \sqrt{(P - P_c)(P - \bar{P}_c)}. \tag{14}$$

Differentiating Eq. (14) with respect to P yields a minimum of the energy gap at

$$P = \frac{P_c + \bar{P}_c}{2} = \mathrm{Re}[P_c] = 0. \tag{15}$$

The presence of the avoided crossing at $P = 0$ can be verified by plotting the eigenvalues $\lambda_{\pm} = \frac{1}{2}(7P_r \pm \sqrt{P_r^2 + P^2})$ for any

$P_r \neq 0$. For $P_r=0$ the avoided crossing turns into a crossing. It should be noted in the example above that a pair (the complex root and its conjugate) of roots give rise to a single avoided crossing.

We have provided above a specific instance of the general rule that an avoided crossing occurs when the parameter P equals the real part of a complex root P_c of the discriminant. However for matrices larger than 2×2 the rule is no longer exact and one of two conditions need to be satisfied for it to hold [13]. The first condition is that there should not be a second avoided crossing nearby, involving either of the original eigenvalues. If either of the eigenvalues undergoes another avoided crossing in the vicinity of the first, the two avoided crossings can "interact" and be displaced from the corresponding positions indicated by the complex roots of the discriminant. The second condition allows the rule to hold even if there is an avoided crossing in the vicinity. The condition is that the original crossing should be very narrowly avoided. P_c is very close to the real axis in this case.

It is worth emphasizing that the proximity of two avoided crossings along the energy axis in the spectrum cannot be calculated by use of the discriminant alone. Although two avoided crossings can correspond to close-lying complex roots of the discriminant, they may occur between entirely different pairs of eigenvalues, and thus may not interact at all. In the language of complex analysis, they occur on different Riemann sheets of the energy surface for the system. However, the discriminant cannot distinguish between these sheets and the spectrum has to be consulted.

B. Counting and locating (avoided) crossings

For the simple example of Eq. (1), Δ turned out to be quadratic in a single parameter, P; in general $D[H(P)]$ is a polynomial of high degree in the N variables P_N. A significant amount of information about the roots of this polynomial can be obtained from its coefficients, as evidenced by our study of the discriminant, which we constructed from the coefficients of the characteristic polynomial. We will now examine the coefficients of the discriminant itself to learn about its roots, which correspond to (avoided) curve crossings. We will present techniques which allow us to count and estimate the locations of the roots of a polynomial using information from its coefficients. We also quote results which allow us to determine the interval in which real roots and the moduli of complex roots lie, as well as the separation between the closest lying of those roots.

1. Bounds on the number of (avoided) crossings

Given a particular Hamiltonian, how many (avoided) crossings does its spectrum contain? This total is particularly useful to know when tracking the movement of the (avoided) crossings as parameters are varied. In the case of a numerical search of the spectrum, this bound enables us to know when to terminate the search.

In order to find the number of (avoided) crossings, we first consider the degree of the discriminant in the relevant parameter. If the Hamiltonian of a physical system is defined in an n-dimensional Hilbert space and is a polynomial of degree q in a parameter P, it can be shown that the discriminant $D[H(P)]$ is a polynomial of degree k in P where

$$k = n(n-1)q \bmod 2. \tag{16}$$

For example, if $n=2$ and $q=3$ then k can take values 6, 4, 2, or 0. The maximum value that k can assume, from Eq. (16), is

$$k_{\max} = n(n-1)q. \tag{17}$$

The reader can derive for herself this bound from the facts that $H(P)$ is a polynomial in P, and therefore every matrix element in its representation is also a polynomial of degree q or less in P. That the degree of the matrix element could be less than q is illustrated with an example from atomic physics in the accompanying paper [8]. In the general case if some of the matrix elements of the Hamiltonian are of a degree lower than q, the discriminant will have a degree lower than $k_{\max}$.

We note that since n and q are integers, $k_{\max}$ is always an even integer. The presence of mod 2 in Eq. (16) implies that k is always an even integer. This restriction follows from the property that if $H(P)$ is a polynomial in P, the degree of $D[H(P)]$ in P is always even. One way to derive this property is from a very useful theorem [28] which states that the discriminant can always be written as the sum of the squares of the moduli of a finite number of terms $A_i(P)$, each of which is a polynomial in the matrix elements of $H[(P)]$, and hence in P:

$$D[H(P)] = |A_1(P)|^2 + |A_2(P)|^2 + \cdots. \tag{18}$$

This condition restricts k, the degree of $D[H(P)]$ in P, to even integral values. This result is a useful cross-check when deriving expressions for discriminants in several parameters—the highest degree of the discriminant should be even in every parameter.

Another important conclusion that can be drawn from Eq. (18) is that if $P=S$ is a real or complex root of $D[H(P)]$ then it has to be a root of each $A_i(P)$; equivalently, $A_i(P)=(P-S)B_i(P)$, where the B_i are also polynomials in P. Thus Eq. (18) becomes

$$D[H(P)] = |P-S|^2[|B_1(P)|^2 + |B_2(P)|^2 + \cdots]. \tag{19}$$

If S is real,

$$|P-S|^2 = (P-S)^2; \tag{20}$$

if S is complex,

$$|P-S|^2 = (P-S)(\overline{P-S}) = (P-S)(P-\bar{S}). \tag{21}$$

Now we recall that (complex) real roots of the discriminant correspond to (avoided) crossings. We see that due to the structure of the discriminant implied by Eq. (19) *each crossing as well as each avoided crossing contributes a factor quadratic in the parameter P to the discriminant*. We have already seen explicit examples of each case. In Sec. III although there was only a single crossing at $P=0$, $\Delta=4P^2$ contained a double root at that point. In Sec. VI A $D[M(P)]=P_r^2+P^2$ [Eq. (13)] also turned out to be a quadratic with a pair of complex conjugate roots, both of which corre-

sponded to a single avoided crossing at $P=\mathrm{Re}[\pm iP_r]=0$.

It is important to note that the above italicized conclusion cannot be derived from the definition of Eq. (7) as the algebraic form of the eigenvalues in the general case of an $n(>4)$-dimensional matrix $H(P)$ is not known; the use of the nontrivial result Eq. (18) is necessary.

