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Classification and normal forms for avoided crossings of quantum-mechanical energy levels

George A Hagedorn

Department of Mathematics and Center for Statistical Mechanics and Mathematical Physics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0123, USA

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Abstract. When using the Born–Oppenheimer approximation for molecular systems, one encounters a quantum mechanical Hamiltonian for the electrons that depends on several parameters that describe the positions of the nuclei. As these parameters are varied, the spectrum of the electron Hamiltonian may vary. In particular, discrete eigenvalues may approach very close to one another at 'avoided crossings' of the electronic energy levels. We give a definition of an avoided crossing and classify generic avoided crossings of minimal multiplicity eigenvalues. There are six distinct types that depend on the dimension of the nuclear-configuration space and on the symmetries of the electron Hamiltonian function.

1. Introduction

In various situations, one encounters quantum mechanical Hamiltonians $h(X)$ that depend on parameters $X \in \mathbb{R}^n$. For example, in the Born–Oppenheimer approximation of molecular physics, the electron Hamiltonian $h(X)$ depends on the nuclear-configuration parameters X. In such situations, the spectrum of $h(X)$ may depend on X in a complicated way.

In this paper we classify and study the local structure of 'avoided crossings' of discrete eigenvalues of quantum mechanical Hamiltonian functions. These occur at values of the parameters X where two discrete eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ of $h(X)$ approach very close to one another, but remain a positive distance apart.

Avoided crossings are of interest because they may dramatically affect the physics of the situation. For example, in the time-dependent Born–Oppenheimer approximation the adiabatic approximation for the electrons can break down at an avoided crossing [3, 4], and this breakdown can provide a mechanism for certain chemical reactions to occur.

The first rigorous results on the structure of crossings and avoided crossings were published in 1929 by Wigner and von Neumann [8]. They were motivated by examples computed by Hund. They first showed that the space of $n \times n$ Hermitian matrices has dimension n^2, and the subset that has a degenerate pair of eigenvalues has dimension $n^2 - 3$. They also showed that the real symmetric $n \times n$ matrices have dimension $\frac{1}{2}n(n-1)$, while those with a degenerate pair of eigenvalues have dimension $\frac{1}{2}n(n-1) - 2$. Thus, one should 'in general' not expect level crossings of Hermitian matrix-valued functions unless one has at least three parameters to adjust, and one should not expect crossings in the real symmetric case unless one has at least two parameters. They also commented that in the presence of symmetries, eigenvalues associated with different symmetry classes could 'in general' cross one another.

Wigner and von Neumann also discussed the dependence of eigenvalues and eigenfunctions of 2×2 matrices $H + \kappa V$ on the single parameter κ. They assumed the eigenvalues $E_1(\kappa)$ and $E_2(\kappa)$ have the same derivative at $\kappa = 0$, and that $E_1(0) = E - \epsilon$ and $E_2(0) = E + \epsilon$. They observed that the graphs of the eigenvalues were hyperbolas, and they discussed the behaviour of the eigenvectors. Their results are special cases of the general discussion presented below.

There is no universal definition of what is meant by an avoided crossing. In this paper we define one to be a 'detuned crossing', i.e. a situation where an actual eigenvalue crossing has been dismantled by a perturbation. We assume the Hamiltonian depends on the nuclear parameters X and an additional 'detuning' parameter δ, such that $h(X, 0)$ has a crossing, but that $h(X, \delta)$ does not for small $\delta > 0$. Our precise definition is the following:

Definition. Suppose $h(X, \delta)$ is a family of self-adjoint operators with a fixed domain $\mathcal{D}$ in a Hilbert Space $\mathcal{H}$, for $X \in \Omega$ and $\delta \in [0, \alpha)$, where Ω is an open subset of $\mathbb{R}^n$. Suppose that the resolvent of $h(X, \delta)$ is a C^2 function of X and δ as an operator from $\mathcal{H}$ to $\mathcal{D}$. Suppose $h(X, \delta)$ has two eigenvalues $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ that depend continuously on X and δ and are isolated from the rest of the spectrum of $h(X, \delta)$. Assume $\Gamma = \{X : E_{\mathcal{A}}(X, 0) = E_{\mathcal{B}}(X, 0)\}$ is a single point or non-empty connected proper submanifold of Ω, but that for all $X \in \Omega$, $E_{\mathcal{A}}(X, \delta) \neq E_{\mathcal{B}}(X, \delta)$ when $\delta > 0$. Then we say $h(X, \delta)$ has an avoided crossing on Γ.

In this definition, we have allowed the possibility that Γ is a manifold. The added generality has essentially no cost, and manifolds can arise in applications because of symmetries of some systems. For example, in the absence of external fields, electron Hamiltonians in molecular systems undergo similarity transformations as nuclear configurations are translated or rotated. The invariance of the eigenvalues under these transformations forces avoided crossings to occur on manifolds of positive dimension.

The motivation for this paper is the study of molecular propagation through avoided crossings [3, 4]. In that situation, the direction of propagation of the nuclei through an avoided crossing defines a special direction in the nuclear configuration space. Generically that direction has a non-trivial component in the hyperplane perpendicular to Γ at any particular point. Throughout the paper, we choose the X_1 coordinate direction to be aligned with that component. The particular normal forms we obtain depend on having this distinguished X_1 direction.

Our classification depends on the codimension of Γ and the symmetries of $h(X, \delta)$. The codimension of $\Gamma \subset \mathbb{R}^n$ is $n - m$, where m is the dimension of Γ, i.e. it is the minimum number of parameters that must be altered to move a generic point of $\mathbb{R}^n$ near Γ onto Γ. Every Hamiltonian function $h(X, \delta)$ has a symmetry group G, which is the set of all (X, δ)-independent unitary and anti-unitary operators that commute with $h(X, \delta)$. An anti-unitary operator is complex conjugation composed with a unitary operator, and such operators have the feature of reversing time.

In this paper, we consider only avoided crossings of energy levels $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ that are generic and have the minimal multiplicity allowed by the symmetry group. If G contains no anti-unitary operators, then each discrete energy level $E(X, \delta)$ of $h(X, \delta)$ is associated with an irreducible representation of G. In this case, the minimal multiplicity allowed is 1.

If G contains anti-unitary operators, then each discrete energy level $E(X, \delta)$ of $h(X, \delta)$ is associated with an irreducible corepresentation of G [5, 7]. In this case, the unitary elements of G form a subgroup H of index 2, and each irreducible corepresentation belongs to one of three types [5, 7].

A corepresentation U of G is of *type I* if its restriction U_H to H is an irreducible representation of H. In this case, minimal multiplicity energy levels of $h(X, \delta)$ again have multiplicity 1.

A corepresentation U of G is of *type II* if U_H is a direct sum of two equivalent irreducible representations of H, i.e. $U_H = D \oplus D$. Furthermore, for any anti-unitary $\mathcal{K} \in G$, the corepresentation U can be cast in the form $U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & D(h) \end{pmatrix}$, $U(\mathcal{K}) = \begin{pmatrix} 0 & -K \\ K & 0 \end{pmatrix}$, and $U(\mathcal{K}h) = U(\mathcal{K})U(h)$, for all $h \in H$. Here K is an anti-unitary operator that satisfies $K^2 = -D(\mathcal{K}^2)$ and $K\, D(\mathcal{K}^{-1}h\mathcal{K})\, K^{-1} = D(h)$ for all $h \in H$. In this case, minimal multiplicity energy levels have multiplicity 2.