We now use the arguments made above to relate the degree of the discriminant to the number of (avoided) crossings for a given Hamiltonian. Recalling the fundamental theorem of algebra, which states that a polynomial of degree k with complex coefficients has exactly k roots, real or complex, we state a sum rule for level crossings: If the discriminant is a polynomial of degree k given by Eq. (16),

$$n_c + n_{\mathrm{ac}} = k/2, \tag{22}$$

where n_c and n_{ac} are the number of crossings and avoided crossings respectively in the spectrum of the corresponding Hamiltonian.

Now as we have mentioned in Sec. VI A above an obvious one-to-one correspondence between avoided crossings and complex roots is sometimes lacking. Therefore the sum rule Eq. (22) is not always exact. However, we may convert it into an upper bound that always holds:

$$n_c + n_{\mathrm{ac}} \leq k/2. \tag{23}$$

Equations (16) and (23) together imply that the number of (avoided) crossings scales no faster than quadratically with the dimension of the Hilbert space, and no faster than linearly with the degree of dependence of the Hamiltonian on a parameter. It is important to note that if the eigenvalues of $H(P)$ have to be found numerically, there is no way to find an exact bound on the number of (avoided) crossings in the spectrum other than calculating the discriminant.

2. Bounds on the location of (avoided) crossings

Given a Hamiltonian can we say where all the (avoided) crossings lie in its spectrum? The coefficients of a polynomial can yield very useful bounds on the location of the roots, a fact that can be used to immediately reduce the parameter space for a search for (avoided) crossings. A variety of bounds can be derived [29]; we will provide one due to Cauchy. Consider a discriminant of the form

$$D[H(P)] = \sum_{i=0}^{n} d_i P^i \tag{24}$$

of degree n and with $n+1$ real coefficients d_i. It can be shown that if S is any root, real or complex, of $D[H(P)]$, then

$$\frac{|d_0|}{|d_0| + H_0} < |S| < 1 + \frac{H_n}{|d_n|}, \tag{25}$$

where

$$H_0 = \max(|d_1|, |d_2|, \ldots, |d_n|) \tag{26}$$

and

$$H_n = \max(|d_0|, |d_1|, \ldots, |d_{n-1}|). \tag{27}$$

The coefficients d_i thus provide a bound for the values of the real roots as well as for the moduli of the complex roots. Let us find the bounds for a sample discriminant

$$D[H(P)] = (P-2)^2(P^2+1) = P^4 - 4P^3 + 5P^2 - 4P + 4. \tag{28}$$

In this case $H_0=H_n=5$. Hence the roots lie in the disk $4/9 < |S| < 6$. which is correct as the roots of Eq. (28) are $2, 2, \pm i$. Let us now choose $D[H(P)]$ to be

$$D[H(P)] = P^4 + P^3 + 5dP^2 + dP + d, \tag{29}$$

where $d>1$ is a real parameter, which we hold fixed while we tune P. In this case $H_0=H_n=5d$. Hence all the (avoided) crossings lie in the disk $1/6 < |S| < 1+5d$. This illustrates how the presence of a second parameter (d) influences the location of (avoided) crossings as the first parameter (P) is tuned.

In the discussion so far we have introduced ways of estimating the total number and locations of both real and complex roots. These methods do not distinguish between real and avoided crossings. We will now discuss three methods of locating real roots, which correspond to crossings exclusively. The methods are described in order of increasing generality as well as sophistication. We will first examine the information that the discriminant of a polynomial contains about its real roots. Then we will introduce Descartes' rule of signs, a useful tool for real root counting often used in elementary algebra. Last, we will describe the advanced method of Sturm-Habicht sequences.

3. Discriminant of the discriminant

The discriminant equals zero at an (avoided) crossing in the spectrum. Does it carry any information about the roots when it is not zero? Some information regarding the real roots of the discriminant can be obtained by calculating the discriminant of the discriminant. To eliminate confusion, we repeat we are now considering the discriminant $D[D[H(P)]]$ of the discriminant $D[H(P)]$ of the characteristic polynomial of $H[(P)]$. The characteristic polynomial is in the variable E, and the discriminant $D[H(P)]$ is a polynomial in the variable P. In this context it is relevant to note that although $D[H(P)] \geq 0$ as proved earlier in Sec. V D, $D[D[H(P)]]$ is allowed to be negative via definition Eq. (7), since the roots of $D[H(P)]$ may not all be real.

If all the roots, real or complex, of $D[H(P)]$ are distinct, then $D[D[H(P)]]$ is not zero; it must then either be positive or negative. It can be shown that the sign of $D[D[H(P)]]$ determines the number of real roots of $D[H(P)]$ modulo 4 [10]. More precisely, if $D[H(P)]$ is a monic (the coefficient of the highest term in P is 1) polynomial of degree k and all of whose roots (real or complex) are distinct, the number t of real roots it can have is given by [10],

$$D[D[H(P)]] > 0 \Leftrightarrow t = k \bmod 4$$

$$D[D[H(P)]] < 0 \Leftrightarrow t = (k-2) \bmod 4. \quad (30)$$

We note that $k>1$ for $D[D[H(P)]]$ to be defined.

Let us consider some examples. In Eq. (30) if $k=2$ and $D[D[H(P)]]>0$ then $D[H(P)]$ has exactly 2 real roots; if $D[D[H(P)]]<0$ then it has exactly none. However if $k=10$ and $D[D[H(P)]]<0$ then it has either 8, 4, or 0 real roots. The information regarding crossings is therefore exact only if the polynomial has no repeated roots and is of degree $1<k<4$ (in case $D[D[H(P)]]>0$) or $1<k<6$ (in case $D[D[H(P)]]<0$). In Sec. VI B above we proved that k has to be even. Hence Eq. (30) yields precise information only in the allowed cases $k=2(2,4)$ for $D[D[H(P)]]$ positive (negative). To gain more information about less specialized polynomials we turn to Descartes' rule below.

4. Descartes' rule of signs

A method from elementary algebra for counting real roots is Descartes' rule of signs [10] which equates the total number of positive real roots of a polynomial with real coefficients to the number of sign changes in its coefficients, modulo 2. The number of negative real roots may be similarly estimated by changing the sign of the variable of the polynomial. As a useful consistency check we mention one of the lemmas of Descartes' rule: The number of sign variations of a polynomial with real coefficients is even if the first and last coefficients have the same sign and odd if they have opposite signs. Note that when counting sign variations terms with missing coefficients can be ignored.