A corepresentation U of G is of *type III* if U_H is a direct sum of two inequivalent irreducible representations of H, i.e. $U_H = D \oplus C$. Furthermore, for any anti-unitary $\mathcal{K} \in G$, the corepresentation U can be cast in the form $U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & C(h) \end{pmatrix}$, $U(\mathcal{K}) = \begin{pmatrix} 0 & -K \\ D(\mathcal{K}^2)K^{-1} & 0 \end{pmatrix}$, and $U(\mathcal{K}h) = U(\mathcal{K})U(h)$, for all $h \in H$. Here $K : \mathcal{H}_D \to \mathcal{H}_C$ is an anti-unitary operator that satisfies $K\, D(\mathcal{K}^{-1}h\mathcal{K})K^{-1} = D(h)$ for all $h \in H$. In this case, minimal multiplicity energy levels have multiplicity 2.

Suppose two energy levels $E_{\mathcal{A}}(X, 0)$ and $E_{\mathcal{B}}(X, 0)$ have a level crossing and are associated with inequivalent representations or corepresentations. Without loss of generality, assume this crossing occurs at at $X = 0$. From the classification theory of level crossings [1, 2], we see that $E_{\mathcal{A}}(X, 0)$ and $E_{\mathcal{B}}(X, 0)$ satisfy no special conditions except that their values coincide at $X = 0$. Thus, the gradient $\nabla_X|_{(X,\delta)=(0,0)}(E_{\mathcal{A}}(X, \delta) - E_{\mathcal{B}}(X, \delta))$ is non-zero under generic conditions. If we restrict X to any line $\mathcal{L}$ through the origin that is not perpendicular to this gradient, we can apply the implicit-function theorem to conclude that for small δ, there is a unique $X(\delta)$ near the origin on $\mathcal{L}$, that satisfies $E_{\mathcal{A}}(X(\delta), \delta) - E_{\mathcal{B}}(X(\delta), \delta) = 0$. Thus, for small δ, the perturbed levels $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ still cross one another, and an avoided crossing does not arise.

Throughout the rest of this paper, we therefore restrict our attention to the situations where $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ correspond to equivalent representations or corepresentations.

2. Type 1 avoided crossings

Type 1 avoided crossings are the simplest avoided crossings. They are characterized by codimension$(\Gamma) = 1$ and the multiplicity of $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ being 1.

Suppose Γ has codimension 1 and $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ are multiplicity 1 levels with equivalent representations or corepresentations. Note that because of the multiplicity, any corepresentations that are present here must be of *type I*. Since the two levels are isolated from the rest of the spectrum, we can construct the rank 2 spectral projection onto the spectral subspace corresponding to both eigenvalues by contour integration of the resolvent of $h(X, \delta)$:

$$P(X, \delta) = \frac{1}{2\pi \mathrm{i}} \int_\gamma (z - h(X, \delta))^{-1}\, \mathrm{d}z$$

where γ surrounds the two eigenvalues.

Without loss of generality, assume $0 \in \mathbb{R}^n$ is an arbitrary generic point of Γ. Since the resolvent of $h(X, \delta)$ is C^2, and we are studying generic situations, Γ has a well defined tangent plane at $X = 0$. Choose a coordinate system in which the $X_2, X_3, \ldots X_n$ axes are tangent to Γ at $X = 0$ and the X_1 axis is perpendicular to Γ at $X = 0$.

Choose $\{\psi_1, \psi_2\}$ to be an orthonormal basis of the range of $P(0,0)$. Define

$$\psi_1(X,\delta) = \frac{P(X,\delta)\psi_1}{\|P(X,\delta)\psi_1\|}$$

and let $P_1(X,\delta)$ be the orthogonal projection onto $\psi_1(X,\delta)$. The projections $P(X,\delta)$ and $P_1(X,\delta)$ commute with one another. Define

$$\psi_2(X,\delta) = \frac{(1 - P_1(X,\delta))P(X,\delta)\psi_2}{\|(1 - P_1(X,\delta))P(X,\delta)\psi_2\|}.$$

Then $\{\psi_1(X,\delta), \psi_2(X,\delta)\}$ is an orthonormal basis for the range of $P(X,\delta)$ for small $\|X\|$ and small δ.

The range of $P(X,\delta)$ is an invariant subspace for $h(X,\delta)$, and in the basis $\{\psi_1(X,\delta), \psi_2(X,\delta)\}$, the restriction of $h(X,\delta)$ to the range of $P(X,\delta)$ is given by a 2×2 matrix $h_1(X,\delta)$. We define

$$h_2(X,\delta) = h_1(X,\delta) - \tfrac{1}{2}(E_{\mathcal{A}}(X,\delta) + E_{\mathcal{B}}(X,\delta))I$$

where I is the 2×2 identity matrix. Then $h_2(X,\delta)$ is a 2×2 traceless self-adjoint matrix-valued function. Since $E_{\mathcal{A}}(0,0) = E_{\mathcal{B}}(0,0)$, $h_2(0,0)$ is the zero matrix.

By the assumed smoothness of the resolvent of $h(X,\delta)$, $h_2(X,\delta)$ is C^2 in X and δ for $\|X\|$ and δ small. Thus, for small $\|X\|$ and δ, by first-order Taylor series,

$$h_2(X,\delta) = BX_1 + C\delta + \mathrm{O}(X^2 + \delta^2)$$

where B and C are 2×2 traceless self-adjoint matrices. By the spectral theorem, we can make an X and δ independent change of basis so that B is diagonal. Since we are studying generic avoided crossings, we assume B is non-zero. Thus, in the new basis, $\{\phi_1(X,\delta), \phi_2(X,\delta)\}$, $h_2(X,\delta)$ is represented by

$$h_3(X,\delta) = \begin{pmatrix} b_1 & 0 \\ 0 & -b_1 \end{pmatrix} X_1 + \begin{pmatrix} b_2 & c_2 + \mathrm{i}d_2 \\ c_2 - \mathrm{i}d_2 & -b_2 \end{pmatrix} \delta + \mathrm{O}(X^2 + \delta^2).$$

By replacing $\phi_2(X,\delta)$ by $\mathrm{e}^{\mathrm{i}\theta}\phi_2(X,\delta)$ for appropriate θ, we can arrange for the imaginary terms in the above expression to vanish. Thus, in a final basis, $h_2(X,\delta)$ is represented by

$$h_4(X,\delta) = \begin{pmatrix} b_1X_1 + b_2\delta & \tilde{c}_2\delta \\ \tilde{c}_2\delta & -b_1X_1 - b_2\delta \end{pmatrix} + \mathrm{O}(X^2 + \delta^2). \tag{1}$$

From this representation, we see that

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\sqrt{(b_1X_1 + b_2\delta)^2 + (\tilde{c}_2\delta)^2} + \mathrm{O}(X^2 + \delta^2)$$

and that $h_1(X,\delta)$ minus half its trace (which depends smoothly on X and δ) is unitarily equivalent to the normal form $h_4(X,\delta)$.

3. Type 2 avoided crossings

Type 2 avoided crossings are very similar to type 1, except that the eigenvalues are degenerate. Type 2 avoided crossings are characterized by having codimension$(\Gamma) = 1$ and the multiplicity of $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ being 2.

Type 2 avoided crossings may occur when the eigenvalues are associated with *type II* or *type III* corepresentations. We begin our discussion with the simpler case of a *type III* corepresentation. In that case, we construct the rank 4 projection $P(X,\delta)$ onto the spectral subspace for $h(X,\delta)$ that corresponds to both eigenvalues by contour integration as for type 1 avoided crossings. The corepresentation decomposes as $U = D \oplus C$, where C and D are inequivalent representations of H. Assume $0 \in \mathbb{R}^n$ is an arbitrary point of Γ, and choose coordinates $X_1, X_2, \dots, X_n$ as in the discussion of type 1 avoided crossings.

Arbitrarily choose two orthonormal vectors ψ_1 and ψ_2 that lie in the range of $P(0,0)$ and in the carrier subspace for the D representation of the subgroup H of the symmetry group G. Define

$$\psi_1(X,\delta) = \frac{P(X,\delta)\psi_1}{\|P(X,\delta)\psi_1\|}$$

and let $P_1(X,\delta)$ be the orthogonal projection onto $\psi_1(X,\delta)$. Then define

$$\psi_2(X,\delta) = \frac{(1-P_1(X,\delta))P(X,\delta)\psi_2}{\|(1-P_1(X,\delta))P(X,\delta)\psi_2\|}.$$

For small $|X|$ and δ, these two vectors form an orthonormal basis for the intersection of the range of $P(X,\delta)$ and the carrier subspace for the D representation of H. We then let $\psi_3(X,\delta) = \mathcal{K}\psi_1(X,\delta)$ and $\psi_4(X,\delta) = \mathcal{K}\psi_2(X,\delta)$, where $\mathcal{K}$ is the anti-unitary operator mentioned in the description of *type III* corepresentations. These last two vectors form an orthonormal basis for the intersection of the range of $P(X,\delta)$ and the carrier subspace for the C representation of H. The four vectors form an orthonormal basis for the range of $P(X,\delta)$.

In this basis, the restriction of

$$h_1(X,\delta) = h(X,\delta) - \tfrac{1}{4}(E_{\mathcal{A}}(X,\delta) + E_{\mathcal{B}}(X,\delta))I$$

to the range of $P(X,\delta)$ is represented by a self-adjoint traceless 4×4 matrix-valued function $h_2(X,\delta)$ whose entries are C^2 functions that vanish for $(X,\delta) = (0,0)$. Since $h(X,\delta)$ commutes with the projections onto the carrier subspaces for the C and D representations and with the action of $\mathcal{K}$, $h_2(X,\delta)$ commutes with

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$\begin{pmatrix} 0 & 0 & \mathrm{e}^{\mathrm{i}\omega} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\omega} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \cdot \text{(conjugation)}$$

where $D(\mathcal{K}^2)$ is a multiplication by $\mathrm{e}^{\mathrm{i}\omega}$. It follows that $h_2(X,\delta)$ must have the form

$$\begin{pmatrix} \alpha(X,\delta) & \beta(X,\delta)+\mathrm{i}\gamma(X,\delta) & 0 & 0 \\ \beta(X,\delta)-\mathrm{i}\gamma(X,\delta) & -\alpha(X,\delta) & 0 & 0 \\ 0 & 0 & \alpha(X,\delta) & \beta(X,\delta)-\mathrm{i}\gamma(X,\delta) \\ 0 & 0 & \beta(X,\delta)+\mathrm{i}\gamma(X,\delta) & -\alpha(X,\delta) \end{pmatrix}.$$

We expand $h_2(X,\delta)$ in its first order Taylor series

$$h_2(X,\delta) = BX_1 + C\delta + \mathrm{O}(X^2+\delta^2)$$

where B and C are 4×4 traceless self-adjoint matrices. By the spectral theorem, we can make an X and δ independent change of basis so that B is diagonal. Since we are studying generic avoided crossings, we assume B is non-zero. Thus, in the new basis, $\{\phi_1(X,\delta), \phi_2(X,\delta), \phi_3(X,\delta), \phi_4(X,\delta)\}$, $h_2(X,\delta)$ is represented by

$$h_3(X,\delta) = \begin{pmatrix} b_1 & 0 & 0 & 0 \\ 0 & -b_1 & 0 & 0 \\ 0 & 0 & b_1 & 0 \\ 0 & 0 & 0 & -b_1 \end{pmatrix} X_1 + \begin{pmatrix} b_2 & c_2+\mathrm{i}d_2 & 0 & 0 \\ c_2-\mathrm{i}d_2 & -b_2 & 0 & 0 \\ 0 & 0 & b_2 & c_2-\mathrm{i}d_2 \\ 0 & 0 & c_2+\mathrm{i}d_2 & -b_2 \end{pmatrix} \delta$$
$$+\mathrm{O}(X^2+\delta^2).$$

By replacing $\phi_2(X,\delta)$ by $\mathrm{e}^{\mathrm{i}\theta}\phi_2(X,\delta)$ and $\phi_4(X,\delta)$ by $\mathrm{e}^{-\mathrm{i}\theta}\phi_4(X,\delta)$ for appropriate θ, we can arrange for the imaginary terms in the above expression to vanish. Thus, in a final basis, $h_2(X,\delta)$ is represented by

$$h_4(X,\delta) = \begin{pmatrix} b_1X_1+b_2\delta & \tilde{c}_2\delta & 0 & 0 \\ \tilde{c}_2\delta & -b_1X_1-b_2\delta & 0 & 0 \\ 0 & 0 & b_1X_1+b_2\delta & \tilde{c}_2\delta \\ 0 & 0 & \tilde{c}_2\delta & -b_1X_1-b_2\delta \end{pmatrix} + \mathrm{O}(X^2+\delta^2). \tag{2}$$

From this representation, we see that

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\sqrt{(b_1X_1+b_2\delta)^2 + (\tilde{c}_2\delta)^2} + \mathrm{O}(X^2+\delta^2)$$

and that $h_1(X,\delta)$ minus a quarter its trace (which depends smoothly on X and δ) is unitarily equivalent to the normal form $h_4(X,\delta)$.

If the corepresentation is *type II* instead of *type III*, the analysis is more complicated, but ultimately leads to the same normal form (2).

When the corepresentation is of *type II*, we choose a unit vector ψ_1 in the range of $P(0,0)$, and define $\psi_2 = \mathcal{K}\psi_1$. Then ψ_2 is a unit vector orthogonal to ψ_1. We choose ψ_3 to be any unit vector in the range of $P(0,0)$ that is orthogonal to both ψ_1 and ψ_2, and let $\psi_4 = \mathcal{K}\psi_3$. The four vectors then constitute an orthonormal basis of the range of $P(0,0)$.

We define

$$\psi_1(X,\delta) = \frac{P(X,\delta)\psi_1}{\|P(X,\delta)\psi_1\|}$$

and let $\psi_2(X,\delta) = \mathcal{K}\psi_1(X,\delta)$. We let $P_{1,2}(X,\delta)$ be the orthogonal projection onto $\psi_1(X,\delta)$ and $\psi_2(X,\delta)$, and define

$$\psi_3(X,\delta) = \frac{(1-P_{1,2}(X,\delta))P(X,\delta)\psi_3}{\|(1-P_{1,2}(X,\delta))P(X,\delta)\psi_3\|}.$$

Finally, we let $\psi_4(X,\delta) = \mathcal{K}\psi_3(X,\delta)$. For small $|X|$ and δ, these four vectors form an orthonormal basis for the range of $P(X,\delta)$.