Rather than present a proof [29], we show how the rule works with the discriminant defined in Eq. (28)

$$(P-2)^2(P^2+1) = P^4 - 4P^3 + 5P^2 - 4P + 4, \quad (31)$$

which has two real roots both at $P=2$. It also has a pair of complex roots at $P=\pm i$. The number of sign changes in the coefficients of the polynomial in Eq. (31) is 4. Descartes' rule implies that the number of *positive* real roots is 4, 2, or 0, of which we know the second to be the correct answer. Now if we make the transformation $P\rightarrow -P$ in Eq. (31) we obtain the polynomial $P^4+4P^3+5P^2+4P+4$. The number of sign changes in the coefficients is 0. Descartes' rule implies that there are no *negative* real roots at all, which is correct.

Descartes' rule yields the exact number of crossings only when the number of sign changes in the discriminant is 0 or 1. The rule is most useful in the former case which corresponds to the total absence of level crossings in the spectrum. An example of this will be provided in the section on atoms in the accompanying paper [8]. However in many cases multiple crossings do exist, and it is desirable to account for their exact number in an arbitrary parameter interval. For this we turn to the method of Sturm-Habicht sequences. These will be of use in determining curve crossings in a diatomic molecule.

5. Sturm-Habicht sequences

A more sophisticated method of locating real roots uses the Sturm-Habicht (SH) sequence of a polynomial with real coefficients such as $D[H(P)]$ [10]. If $D[H(l)]D[H(r)]\neq 0$ the difference in the number of sign variations in the SH sequence at $P=l$ and $P=r$ equals the number of real zeros of $D[H(P)]$ in the interval $P\in[l,r]$ exactly.

We first describe the method generally. Given a polynomial $D[H(P)]$ of degree k, the SH sequence

$$S = S_k, S_{k-1}, \ldots, S_0 \quad (32)$$

contains $k+1$ elements, is numbered in reverse and is constructed as follows [30]. The first element of the sequence is the polynomial itself

$$S_k = D[H(P)]. \quad (33)$$

The second element is the derivative of the polynomial with respect to P

$$S_{k-1} = D'[H(P)]. \quad (34)$$

The remaining $k-1$ elements from $i=k-2$ to $i=0$ are obtained from the prescription

$$S_i = -\frac{\mathcal{R}[s_{i+1}^2 S_{i+2}, S_{i+1}, P]}{s_{i+2}^2}, \quad (35)$$

where s_i is the coefficient of the highest monomial in S_i and $\mathcal{R}[A,B,P]$ is the polynomial remainder obtained upon dividing A by B, both of which are polynomials in P. The S_i are polynomials in P themselves.

From Eq. (35) we can see that technical problems can arise if some $s_i=0$ (the SH sequence is "defective"). The SH sequence can however still be constructed for such a case; details are provided in [30]. We now give a simple example of SH technique using the discriminant

$$D[H(P,c)] = P^4 + P^3 + P^2 + P + c, \quad (36)$$

where the c is a constant which will be assigned a numerical value later. In a physical system, it may correspond to a tunable parameter other than P. $D[H(P,c)]$ in Eq. (36) is a quartic in P and hence there will be five elements in the SH sequence. Following the prescriptions in Eqs. (33)–(35) above we find

$$S_4 = P^4 + P^3 + P^2 + P + c,$$

$$S_3 = 4P^3 + 3P^2 + 2P + 1,$$

$$S_2 = -5P^2 - 10P - 16c - 1,$$

$$S_1 = 20(c-1)P - 25c,$$

$$S_0 = 256c^3 - 203c^2 + 88c - 16. \quad (37)$$

From Eq. (37) we obtain

$$s_4 = 1,$$

$$s_3 = 4,$$

$$s_2 = -5,$$

$$s_1 = 20(c-1),$$

$$s_0 = 256c^3 - 203c^2 + 88c - 16. \tag{38}$$

If we wish to know the total number of real roots for Eq. (36) exactly, then we must examine the sign of each term in the SH sequence (37) at $P=\pm\infty$. Our task is simplified by the fact that at these limits the sign of each element in the sequence (37) is determined by the highest monomial and its coefficient. Thus we need examine only the sequence defined by Eq. (38) $[P^4, 4P^3, -5P^2, 20(c-1)P, 256c^3-203c^2+88c-16]$. For $c>1$, the coefficient of the fourth term in this sequence is positive. For $c>0.32$ the last term in the sequence is positive. Let us consider the case $c>1$. At $P=-\infty$ the signs of the terms in the sequence are

$$(+,-,-,-,+). \tag{39}$$

There are $\delta_{-\infty}=2$ sign changes in this sequence. At $P=+\infty$ the signs of the terms in the sequence are

$$(+,+,-,+,+). \tag{40}$$

There are $\delta_{+\infty}=2$ sign changes in this sequence. The exact number of real roots of $D[H(P)]$ is then given by

$$\delta_{-\infty} - \delta_{+\infty} = 0, \tag{41}$$

which implies that there are no level crossings for any P and $c>1$. This is an example of a case where two parameters are tunable in a physical system and the method of SH sequences allows us to identify a large portion of the corresponding two-parameter space which does not contain any crossings at all. More generally algebraic technique allows us to systematically account for the effects of multiple parameters in the problem when looking for level crossings.

A similar analysis using the sequence (37) for $c=0.2$ yields exactly two real roots for Eq. (36). They can be verified to be $P=-0.86,-0.25$ by solving Eq. (36). It is worth noting that the ordering of the terms in the left-hand side (LHS) of Eq. (41) is important. If the interval of interest is $[l,r]$ then the SH method prescribes the number of real roots to be $\delta_l-\delta_r$. If this quantity turns out to be negative the coefficients of $D[H(P)]$ can no longer be considered purely real [10].

We make three observations about the method of SH sequences, stated in order of increasing importance. First, it is important to note that the SH sequence does not immediately provide the numerical value of the real root, it only indicates its presence in an interval. However, by using successively smaller intervals in a search one may isolate the root and obtain its value [10].

Second, it is of use to know that the coefficients of the polynomials in the SH sequence can be related to the *subdiscriminants* of $D[H(P)]$ [10], which will be discussed below. In fact S_0 in Eq. (37) is the discriminant of $D[H(P,c)]$ as defined in Eq. (36), i.e., $S_0=D[D[H(P,c)]]$. Knowledge of this fact can be employed to save computational time and effort. For instance, if the total number of roots is the only information desired, as in the example above, then only the coefficients of the leading monomials in the SH sequence, i.e., the s_i need be computed. This can be done by calculating the relevant subdiscriminants.

Third, often the greatest use of SH technique is to be able to isolate large intervals of (multi)parameter space which do not contain any real roots. This corresponds to regimes in the spectrum that do not have crossings. The use of SH technique to find such intervals has the advantage that each specific numerical parameter value does not have to be investigated, in contrast to searching the spectrum.

Fourth, the SH analysis shows how it is possible to gain information about crossings even if the Hamiltonian is not fully specified. In fact it may happen that an experiment requires staying away from the crossings in a system described by the Hamiltonian $H(P,c)$, and c is a parameter about which the only information we have is $c>10$. Then, even though $H(P,c)$ is not fully known, the SH analysis in the example above implies that a crossing will never be encountered, since $c>1$.

6. Minimum separation between crossings

Given a Hamiltonian, what is the minimum separation between two (avoided) crossings in its spectrum? The coefficients of a polynomial can provide a lower bound for the separation between any two roots of the polynomial. This bound is of use in implementing any root-isolation procedure, including the method of SH sequences delineated above. It also provides a measure for the proximity of avoided crossings, which as we have seen in Sec. VI A can be important for their "interaction."

Consider a discriminant $D[H(P)]$ of the form

$$D[H(P)] = \sum_{i=0}^{k} d_i P^i, \tag{42}$$

where $k\geq 2$ is the degree of the discriminant and d_i are its coefficients. We define the Euclidean norm of $D[H(P)]$ as

$$\|D[H(P)]\| = \sqrt{\sum_{i=0}^{k} |d_i|^2}. \tag{43}$$

It can be shown that if S and S' are any two roots of $D[H(P)]$, then [31]

$$|S-S'| > \frac{\sqrt{3|D[D[H(P)]]|}}{k^{(k+2)/2}} \|D[H(P)]\|^{1-k}, \tag{44}$$

where it should be noticed that the discriminant of $D[H(P)]$ is under a radical as well as within a modulus.

Let us evaluate this bound for the discriminant

$$D[H(P)] = (P+1)(P-2)(P^2+1), \tag{45}$$

whose roots are -1, 2, and $\pm i$. The discriminant of $D[H(P)]$ is -3600, the Euclidean norm $\sqrt{8}$. This implies a minimum separation ~ 0.07.

The usefulness of Eq. (44) is limited in the cases where $D[D[H(P)]]=0$, i.e., when there is more than one crossing at the same parameter value, a phenomenon which is certainly not rare. In such cases it is sometimes possible to remove the repeated factors by hand and apply Eq. (44) to the remaining polynomial factor. MATHEMATICA for instance has the command FactorSquareFree which performs this function.

7. Degeneracy of an (avoided) crossing

Can we tell, without looking at the spectrum, exactly how many eigenvalues are coincident or avoid each other at a particular parameter value? We divide the answer to this question into two parts. In the first part we show how much information can be extracted from the discriminant itself. In the second part we introduce subdiscriminants and quantify the information that can be extracted from them.

(a) Discriminants. It will be sufficient to consider crossings only. Before we answer the question posed above, it is useful to reiterate the definition of a crossing: We define a crossing to be the intersection of two eigenvalues. If m eigenvalues coincide at the same value of the parameter, the number of crossings is given by the ways to pick a pair out of m curves, i.e., the binomial factor $\binom{m}{2}$. Since every crossing leads to a quadratic factor in the discriminant according to Sec. VI B, the corresponding exponent of the parameter in the discriminant will be $2\binom{m}{2}=m(m-1)$. Given the form of the discriminant, we can follow this chain of reasoning backwards in order to extract the number m of intersecting eigenvalues. For example in Sec. III, we found $\Delta=4P^2$. In this case, the exponent of P implies that

$$2\binom{m}{2}=2. \tag{46}$$

This has the solution $m=2$ and points to the intersection of *two* eigenvalues at $P=0$.

The retrodictive power of this analysis decreases for more general cases. One such case is where the eigenvalues all do not coincide at the same value of the corresponding physical observable (energy for example), although they may coincide for the same value of the parameter P.

Let us consider the simplest possible situation of this type by considering an example where the dimension of the Hilbert space is n. We assume that m eigenvalues are coincident at a single point and also that the remaining $n-m$ eigenvalues are coincident at another value of the corresponding physical observable. Both intersections occur at the same value of the parameter, say $P=a$. Then the discriminant has a factor

$$(P-a)^{2\left[\binom{m}{2}+\binom{n-m}{2}\right]}=(P-a)^c. \tag{47}$$

Given c (from the form of the discriminant), the two partitions of n can be uniquely found to be

$$m=\frac{n}{2}\pm[2c-n(n-2)]^{1/2}. \tag{48}$$

For $n=2$, $c=2$, we get $m=0,2$, which corresponds to the specific case of Eq. (46). So even in this case we can retrodict. We now consider the general case of partitioning n eigenvalues among r crossing points—all at the same parameter value—in order to see if the number of crossings is unique for each partition. For a matrix $H(P)$ with n eigenvalues distributed amongst r crossing points, such that $n_i(\geq 2)$ eigenvalues coincide at the ith point, the total number of crossings equals the half the corresponding exponent in the discriminant, which we label c:

$$\binom{n_1}{2}+\binom{n_2}{2}+\cdots\binom{n_r}{2}=\frac{c}{2}. \tag{49}$$

Simplifying, we see that the equation to be solved becomes

$$n_1^2+n_2^2+\cdots+n_r^2=c+n, \tag{50}$$

where we have used the fact that $\Sigma_{i=1}^{r}n_i=n$. Since $c+n$ is a fixed (known) integer, the question now becomes: "For every partition of n into a sum of integers each greater than two, is the sum of the squares of those integers unique?" Interestingly we have not been able to answer in the negative for any specific r, although we have not tried to prove the result for arbitrary r. The answer may already exist in number theory, and would enable us to retrodict the crossing degeneracy exactly albeit for a special category of spectra, where from physical considerations we can argue for the absence of any nondegenerate states at some value of the parameter P. However, it should be noted that we will still be unable to distinguish between different orderings of the n_i on the ordinate of the spectrum. For example we will not be able to tell, in order of decreasing (say) energy, if 3,2,6 or 6,3,2 eigenvalues are meeting in the spectrum at 3 different points for the same value of the parameter.