In this basis, the restriction of

$$h_1(X,\delta) = h(X,\delta) - \tfrac{1}{4}(E_{\mathcal{A}}(X,\delta) + E_{\mathcal{B}}(X,\delta))$$

to the range of $P(X,\delta)$ is represented by a self-adjoint traceless 4×4 matrix-valued function $h_5(X,\delta)$ whose entries are C^2 functions that vanish for $(X,\delta)=(0,0)$. Since $h(X,\delta)$ commutes with the action of $\mathcal{K}$, $h_5(X,\delta)$ commutes with

$$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot (\text{conjugation}).$$

It follows that $h_5(X,\delta)$ must have the form

$$\begin{pmatrix} \alpha(X,\delta) & 0 & \beta(X,\delta)+\mathrm{i}\gamma(X,\delta) & \epsilon(X,\delta)+\mathrm{i}\zeta(X,\delta) \\ 0 & \alpha(X,\delta) & -\epsilon(X,\delta)+\mathrm{i}\zeta(X,\delta) & \beta(X,\delta)-\mathrm{i}\gamma(X,\delta) \\ \beta(X,\delta)-\mathrm{i}\gamma(X,\delta) & -\epsilon(X,\delta)-\mathrm{i}\zeta(X,\delta) & -\alpha(X,\delta) & 0 \\ \epsilon(X,\delta)-\mathrm{i}\zeta(X,\delta) & \beta(X,\delta)+\mathrm{i}\gamma(X,\delta) & 0 & -\alpha(X,\delta) \end{pmatrix}.$$

We expand $h_5(X,\delta)$ in its first order Taylor series

$$h_5(X,\delta) = BX_1 + C\delta + \mathrm{O}(X^2+\delta^2)$$

where B and C are 4×4 traceless self-adjoint matrices. By the spectral theorem, we can make an X and δ independent change of basis so that B is diagonal. Since we are studying generic avoided crossings, we assume B is non-zero. Thus, in the new basis, $\{\phi_1(X,\delta),\phi_2(X,\delta),\phi_3(X,\delta),\phi_4(X,\delta)\}$, $h_5(X,\delta)$ is represented by

$$\begin{aligned} h_6(X,\delta) = {} & \begin{pmatrix} b_1 & 0 & 0 & 0 \\ 0 & b_1 & 0 & 0 \\ 0 & 0 & -b_1 & 0 \\ 0 & 0 & 0 & -b_1 \end{pmatrix} X_1 \\ & + \begin{pmatrix} b_2 & 0 & c_2+\mathrm{i}d_2 & e_2+\mathrm{i}f_2 \\ 0 & b_2 & -e_2+\mathrm{i}f_2 & c_2-\mathrm{i}d_2 \\ c_2-\mathrm{i}d_2 & -e_2-\mathrm{i}f_2 & -b_2 & 0 \\ e_2-\mathrm{i}f_2 & c_2+\mathrm{i}d_2 & 0 & -b_2 \end{pmatrix}\delta + \mathrm{O}(X^2+\delta^2). \end{aligned}$$

By analogy with the construction for type 1 avoided crossings, we now alter the basis to force certain coeficients to vanish. Instead of multiplying some basis vectors by phases, we apply a unitary operator in a two-dimensional subspace. We define a unitary operator on $\mathbb{C}^2$ by

$$U = \frac{1}{\sqrt{c_2^2+d_2^2+e_2^2+f_2^2}}\begin{pmatrix} c_2+\mathrm{i}d_2 & e_2+\mathrm{i}f_2 \\ -e_2+\mathrm{i}f_2 & c_2-\mathrm{i}d_2 \end{pmatrix}$$

and replace $\phi_3(X,\delta)$ and $\phi_4(X,\delta)$ by $U\phi_3(X,\delta)$ and $U\phi_4(X,\delta)$, respectively. In the new basis, $h_5(X,\delta)$ is represented by

$$h_7(X,\delta) = \begin{pmatrix} b_1X_1+b_2\delta & 0 & \tilde{c}_2\delta & 0 \\ 0 & b_1X_1+b_2\delta & 0 & \tilde{c}_2\delta \\ \tilde{c}_2\delta & 0 & -b_1X_1b_2\delta & 0 \\ 0 & \tilde{c}_2\delta & 0 & -b_1X_1-b_2\delta \end{pmatrix} + \mathrm{O}(X^2+\delta^2).$$

Then, by interchanging the second and third basis vectors, we obtain a final basis in which $h_5(X,\delta)$ is represented by

$$h_8(X,\delta) = \begin{pmatrix} b_1X_1+b_2\delta & \tilde{c}_2\delta & 0 & 0 \\ \tilde{c}_2\delta & -b_1X_1-b_2\delta & 0 & 0 \\ 0 & 0 & b_1X_1+b_2\delta & \tilde{c}_2\delta \\ 0 & 0 & \tilde{c}_2\delta & -b_1X_1-b_2\delta \end{pmatrix} + \mathrm{O}(X^2+\delta^2)$$

which has the same form as (2).

So, in either case, we see that

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\sqrt{(b_1X_1 + b_2\delta)^2 + (\tilde{c}_2\delta)^2} + \mathrm{O}(X^2+\delta^2)$$

and that $h_1(X,\delta)$ minus a quarter of its trace (which depends smoothly on X and δ) is unitarily equivalent to the normal form (2).

4. Type 3 avoided crossings

Type 3 avoided crossings are characterized by having codimension(Γ) $=$ 2 and the multiplicity of $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ being 1.

We claim that type 3 avoided crossings do not generically occur if the symmetry group contains anti-unitary operators.

To prove this claim, suppose the symmetry group does contain anti-unitary operators, and that the multiplicities of the eigenvalues are 1. Assume, without loss of generality that $0 \in \mathbb{R}^n$ is a generic point of Γ. Then the corepresentation must be of *type I*, and the level crossing of $h(X,\delta)$ at $(X,\delta) = (0,0)$ must be of *type I* in the classification given in [1, 2]. It follows [1, 2] that the restriction of $h(X,\delta)$ to the spectral subspace associated with $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ is unitarily equivalent to a real symmetric 2×2 matrix

$$\begin{pmatrix} \alpha(X,\delta)+\beta(X,\delta) & \gamma(X,\delta) \\ \gamma(X,\delta) & \alpha(X,\delta)-\beta(X,\delta) \end{pmatrix}$$

whose eigenvalues cross if and only if $\beta(X,\delta) = \gamma(X,\delta) = 0$. Generically the two gradients $\nabla_X|_{(X,\delta)=(0,0)}\beta(X,\delta)$ and $\nabla_X|_{(X,\delta)=(0,0)}\gamma(X,\delta)$ are non-zero. If X is restricted to a plane $\mathcal{P}$ that is not perpendicular to either of these gradients, then we can apply the implicit-function theorem to conclude that for small δ, there is a unique $X(\delta)$ near the origin on $\mathcal{P}$, that satisfies $\beta(X(\delta),\delta) = \gamma(X(\delta),\delta) = 0$. Thus, for small δ, the perturbed levels $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ still cross one another, and an avoided crossing does not arise. This proves the claim.

Without loss of generality, assume that $0 \in \mathbb{R}^n$ is a generic point of Γ. Since Γ has a well defined tangent plane at $X = 0$, we can choose an orthogonal coordinate system in which the X_1 and X_2 coordinate axes are perpendicular to Γ and the $X_3, X_4, \ldots, X_n$ axes are tangent to Γ. We further assume that the X_1-axis is in the distinguished direction perpendicular to Γ at the origin, as mentioned in the introduction.