If some of the eigenvalues do not cross at all, different partitions can readily be shown to yield the same exponent c. Consider $n=6$. In one case let six eigenvalues coincide pairwise at three different crossing points (for the same value of P). This yields $c=2\times3\times\binom{2}{2}=6$. In the second case, let three eigenvalues coincide at a single crossing point, and the remaining three not at all. This yields $c=2\times\binom{3}{2}=6$ also. Hence in this case it is not possible to deduce the number of eigenvalues crossing at a parameter value uniquely.

As far as the discriminant is concerned, the answer to the question posed in the beginning of this section can thus be answered as follows. It is not generally possible to decipher uniquely from the discriminant how many eigenvalues are coincident at a particular parameter value without looking at the spectrum. However, if the spectrum can be consulted the combinatoric accounting of the exponents of the factors in the discriminant provides a very useful check on the correctness of the discriminant itself. This is particularly true if the comparison is made for values of the parameter which correspond to known symmetries—and hence degeneracies—of the spectrum. An example of this will be provided in the section on atoms in [8].

(b) Subdiscriminants. There exist mathematical objects that rigorously count the number of times a root is repeated for a given polynomial [10]. These are called *subdiscriminants* ($\mathcal{S}_q^D$) and are generalizations of the discriminant ($\mathcal{S}_0^D$), which tells us if any root occurs at least twice. For a p-fold ($p\geq2$) root of the characteristic polynomial Eq. (6), subdiscriminants up to $\mathcal{S}_{p-2}^D$ will be zero.

In terms of the eigenvalues of $H(P)$ the qth subdiscriminant is defined as [10]

$$\mathcal{S}_q^D[H(P)] = \sum_{\substack{I\subset\{1,\ldots,n\} \\ \#(I)=n-q}} \prod_{\substack{(i,j)\in I \\ i<j}}^{n-q} (\lambda_i - \lambda_j)^2. \tag{51}$$

Here $\subset$ means "is a subset of," # means "number of elements in," and $\in$ means "is a member of." The summation is over I, which is chosen to be an $(n-q)$ tuple of numbers chosen from the set $\{1,\ldots,n\}$. The product is over all the choices of I. For simplicity we will often suppress the $H(P)$ label on the $\mathcal{S}^D$'s in what follows, i.e., we will refer to $\mathcal{S}_q^D[H(P)]$ simply as $\mathcal{S}_q^D$.

We further explain the notation of Eq. (51) by providing an example. If we calculate $\mathcal{S}_0^D$, i.e., with $q=0$, there is then only one way to choose I: It is a single n-tuple $\{1,\ldots,n\}$ containing all values from 1 to n. The product is then evaluated by letting i,j run over all the n values in I subject to the constraint $i<j$. We can then see that the $\mathcal{S}_0^D$ actually gives us back the discriminant of Eq. (7):

$$\mathcal{S}_0^D[H(P)] = \prod_{i<j}^{n} (\lambda_i - \lambda_j)^2. \tag{52}$$

Let us now pick a case where $q\neq 0$. We assign a value to n in order to make the example transparent. Let $n=3$. In this case, explicitly from Eq. (52)

$$\mathcal{S}_0^D = (\lambda_1 - \lambda_2)^2(\lambda_2 - \lambda_3)^2(\lambda_1 - \lambda_3)^2, \tag{53}$$

which equals zero when any two of the roots are equal. Let us consider $q=1$. The number of elements in I is now $n-q=3-1=2$ and the summation is over the three 2-tuples $\{1,2\},\{2,3\}$, and $\{1,3\}$. Taking the product so that i,j run over the values in each 2-tuple so that $i<j$ holds, we find

$$\mathcal{S}_1^D = (\lambda_1 - \lambda_2)^2 + (\lambda_2 - \lambda_3)^2 + (\lambda_1 - \lambda_3)^2, \tag{54}$$

which equals zero only when all three roots are equal, i.e., when the corresponding Hamiltonian has a threefold root. In this case, of course $\mathcal{S}_0^D$ from Eq. (53) is also zero. Thus for a threefold root $\mathcal{S}_q^D$'s up to $q=3-2=1$ are zero. We see that the subdiscriminants account for root multiplicities in a natural way, and thus inform us of the number of (avoided) crossings at a particular parameter value. However, as in Sec. VI B(a) we cannot distinguish between (avoided) crossings that occur at different values of the energy but the same value of the parameter. For this, the spectrum has to be consulted. The method of subdiscriminants is useful when the discriminant does not display the multiplicities of its roots explicitly. Some caution needs to be exercised when using this method if the same parameter value corresponds to crossings as well as avoided crossings.

Subdiscriminants may be found without consulting the spectrum and an analog exists to Eq. (9) for discriminants, written using the determinant of the $(n-q)\times(n-q)$ Hermite matrix of the characteristic polynomial $G(E)$ in Eq. (6) [10]:

$$\mathcal{S}_q^D[H(P)] = \begin{vmatrix} N_0 & N_1 & \cdots & & \cdots & N_{n-q-1} \\ N_1 & \cdots & & \cdots & N_{n-q-1} & N_{n-q} \\ \cdots & & & & & \\ \cdots & N_{n-q-1} & N_{n-q} & \cdots & & \cdots \\ N_{n-q-1} & N_{n-q} & \cdots & & \cdots & N_{2n-2q-2} \end{vmatrix}, \tag{55}$$

where the (i,j)th matrix element is given by the Newton sum N_{i+j-2} defined by

$$N_w = \sum_{i=1}^{n} \lambda_i^w. \tag{56}$$

The Newton sums are basically sums of powers of the eigenvalues of $D[H(P)]$; they can also be obtained purely from the coefficients C_i of Eq. (6) from the recurrence relations:

$$N_0 = n,$$

$$C_n N_1 + C_{n-1} = 0,$$

$$C_n N_2 + C_{n-1} N_1 + 2C_{n-2} = 0. \tag{57}$$

More generally,

$$C_n N_d + C_{n-1} N_{d-1} + \cdots + C_{n-d+1} N_1 + dC_{n-d} = 0. \tag{58}$$

Subdiscriminants are specializations of subresultants, which are defined in *Mathematica* and *Maple*. Using such functions we can verify that the first two subdiscriminants of the polynomial

$$P(P-a)^3 = P^4 - 3aP^3 + 3a^2P^2 - a^3P, \tag{59}$$

where a is a real constant, vanish. This confirms the existence of the threefold root at $P=a$.