We choose $\psi_1(X,\delta)$ and $\psi_2(X,\delta)$, and define $h_2(X,\delta)$ as in our discussion of type 1 avoided crossings. We then expand $h_2(X,\delta)$ in its first-order Taylor series:

$$h_2(X,\delta) = BX_1 + CX_2 + D\delta + \mathrm{O}(X^2+\delta^2)$$

where B, C, and D are traceless 2×2 self-adjoint matrices. By performing an X and δ independent change of basis from $\psi_1(X,\delta)$ and $\psi_2(X,\delta)$ to some $\phi_1(X,\delta)$ and $\phi_2(X,\delta)$, we may force B to be diagonal. In the new basis, $h_2(X,\delta)$ is represented by

$$h_3(X,\delta) = \begin{pmatrix} b_1X_1+b_2X_2+b_3\delta & c_2X_2+\mathrm{i}d_2X_2+c_3\delta+\mathrm{i}d_3\delta \\ c_2X_2-\mathrm{i}d_2X_2+c_3\delta-\mathrm{i}d_3\delta & -b_1X_1-b_2X_2-b_3\delta \end{pmatrix} + \mathrm{O}(X^2+\delta^2).$$

We choose θ so that $c_2+\mathrm{i}d_2 = \tilde{c}_2\mathrm{e}^{\mathrm{i}\theta}$, where $\tilde{c}_2$ is real and positive. We then replace $\phi_2(X,\delta)$ by $\mathrm{e}^{\mathrm{i}\theta}\phi_2(X,\delta)$. In the resulting basis, $h_2(X,\delta)$ is represented by

$$h_4(X,\delta) = \begin{pmatrix} b_1X_1+b_2X_2+b_3\delta & \tilde{c}_2X_2+\tilde{c}_3\delta+\mathrm{i}\tilde{d}_3\delta \\ \tilde{c}_2X_2+\tilde{c}_3\delta-\mathrm{i}\tilde{d}_3\delta & -b_1X_1-b_2X_2-b_3\delta \end{pmatrix} + \mathrm{O}(X^2+\delta^2) \qquad (3)$$

where $\tilde{c}_3 + \mathrm{i}\tilde{d}_3 = \mathrm{e}^{-\mathrm{i}\theta}(c_2 + \mathrm{i}d_2)$. From this we see that

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\sqrt{(b_1X_1 + b_2X_2 + b_3\delta)^2 + (\tilde{c}_2X_2 + \tilde{c}_3\delta)^2 + (\tilde{d}_3\delta)^2} + \mathrm{O}(X^2 + \delta^2)$$

and that $h_1(X,\delta)$ minus half of its trace (which depends smoothly on X and δ) is unitarily equivalent to the normal form (3).

5. Type 4 avoided crossings

Type 4 avoided crossings are characterized by having codimension$(\Gamma) = 2$ and the multiplicity of $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ being 2.

In this situation, our minimal multiplicity assumption dictates that the symmetry group G contains anti-unitary operators, and that the corepresentation for these eigenvalues be of *type II* or *type III*. In either case, we choose a coordinate system for X as in our discussion of type 3 avoided crossings.

If $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ are associated with a *type III* corepresentation, we choose basis vectors as in our discussion of type 2 avoided crossings. The resulting matrix $h_2(X,\delta)$ has the same form as in the discussion of type 2 avoided crossings. We expand this matrix-valued function in its first-order Taylor series and diagonalize the matrix that is the coefficient of X_1. At that point $h_2(X,\delta)$ is represented in a basis $\{\phi_1(X,\delta), \phi_2(X,\delta), \phi_3(X,\delta), \phi_4(X,\delta)\}$ by the matrix

$$h_3(X,\delta) = \begin{pmatrix} b_1X_1 + b_2X_2 + b_3\delta & c_2X_2 + \mathrm{i}d_2X_2 + c_3\delta + \mathrm{i}d_3\delta & 0 & 0 \\ c_2X_2 - \mathrm{i}d_2X_2 + c_3\delta - \mathrm{i}d_3\delta & -b_1X_1 - b_2X_2 - b_3\delta & 0 & 0 \\ 0 & 0 & b_1X_1 + b_2X_2 + b_3\delta & c_2X_2 - \mathrm{i}d_2X_2 + c_3\delta - \mathrm{i}d_3\delta \\ 0 & 0 & c_2X_2 + \mathrm{i}d_2X_2 + c_3\delta + \mathrm{i}d_3\delta & -b_1X_1 - b_2X_2 - b_3\delta \end{pmatrix}$$
$$+\mathrm{O}(X^2 + \delta^2).$$

We then choose θ as in the discussion of type 3 avoided crossings and replace $\phi_2(X,\delta)$ by $\mathrm{e}^{\mathrm{i}\theta}\phi_2(X,\delta)$ and $\phi_4(X,\delta)$ by $\mathrm{e}^{-\mathrm{i}\theta}\phi_4(X,\delta)$. In this final basis, $h_2(X,\delta)$ is represented by the normal form

$$h_4(X,\delta) = \begin{pmatrix} b_1X_1 + b_2X_2 + b_3\delta & \tilde{c}_2X_2 + \tilde{c}_3\delta + \mathrm{i}\tilde{d}_3\delta & 0 & 0 \\ \tilde{c}_2X_2 + \tilde{c}_3\delta - \mathrm{i}\tilde{d}_3\delta & -b_1X_1 - b_2X_2 - b_3\delta & 0 & 0 \\ 0 & 0 & b_1X_1 + b_2X_2 + b_3\delta & \tilde{c}_2X_2 + \tilde{c}_3\delta - \mathrm{i}\tilde{d}_3\delta \\ 0 & 0 & \tilde{c}_2X_2 + \tilde{c}_3\delta + \mathrm{i}\tilde{d}_3\delta & -b_1X_1 - b_2X_2 - b_3\delta \end{pmatrix} + \mathrm{O}(X^2 + \delta^2) \tag{4}$$

where $\tilde{c}_3 + \mathrm{i}\tilde{d}_3 = \mathrm{e}^{-\mathrm{i}\theta}(c_2 + \mathrm{i}d_2)$. As in the case of a type 3 avoided crossing,

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\sqrt{(b_1X_1 + b_2X_2 + b_3\delta)^2 + (\tilde{c}_2X_2 + \tilde{c}_3\delta)^2 + (\tilde{d}_3\delta)^2} + \mathrm{O}(X^2 + \delta^2).$$

When the corepresentation is of *type II*, the situation is more complicated. We again mimic the discussion of type 2 avoided crossings to choose an appropriate basis; we expand in first-order Taylor series; and we diagonalize the matrix that is the X_1 coefficient in that Taylor series. We then find that $h_2(X,\delta)$ is represented in a basis $\{\phi_1(X,\delta), \phi_2(X,\delta), \phi_3(X,\delta), \phi_4(X,\delta)\}$ by the matrix $h_5(X,\delta)$ that is given below.

$$h_5(X,\delta) = \begin{pmatrix} b_1X_1 + b_2X_2 + b_3\delta & 0 & (c_2 + \mathrm{i}d_2)X_2 + (c_3 + \mathrm{i}d_3)\delta & (e_2 + \mathrm{i}f_2)X_2 + (e_3 + \mathrm{i}f_3)\delta \\ 0 & b_1X_1 + b_2X_2 + b_3\delta & (-e_2 + \mathrm{i}f_2)X_2 + (-e_3 + \mathrm{i}f_3)\delta & (c_2 - \mathrm{i}d_2)X_2 + (c_3 - \mathrm{i}d_3)\delta \\ (c_2 - \mathrm{i}d_2)X_2 + (c_3 - \mathrm{i}d_3)\delta & (-e_2 - \mathrm{i}f_2)X_2 + (-e_3 - \mathrm{i}f_3)\delta & -b_1X_1 - b_2X_2 - b_3\delta & 0 \\ (e_2 - \mathrm{i}f_2)X_2 + (e_3 - \mathrm{i}f_3)\delta & (c_2 + \mathrm{i}d_2)X_2 + (c_3 + \mathrm{i}d_3)\delta & 0 & -b_1X_1 - b_2X_2 - b_3\delta \end{pmatrix}$$
$$+\mathrm{O}(X^2 + \delta^2).$$

We next make a similarity transformation of the form

$$h_6(X,\delta) = \begin{pmatrix} U_1 & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & U_2 \end{pmatrix} h_5(X,\delta) \begin{pmatrix} U_1 & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & U_2 \end{pmatrix}^{-1}$$

where U_1 and U_2 are certain constant 2×2 unitary matrices. There is a well known 2-to-1 Lie-group homomorphism [6] from $SU(2) \times SU(2)$ onto $SO(4)$, $(U_1, U_2) \longmapsto O_{U_1,U_2}$, which satisfies

$$\begin{pmatrix} \tilde{c} + \mathrm{i}\tilde{d} & \tilde{e} + \mathrm{i}\tilde{f} \\ -\tilde{e} + \mathrm{i}\tilde{f} & \tilde{c} - \mathrm{i}\tilde{d} \end{pmatrix} = U_1 \begin{pmatrix} c + \mathrm{i}d & e + \mathrm{i}f \\ -e + \mathrm{i}f & c - \mathrm{i}d \end{pmatrix} U_2^{-1}$$

if and only if

$$(\,\tilde{c} \quad \tilde{d} \quad \tilde{e} \quad \tilde{f}\,) = (\,c \quad d \quad e \quad f\,)\, O_{U_1,U_2}.$$

Since the homomorphism is onto $SO(4)$, we can choose U_1 and U_2 so that the transpose of O_{U_1,U_2} satisfies

$$O_{U_1,U_2}^{\mathrm{T}} \begin{pmatrix} c_2 & c_3 \\ d_2 & d_3 \\ e_2 & e_3 \\ f_2 & f_3 \end{pmatrix} = \begin{pmatrix} \tilde{c}_2 & \tilde{c}_3 \\ 0 & \tilde{d}_3 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

with $\tilde{c}_2 > 0$ and $\tilde{d}_3 > 0$. (Since all rotations arise, we simply choose one which maps the first vector into the positive X_1 direction and the second vector into the X_1–X_2 plane with positive second component.) By doing this, we see that $h_2(X, \delta)$ is represented by

$$h_6(X, \delta) = \begin{pmatrix} b_1X_1 + b_2X_2 + b_3\delta & 0 & \tilde{c}_2X_2 + \tilde{c}_3\delta + \mathrm{i}\tilde{d}_3\delta & 0 \\ 0 & b_1X_1 + b_2X_2 + b_3\delta & 0 & \tilde{c}_2X_2 + \tilde{c}_3\delta - \mathrm{i}\tilde{d}_3\delta \\ \tilde{c}_2X_2 + \tilde{c}_3\delta - \mathrm{i}\tilde{d}_3\delta & 0 & -b_1X_1 - b_2X_2 - b_3\delta & 0 \\ 0 & \tilde{c}_2X_2 + \tilde{c}_3\delta + \mathrm{i}\tilde{d}_3\delta & 0 & -b_1X_1 - b_2X_2 - b_3\delta \end{pmatrix} + \mathrm{O}(X^2 + \delta^2).$$

Then, by interchanging the second and third basis vectors, we again obtain the normal-form matrix $h_4(X, \delta)$ given by (4), and

$$E_{\mathcal{A}}(X, \delta) - E_{\mathcal{B}}(X, \delta) = 2\sqrt{(b_1X_1 + b_2X_2 + b_3\delta)^2 + (\tilde{c}_2X_2 + \tilde{c}_3\delta)^2 + (\tilde{d}_3\delta)^2} \\ +\mathrm{O}(X^2 + \delta^2).$$

6. Type 5 avoided crossings

Type 5 avoided crossings are characterized by having codimension$(\Gamma) = 3$.

We claim that when the codimension$(\Gamma) \geqslant 3$, generic avoided crossings cannot arise unless the G contains anti-unitary operators and the corepresentation for the eigenvalues is of *type II*. This forces the minimal multiplicity of the eigenvalues to be 2.

To prove this claim, we assume that $0 \in \mathbb{R}^n$ is a generic point of Γ and examine several cases:

Case 1. Suppose the corepresentation for $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ is of *type I*. In this case we repeat the implicit-function theorem argument from the beginning of our discussion of type 3 avoided crossings to see that crossings are stable under generic perturbations, and that no avoided crossing arises.

Case 2. Suppose G contains no anti-unitary operators. Then the level crossing of $h(X, \delta)$ at $(X, \delta) = (0, 0)$ must be of type B in the classification given in [1, 2]. Furthermore, the restriction of $h(X, \delta)$ to the spectral subspace associated with $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ is unitarily equivalent to a 2×2 matrix

$$\begin{pmatrix} \alpha(X, \delta) + \beta(X, \delta) & \gamma(X, \delta) + \mathrm{i}\omega(X, \delta) \\ \gamma(X, \delta) - \mathrm{i}\omega(X, \delta) & \alpha(X, \delta) - \beta(X, \delta) \end{pmatrix}$$

whose eigenvalues cross if and only if $\beta(X,\delta) = \gamma(X,\delta) = \omega(X,\delta) = 0$. Generically the three gradients $\nabla_X|_{(X,\delta)=(0,0)}\beta(X,\delta)$, $\nabla_X|_{(X,\delta)=(0,0)}\gamma(X,\delta)$, and $\nabla_X|_{(X,\delta)=(0,0)}\omega(X,\delta)$ are non-zero. If X is restricted to a three-dimensional subspace $\mathcal{S}$ that is not perpendicular to any of these gradients, then we can apply the implicit-function theorem to conclude that for small δ, there is a unique $X(\delta)$ near the origin in $\mathcal{S}$, that satisfies $\beta(X(\delta),\delta) = \gamma(X(\delta),\delta) = \omega(X(\delta),\delta) = 0$. Thus, for small δ, the perturbed levels $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ still cross one another, and an avoided crossing does not arise.

Case 3. Suppose the corepresentation for $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ is of *type III*. Then the level crossing of $h(X,\delta)$ at $(X,\delta) = (0,0)$ must be of type K in the classification given in [1, 2]. Furthermore, the restriction of $h(X,\delta)$ to the spectral subspace associated with $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ is unitarily equivalent to a 4×4 matrix

$$\begin{pmatrix} \alpha(X,\delta)+\beta(X,\delta) & \gamma(X,\delta)+\mathrm{i}\omega(X,\delta) & 0 & 0 \\ \gamma(X,\delta)-\mathrm{i}\omega(X,\delta) & \alpha(X,\delta)-\beta(X,\delta) & 0 & 0 \\ 0 & 0 & \alpha(X,\delta)+\beta(X,\delta) & \gamma(X,\delta)-\mathrm{i}\omega(X,\delta) \\ 0 & 0 & \gamma(X,\delta)+\mathrm{i}\omega(X,\delta) & \alpha(X,\delta)-\beta(X,\delta) \end{pmatrix}$$

whose eigenvalues cross if and only if $\beta(X,\delta) = \gamma(X,\delta) = \omega(X,\delta) = 0$. The implicit-function theorem argument from case 2 now shows that generic crossings are stable and that no avoided crossing arises.

Since the only other possibility is that G contains anti-unitary operators and the corepresentation for the eigenvalues is of *type II*, this proves our claim.