C. Symmetries and crossings

If the discriminant is a polynomial whose roots can be found algebraically, which is usually not the case, the values of the parameter at which (avoided) crossings occur can be found in terms of the remaining parameters of the physical system. Apart from allowing us to track the crossing trajectories for the full parameter space of the physical system, these analytic expressions can also reveal other useful information. For example if the analytic expressions for a number of crossings imply they are close-lying, but can never be made to coincide exactly, they point to a symmetry of the physical system that is only approximate and not exact. An example of this is given using atoms in the accompanying paper [8].

The roots of the discriminant $D[H(P)]$ can be obtained in terms of radicals only if the Galois group of the discriminant is solvable [32]. Is this the case only if the original Hamiltonian is solvable, or more specifically, only if the Galois group of the characteristic polynomial $G(E)$ [Eq. (6)] is solvable? At present we are not aware of an answer to this question.

A further question to be discussed in Sec. VIII C below is whether the symmetry of the discriminant in a certain parameter is also true of the spectrum. For example if the discriminant is even in P, is the spectrum also invariant under the transformation $P \rightarrow -P$? If so, the discriminant could be used to find the symmetry of the spectrum even when the Hamiltonian cannot be analytically solved, i.e., for arbitrary size n.

D. Visualizing crossings

Crossings can sometimes be difficult to visually distinguish in a spectrum, especially if there are many eigenvalues spaced closely together. In this section we show how the discriminant can provide a visual aid to locating crossings that is often superior to the spectrum.

Although the discriminant equals zero whenever there is a crossing in the spectrum, typically it is not easy to locate these zeros in a plot of the discriminant. The reason for this difficulty can be seen from the following example. Imagine a Hamiltonian defined on a Hilbert space of dimension 5, and depending linearly on a parameter P. Using $n=5$ and $q=1$ in Eq. (16) we find the degree of the discriminant could be as large as 20 in P. For such a nonlinear polynomial it is not easy to capture on a single scale the full range of features as each of the monomials dominates in a different regime of the parameter P. A smoother representation better suited to our purpose is provided by

$$L[D[H(P)]] = \log[D[H(P)] + 1] \tag{60}$$

which dips to zero at every level crossing, where $D[H(P)] = 0$. The argument of the logarithm is bound from below by one and the logarithm itself by zero due to the nonnegativity property of the discriminant ($D[H(P)] \geq 0$) discussed in Sec. IV. In Eq. (60) the logarithm has been taken to the base e.

Plots illustrating Eq. (60) are shown in the accompanying paper, along with the relevant spectra. Before moving on we pause to mention two issues. First, in practice we have often found it necessary to scale $D[H(P)]$ with some number $N_S > 0$ in order to optimize the visibility of the logarithm in Eq. (60). That is we usually plot $\log[D[H(P)]/N_S + 1]$ and adjust N_S to obtain good visibility.

Second, in all the spectra we plot, Eq. (60) does not display avoided crossings. The reason for this is as follows. In principle, a polynomial that is everywhere non-negative (such as $D[H(P)]$) exhibits a minimum at values of the parameter that correspond to complex pairs of roots. Equation (60) is indeed capable of revealing this behavior, but it turns out that all the avoided crossings in our spectra are very shallow, and the minima corresponding to them are washed out by stronger features due to crossings nearby. Such "hidden" avoided crossings are quite well known in molecular physics [33] and are referred to in the accompanying paper [8].

VII. THE WIGNER–VON NEUMANN THEOREM

The simple 2×2 example demonstrated in Sec. III above allows us to make contact with the seminal paper of Wigner and von Neumann [2] which established the rules for curve crossing in systems described by parametrized matrices.

Rewriting Eq. (1) as

$$M(P) = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & V \\ V & 0 \end{pmatrix}, \tag{61}$$

we interpret it to be a representation of the operator equation

$$\hat{M}(P) = \hat{M}_o(P) + \hat{V}(P). \tag{62}$$

The (avoided) crossings in the spectrum of the operator $\hat{M}(P)$ are related to its symmetries by assuming that its representation in Eq. (61) was made using the eigenbasis $|C\rangle$ of some operator $\hat{C}$ which commutes with both $\hat{M}_o(P)$ and $\hat{M}(P)$ and therefore also with $\hat{V}(P)$, i.e.,

$$[\hat{C}, \hat{M}(P)] = [\hat{C}, \hat{M}_o(P)] = [\hat{C}, \hat{V}(P)] = 0. \tag{63}$$

Evaluating the matrix element of the last relation in Eq. (63) we find

$$\langle C'' | \hat{V}(P) | C' \rangle = 0, \tag{64}$$

unless $C' = C''$. Equation (64) implies that barring "accidents" the matrix elements of $\hat{V}(P)$ vanish unless the two states in the Hilbert space of $\hat{M}(P)$ have the same symmetry. Here by symmetry we mean the eigenvalue of $\hat{C}$. In particular the matrix elements of $\hat{V}(P)$ equal zero if the states are *not* of the same symmetry. We are now ready to examine the relation of curve crossing to symmetry. Looking at the representation of $\hat{M}(P)$ in Eq. (61) we see that in order to have a level crossing between the eigenvalues $\lambda_\pm$ of the real symmetric matrix $M(P)$ the conditions are

$$E_1 - E_2 = 0,$$

$$V = 0. \tag{65}$$

If the two eigenstates of $M(P)$ are of different symmetry then $V \equiv 0$ and only the first condition remains to be satisfied [15]. This can be arranged using a single tunable parameter. On the other hand, if the two states are of the same symmetry then $V \neq 0$ except accidentally. In this case two tunable parameters are required to effect a crossing between $\lambda_\pm$. If $M(P)$ were to be a Hermitian matrix, a single tunable parameter would still suffice to make two eigenstates of different symmetry cross. However, the number of tunable parameters required to make two eigenstates of the same symmetry cross would be three [34]. This is so because V is no longer purely real and two parameters are required to make its real and imaginary parts separately equal to zero.

The arguments given above are the essence of the Wigner-Neumann noncrossing rule, which is sometimes broadly stated as "states of the same symmetry do not cross, except accidentally." In the accompanying paper we will show the results of algebraic technique are not only compatible with the Wigner–von Neumann theorem, but in fact provide explicit and interesting examples of it. For example, for the real symmetric atomic Breit-Rabi Hamiltonian where the magnetic field is the only tunable parameter, we confirm that all

crossings occur between states of different symmetry, i.e., there are no accidental crossings. Further, all avoided crossings occur between states of like symmetry. In this case by symmetry we mean the eigenvalues of the projection of the angular momentum along the direction of the magnetic field.