The analysis of type 5 avoided crossings is very similar to the analysis of type 4 avoided crossings when the relevant corepresentation of G is of *type II*. Without loss of generality, assume that $0 \in \mathbb{R}^n$ is a generic point of Γ. Since Γ has a well defined tangent plane at $X = 0$, we can choose an orthogonal coordinate system in which the X_1, X_2, and X_3 coordinate axes are perpendicular to Γ and the $X_4, X_5, \ldots, X_n$ axes are tangent to Γ. We further assume that the X_1 is the distinguished direction perpendicular to Γ at the origin, as mentioned in the introduction.

Since $E_{\mathcal{A}}(X,\delta)$ and $E_{\mathcal{B}}(X,\delta)$ are associated with a *type II* corepresentation, we choose basis vectors as in our discussion of type 2 avoided crossings. The resulting matrix $h_2(X,\delta)$ has the same form as in the discussion of type 2 avoided crossings. We expand this matrix-valued function in its first-order Taylor series and diagonalize the matrix that is the coefficient of X_1. At that point $h_2(X,\delta)$ is represented in a basis $\{\phi_1(X,\delta), \phi_2(X,\delta), \phi_3(X,\delta), \phi_4(X,\delta)\}$ by the matrix $h_3(X,\delta)$ given below.

$$h_3(X,\delta)$$
$$= \begin{bmatrix} \left[\sum_{j=1}^{3} b_j X_j\right] + b_4\delta & 0 & \left[\sum_{j=2}^{3}(c_j+\mathrm{i}d_j)X_j\right] + (c_4+\mathrm{i}d_4)\delta & \left[\sum_{j=2}^{3}(e_j+\mathrm{i}f_j)X_j\right] + (e_4+\mathrm{i}f_4)\delta \\ 0 & \left[\sum_{j=1}^{3} b_j X_j\right] + b_4\delta & \left[\sum_{j=2}^{3}(-e_j+\mathrm{i}f_j)X_j\right] + (-e_4+\mathrm{i}f_4)\delta & \left[\sum_{j=2}^{3}(c_j-\mathrm{i}d_j)X_j\right] + (c_4-\mathrm{i}d_4)\delta \\ \left[\sum_{j=2}^{3}(c_j-\mathrm{i}d_j)X_j\right] + (c_4-\mathrm{i}d_4)\delta & \left[\sum_{j=2}^{3}(-e_j-\mathrm{i}f_j)X_j\right] + (-e_4-\mathrm{i}f_4)\delta & -\left[\sum_{j=1}^{3} b_j X_j\right] - b_4\delta & 0 \\ \left[\sum_{j=2}^{3}(e_j-\mathrm{i}f_j)X_j\right] + (e_4-\mathrm{i}f_4)\delta & \left[\sum_{j=2}^{3}(c_j+\mathrm{i}d_j)X_j\right] + (c_4+\mathrm{i}d_4)\delta & 0 & -\left[\sum_{j=1}^{3} b_j X_j\right] - b_4\delta \end{bmatrix}$$
$$+\mathrm{O}(X^2+\delta^2).$$

We again make a similarity transformation of the form

$$h_4(X,\delta) = \begin{pmatrix} U_1 & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & U_2 \end{pmatrix} h_3(X,\delta) \begin{pmatrix} U_1 & \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} \\ \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & U_2 \end{pmatrix}^{-1}$$

where U_1 and U_2 are certain constant 2×2 unitary matrices. We use the same Lie-group homomorphism as in the type 4 avoided-crossing case, but this time choose $O_{U_1,U_2} \in SO(4)$ so that

$$O_{U_1,U_2}^T \begin{pmatrix} c_2 & c_3 & c_4 \\ d_2 & d_3 & d_4 \\ e_2 & e_3 & e_4 \\ f_2 & f_3 & f_4 \end{pmatrix} = \begin{pmatrix} \tilde{c}_2 & \tilde{c}_3 & \tilde{c}_4 \\ 0 & \tilde{d}_3 & \tilde{d}_4 \\ 0 & 0 & \tilde{e}_4 \\ 0 & 0 & 0 \end{pmatrix}$$

with $\tilde{c}_2 > 0$, $\tilde{d}_3 > 0$, and $\tilde{e}_4 > 0$. By doing this, we see that $h_2(X, \delta)$ is represented by the matrix $h_4(X, \delta)$ given below.

$$\begin{aligned} h_4(X, \delta) \\ = \left[\begin{array}{cccc} b_1X_1 + b_2X_2 + b_3X_3 + b_4\delta & 0 & \tilde{c}_2X_2 + (\tilde{c}_3 + \mathrm{i}\tilde{d}_3)X_3 + (\tilde{c}_4 + \mathrm{i}\tilde{d}_4)\delta & \tilde{e}_4\delta \\ 0 & b_1X_1 + b_2X_2 + b_3X_3 + b_4\delta & -\tilde{e}_4\delta & \tilde{c}_2X_2 + (\tilde{c}_3 - \mathrm{i}\tilde{d}_3)X_3 + (\tilde{c}_4 - \mathrm{i}\tilde{d}_4)\delta \\ \tilde{c}_2X_2 + (\tilde{c}_3 - \mathrm{i}\tilde{d}_3)X_3 + (\tilde{c}_4 - \mathrm{i}\tilde{d}_4)\delta & -\tilde{e}_4\delta & -b_1X_1 - b_2X_2 - b_3X_3 - b_4\delta & 0 \\ \tilde{e}_4\delta & \tilde{c}_2X_2 + (\tilde{c}_3 + \mathrm{i}\tilde{d}_3)X_3 + (\tilde{c}_4 + \mathrm{i}\tilde{d}_4)\delta & 0 & -b_1X_1 - b_2X_2 - b_3X_3 - b_4\delta \end{array} \right] \\ +\mathrm{O}(X^2 + \delta^2). \end{aligned}$$

In the above expression we can further arrange for $\tilde{c}_3 = 0$ by rotating the X_2 and X_3 coordinate axes (recall that we assume the X_1 axis points in a distinguished direction). To see that this can always be done, note that $\tilde{c}_3 = 0$ is equivalent to having $\begin{pmatrix} \tilde{c}_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ orthogonal to $\begin{pmatrix} \tilde{c}_3 \\ \tilde{d}_3 \\ 0 \\ 0 \end{pmatrix}$. This, in turn, is equivalent to having $\begin{pmatrix} c_2 \\ d_2 \\ e_2 \\ f_2 \end{pmatrix}$ orthogonal to $\begin{pmatrix} c_3 \\ d_3 \\ e_3 \\ f_3 \end{pmatrix}$.

Rotations of the X_2 and X_3 axes have the effect of multiplying

$$Z = \begin{pmatrix} c_2 & c_3 \\ d_2 & d_3 \\ e_2 & e_3 \\ f_2 & f_3 \end{pmatrix}$$

on the right by a rotation

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

Thus, we need only show that θ can be chosen so that

$$Z \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \text{ is orthogonal to } Z \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}.$$

However, $Z^{\mathrm{T}}Z$ is a real symmetric 2×2 matrix, whose eigenvectors have the form $\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ and $\begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$. One then easily computes that

$$\begin{aligned} \left\langle Z \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, Z \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \right\rangle &= \left\langle \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, Z^{\mathrm{T}}Z \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \right\rangle \\ &= \mu \left\langle \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix} \right\rangle \\ &= 0 \end{aligned}$$

where μ is an eigenvalue of $Z^{\mathrm{T}}Z$. For this choice of θ, we have the desired orthogonality.