The Wigner–von Neumann noncrossing rule is very useful as a general guideline, and in the construction of correlation diagrams in particular. However when (avoided) crossings do occur it does not provide precise quantitative information about their location, number or degeneracy. It was partly a dissatisfaction with the Wigner–von Neumann theorem that led us to investigate techniques that could yield more quantitative information about (avoided) crossings, accidental or otherwise.

VIII. DISCUSSION

Here we discuss three aspects of the work presented above. First, we mention the original contributions of this article in order to distinguish them from the material that has been collated from the existing literature. Second, we present a critique of algebraic theory. Last, we point out some interesting directions for future research.

A. Original contributions

To the best of our knowledge, the following results presented in this article are original: In Sec. V B, the discussion of the direct product basis as the algebraically most convenient representation for (avoided) crossing analysis; in Sec. V C the mention of the translational invariance of the discriminant under addition of an arbitrary function to the diagonal elements of $H(P)$; in Sec. VI B 1 the use of Eq. (18) to connect the presence of every (avoided) crossing to a quadratic factor in the discriminant and hence to derive the bound on the total number of (avoided) crossings in Eq. (23); in Sec. VI B 5 the use of Sturm-Habicht sequences to show that crossings can be found even if information about the Hamiltonian of the system is incomplete; in Sec. VI B 7(a) the derivation of the combinatoric connection between the (algebraic) degeneracies of the roots of the discriminant and the (spectral) degeneracies of the Hamiltonian; and in Sec. VI D the method of visualizing crossings using the discriminant.

B. Critique

We list criticisms of algebraic technique in the order of appearance of the results in the article.

In Sec. II it is claimed that algebraic technique is a good way to distinguish between finely avoided crossings and actual crossings. As pointed out in [35] for some purposes the distinction is not worth making, since crossings are unstable to arbitrary, small perturbations. Such instabilities can even arise if the spectrum is calculated with a truncated Hilbert space, and are not due to any physical effect. An example of this is the H_2^+ molecular ion which can be solved exactly and yields symmetry-allowed crossings. When basis sets are used to calculate the spectrum however, these crossings turn into avoided intersections [15]. As mentioned in the same section (Sec. II) a shortcoming of algebraic technique is that it does not yield information about eigenvalues, eigenvectors or the physical variable such as energy being described by the spectrum. It cannot provide information about how big the gap in an avoided crossing is, for instance.

In Sec. VI A it is pointed out that the proximity of (avoided) crossings along the ordinate of the spectrum cannot be obtained from the discriminant. Two crossings may occur for the same value of the energy spectrum abscissa, (i.e., parameter) but may be widely separated in energy.

In Sec. VI B 7 it was found that although algebraic technique can tell us the exact number of crossings at any parameter value, it cannot describe the way in which eigenvalues are distributed among the crossings except in very special cases.

Not addressed in the treatment above is a difficulty we encountered while applying algebraic technique to some typical atomic problems: Sometimes for a given Hamiltonian the discriminant is identically zero. This occurs when some remaining symmetry has not been removed from the problem, and makes algebraic study of the (avoided) crossings impossible. In this case an expression for the discriminant may be recovered either by putting in a symmetry-breaking term in the Hamiltonian "by hand,"—or by treating the two subspaces with different symmetry independently as uncoupled problems. A typical example in this class is the Stark Hamiltonian for a polar molecule [36], where even after the application of an electric field there remains a degeneracy between the $\pm M$ subspaces where $|M|$ is the projection of the angular momentum along the electric field. A transverse field can be introduced "by hand,"—or the $\pm M$ manifolds can be treated separately (as they do not interact with each other in the problem) in order to recover the discriminant.

As an overall comment we reemphasize that the sharpest restrictions on algebraic technique arise from the expense of the symbolic computation required to make it useful.

C. Future directions

We discuss a number of interesting questions raised by the work presented in this article. The roots of a polynomial can be solved in terms of radicals if the Galois group of the polynomial is solvable [32]. Thus the eigenvalues of $H(P)$ can be obtained in terms of radicals if $G(E)$ [Eq. (2)] has a solvable Galois group. Similarly, the roots of $D[H(P)]$ can be obtained in terms of radicals if its Galois group is solvable. An interesting question is the link between the solvability of the two polynomials $G(E)$ and $D[H(P)]$. Does one imply the other, and is the converse true? Is it possible to obtain the parameter values for the (avoided) crossings in terms of radicals even if the eigenvalues of the Hamiltonian cannot be so obtained?

A question similar in nature to the one asked above is as follows: Is the spectrum always symmetric in some parameter P if the discriminant is also? We have seen explicit examples of this in Sec. III where $\Delta=4P^2$ and in Sec. VI where $D[M(P)]=P_r^2+P^2$. In [8] we will see a case where the discriminant is asymmetric, as is the spectrum. The answer to the question posed would seem to lie in the examination of

the C_i in Eq. (2). If they are even functions of P, both $D[H(P)]$ and the eigenvalues of $H(P)$ should be as well. However it is not clear if the conclusion is necessarily the opposite if all or some of the C_i are odd or of no particular symmetry in P. Further, a spectrum can be symmetric in a parameter even if the individual eigenvalues are not. An example of this is the Breit-Rabi spectrum presented in the accompanying paper [8]. If a link can be made in the general case, the discriminant can be used to predict the symmetry of the Hamiltonian with respect to the parameter P. This would be especially useful if the spectrum cannot be solved algebraically.

There is also the open question mentioned at the end of Sec. VI B 7(a). It would be interesting to see if the partitioning of m eigenvalues among r crossing points with a minimum of two eigenvalues per point can be done to yield a unique number of crossings for each partition. This would imply we can extract the crossing degeneracies uniquely from the discriminant in a special case where there no nondegenerate states exist at a particular parameter value. How to do this efficiently for large m is a separate question, as the number of partitions $p(n)$ grows quickly with n as $p(n) \sim e^{\pi\sqrt{2n/3}}/(4n\sqrt{3})$ [37].

Most of the examples in this article as well as the realistic problems in the accompanying paper deal with one or two tunable parameters. Obvious extensions of our work include generalizations to a larger number of parameters (i.e., multivariate polynomials) of Sturm-Habicht technique, for instance. Also, an important class of systems to which algebraic technique should be extended is that of *open* or dissipative systems [38] such as in microwave cavities. In these systems, the eigenvalues have finite linewidths which may be exchanged at an avoided crossing, leading to interesting effects such as resonance trapping [39]. Such systems are most generally described by non-Hermitian matrices. This requires a treatment where $H(P)$ is no longer Hermitian and many of the conclusions of this article will have to be suitably modified.

As a closing remark we mention that a variety of mathematics seems to be linked to questions regarding level-crossing in physical systems. In this article we have used linear algebra, complex analysis, combinatorics and algebraic geometry, and touched upon the theory of partitions. From our perusal of other sources it seems there are more links. We end the section with the following intriguing quote [40]: "The place of discriminants in the general theory of hypergeometric functions is similar to the place of quasiclassical approximation in quantum mechanics."

IX. CONCLUSION

Mathematical techniques for algebraically locating and analyzing (avoided) crossings in physical systems have been developed in some detail. The chief tool used in this approach is the discriminant, an elegant bookkeeping device for matrix Hamiltonians of size less than 5×5 and a very useful diagnostic for systems of larger dimension.

Given a physical system, we have shown how to find a bound on the number of (avoided) crossings in its spectrum, the scaling of this bound with the size of the Hilbert space, and the parametric dependencies of the Hamiltonian, the interval in which the (avoided) crossings all lie in parameter space, the number of crossings at any given parameter value, and the minimum separation between the (avoided) crossings. We have also shown how crossings can reveal the symmetries of the physical system, how (avoided) crossings can always be found without solving for the eigenvalues, how they may sometimes be found even in case the Hamiltonian is not fully known, and how crossings may be visualized in a more direct way than revealed by the spectrum. In the accompanying paper [8] we apply these techniques to atoms and molecules in the context of Feshbach resonances.

ACKNOWLEDGMENTS

M.B. would like to thank Dr. S. R. Muniz for encouraging him to pursue this research, and Dr. L. Baksmaty, Professor S. Basu, and Dr. M. Trott for technical help. This research was funded by DOE and ARO.

[1] W. R. Hamilton, Dublin Univ. Rev. Q. Mag **1**, 795 (1833).
[2] J. von Neumann and E. P. Wigner, Z. Phys. **30**, 467 (1929).
[3] L. Landau, Phys. Z. Sowjetunion **2**, 46 (1932).
[4] C. Zener, Proc. R. Soc. London, Ser. A **137**, 696 (1932).
[5] M. V. Berry and M. Wilkinson, Proc. R. Soc. London, Ser. A **392**, 15 (1984).
[6] J. R. Walkup, M. Dunn, D. K. Watson, and T. C. Germann, Phys. Rev. A **58**, 4668 (1998).
[7] R. G. Unanyan, N. V. Vitanov, and K. Bergmann, Phys. Rev. Lett. **87**, 137902 (2001).
[8] M. Bhattacharya and C. Raman, following paper, Phys. Rev. A **75**, 033406 (2007).
[9] M. Bhattacharya and C. Raman, Phys. Rev. Lett. **97**, 140405 (2006).
[10] S. Basu, R. Pollack, and M. F. Roy, *Algorithms in Real Algebraic Geometry* (Springer-Verlag, Berlin, 2003).
[11] I. Freund, J. Opt. A, Pure Appl. Opt. **6**, S229 (2004).
[12] V. V. Stepanov and G. Muller, Phys. Rev. E **58**, 5720 (1998).
[13] W. D. Heiss and W. H. Steeb, J. Math. Phys. **32**, 3003 (1991).
[14] T. J. Davis, Eur. Phys. J. D **18**, 27 (2002).
[15] D. R. Yarkony, Rev. Mod. Phys. **68**, 985 (1996).
[16] C. M. Bender, H. J. Happ, and B. Svetitsky, Phys. Rev. D **9**, 2324 (1974).
[17] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientsists and Engineers* (McGraw-Hill, New York, 1978).
[18] A. Nishino and T. Deguchi, Phys. Rev. B **68**, 075114 (2003).
[19] N. Johansson and E. Sjöqvist, Phys. Rev. Lett. **92**, 060406 (2004).
[20] N. Johansson and E. Sjöqvist, Phys. Rev. A **71**, 012106

(2005).
[21] A. A. Kotze and W. D. Heiss, J. Phys. A **27**, 3059 (1994).
[22] R. Gonzalez-Ferez and J. S. Dehesa, Phys. Rev. Lett. **91**, 113001 (2003).
[23] H. C. Longuet-Higgins, Proc. R. Soc. London, Ser. A **344**, 147 (1975).
[24] A. J. Stone, Proc. R. Soc. London, Ser. A **351**, 141 (1976).
[25] E. A. Yuzbashyan, W. Happer, B. A. Altshuler, and S. B. Sastry, J. Phys. A **36**, 2577 (2003).
[26] P. D. Lax, *Linear Algebra* (Wiley, New York, 1997).
[27] J. P. Tignol, *Galois' Theory of Algebraic Equations* (World Scientific, Singapore, 2001).
[28] N. V. Ilyushechkin, Mat. Zametki **51**, 230 (1992).
[29] A. G. Akritas, *Elements of Computer Algebra* (Wiley, New York, 1989).
[30] A. Cohen, H. Cuypers, and H. Sterk, *Some Tapas of Computer Algebra* (Springer, Berlin, 1999).
[31] M. Mignotte, *Mathematics for Computer Algebra* (Springer-Verlag, Berlin, 1991).
[32] D. Cox, *Galois Theory* (Wiley, New York, 2004).
[33] T. P. Grozdanov and E. A. Solov'ev, Phys. Rev. A **42**, 2703 (1990).
[34] E. Teller, J. Phys. Chem. **41**, 109 (1937).
[35] C. A. Mead, J. Chem. Phys. **70**, 2276 (1978).
[36] T. Hain, R. M. Moison, and T. J. Curtiss, J. Chem. Phys. **111**, 6797 (1999).
[37] T. Apostol, *Modular functions and Dirichlet Series in Number Theory* (Springer-Verlag, Berlin, 1990).
[38] J. Wiersig, Phys. Rev. Lett. **97**, 253901 (2006).
[39] E. Persson, I. Rotter, H. J. Stöckmann, and M. Barth, Phys. Rev. Lett. **85**, 2478 (2000).
[40] I. M. Gelfand, M. M. Kapranov, and A. V. Zelevinsky, *Discriminants, Resultants, and Multidimensional Determinants* (Birkhauser, Boston, 1994).