Thus, we have the final normal-form matrix $h_5(X, \delta)$ given by equation (5).

$$
\begin{aligned}
&h_5(X,\delta)\\
&= \begin{bmatrix} b_1X_1+b_2X_2+b_3X_3+b_4\delta & 0 & \tilde{c}_2X_2+\mathrm{i}\tilde{d}_3X_3+(\tilde{c}_4+\mathrm{i}\tilde{d}_4)\delta & \tilde{e}_4\delta \\ 0 & b_1X_1+b_2X_2+b_3X_3+b_4\delta & -\tilde{e}_4\delta & \tilde{c}_2X_2-\mathrm{i}\tilde{d}_3X_3+(\tilde{c}_4-\mathrm{i}\tilde{d}_4)\delta \\ \tilde{c}_2X_2-\mathrm{i}\tilde{d}_3X_3+(\tilde{c}_4-\mathrm{i}\tilde{d}_4)\delta & -\tilde{e}_4\delta & -b_1X_1-b_2X_2-b_3X_3-b_4\delta & 0 \\ \tilde{e}_4\delta & \tilde{c}_2X_2+\mathrm{i}\tilde{d}_3X_3+(\tilde{c}_4+\mathrm{i}\tilde{d}_4)\delta & 0 & -b_1X_1-b_2X_2-b_3X_3-b_4\delta \end{bmatrix}\\
&\qquad +\mathrm{O}(X^2+\delta^2). \qquad (5)
\end{aligned}
$$

From this expression, one sees that the difference between the eigenvalues is

$$
\begin{aligned}
&E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta)\\
&\qquad = 2\sqrt{(b_1X_1+b_2X_2+b_3X_3+b_4\delta)^2+(\tilde{c}_2X_2+\tilde{c}_4\delta)^2+(\tilde{d}_3X_3+\tilde{d}_4\delta)^2+(\tilde{e}_4\delta)^2}\\
&\qquad\quad +\mathrm{O}(X^2+\delta^2).
\end{aligned}
$$

7. Type 6 avoided crossings

Type 6 avoided crossings are characterized by having codimension$(\Gamma) = 4$. As in the type 5 situation, the symmetry group G must contain anti-unitary operators and the corepresentation for the eigenvalues must be of *type II*. The minimal multiplicity of the eigenvalues is 2.

The analysis of this situation is completely analogous to the type 5 avoided-crossing case. The only changes result from our having four relevant X coordinates instead of three. In this situation, the matrix $h_3(X, \delta)$ is presented below.

$$
\begin{aligned}
&h_3(X,\delta)\\
&= \begin{bmatrix} \left[\sum_{j=1}^4 b_jX_j\right]+b_5\delta & 0 & \left[\sum_{j=2}^4 (c_j+\mathrm{i}d_j)X_j\right]+(c_5+\mathrm{i}d_5)\delta & \left[\sum_{j=2}^4 (e_j+\mathrm{i}f_j)X_j\right]+(e_5+\mathrm{i}f_5)\delta \\ 0 & \left[\sum_{j=1}^4 b_jX_j\right]+b_5\delta & \left[\sum_{j=2}^4 (-e_j+\mathrm{i}f_j)X_j\right]+(-e_5+\mathrm{i}f_5)\delta & \left[\sum_{j=2}^4 (c_j-\mathrm{i}d_j)X_j\right]+(c_5-\mathrm{i}d_5)\delta \\ \left[\sum_{j=2}^4 (c_j-\mathrm{i}d_j)X_j\right]+(c_5-\mathrm{i}d_5)\delta & \left[\sum_{j=2}^4 (-e_j-\mathrm{i}f_j)X_j\right]+(-e_5-\mathrm{i}f_5)\delta & -\left[\sum_{j=1}^4 b_jX_j\right]-b_5\delta & 0 \\ \left[\sum_{j=2}^4 (e_j-\mathrm{i}f_j)X_j\right]+(e_5-\mathrm{i}f_5)\delta & \left[\sum_{j=2}^4 (c_j+\mathrm{i}d_j)X_j\right]+(c_5+\mathrm{i}d_5)\delta & 0 & -\left[\sum_{j=1}^4 b_jX_j\right]-b_5\delta \end{bmatrix}\\
&\qquad +\mathrm{O}(X^2+\delta^2).
\end{aligned}
$$

In analogy with the type 5 discussion, we may rotate the X_2, X_3, and X_4 coordinate axes in order to force the vectors $\begin{pmatrix} c_2\\ d_2\\ e_2\\ f_2 \end{pmatrix}$, $\begin{pmatrix} c_3\\ d_3\\ e_3\\ f_3 \end{pmatrix}$, and $\begin{pmatrix} c_4\\ d_4\\ e_4\\ f_4 \end{pmatrix}$ to be mutually perpendicular. After doing so, we choose unitary matrices U_1 and U_2 so that

$$
O_{U_1,U_2}^{\mathrm{T}} \begin{pmatrix} c_2 & c_3 & c_4 & c_5 \\ d_2 & d_3 & d_4 & d_5 \\ e_2 & e_3 & e_4 & e_5 \\ f_2 & f_3 & f_4 & f_5 \end{pmatrix} = \begin{pmatrix} \tilde{c}_2 & \tilde{c}_3 & \tilde{c}_4 & \tilde{c}_5 \\ 0 & \tilde{d}_3 & \tilde{d}_4 & \tilde{d}_5 \\ 0 & 0 & \tilde{e}_4 & \tilde{e}_5 \\ 0 & 0 & 0 & \tilde{f}_5 \end{pmatrix}.
$$

Because of the mutual orthogonality arranged by the rotation of coordinate axes, $\tilde{c}_3$, $\tilde{c}_4$, and $\tilde{d}_4$ must also vanish.

Thus, we obtain the normal form matrix $h_4(X, \delta)$ in equation (6).

$$h_4(X,\delta) = \begin{bmatrix} \left[\sum_{j=1}^{4} b_j X_j\right] + b_5\delta & 0 & \tilde{c}_2 X_2 + \mathrm{i}\tilde{d}_3 X_3 + (\tilde{c}_5 + \mathrm{i}\tilde{d}_5)\delta & \tilde{e}_4 X_4 + (\tilde{e}_5 + \mathrm{i}\tilde{f}_5)\delta \\ 0 & \left[\sum_{j=1}^{4} b_j X_j\right] + b_5\delta & -\tilde{e}_4 X_4 + (-\tilde{e}_5 + \mathrm{i}\tilde{f}_5)\delta & \tilde{c}_2 X_2 - \mathrm{i}\tilde{d}_3 X_3 + (\tilde{c}_5 - \mathrm{i}\tilde{d}_5)\delta \\ \tilde{c}_2 X_2 - \mathrm{i}\tilde{d}_3 X_3 + (\tilde{c}_5 - \mathrm{i}\tilde{d}_5)\delta & -\tilde{e}_4 X_4 + (-\tilde{e}_5 - \mathrm{i}\tilde{f}_5)\delta & -\left[\sum_{j=1}^{4} b_j X_j\right] - b_5\delta & 0 \\ \tilde{e}_4 X_4 + (\tilde{e}_5 - \mathrm{i}\tilde{f}_5)\delta & \tilde{c}_2 X_2 + \mathrm{i}\tilde{d}_3 X_3 + (\tilde{c}_5 + \mathrm{i}\tilde{d}_5)\delta & 0 & -\left[\sum_{j=1}^{4} b_j X_j\right] - b_5\delta \end{bmatrix} + \mathrm{O}(X^2 + \delta^2). \tag{6}$$

From this representation, we can then compute the difference between the eigenvalues:

$$E_{\mathcal{A}}(X,\delta) - E_{\mathcal{B}}(X,\delta) = 2\left\{\left(\left[\sum_{j=1}^{4} b_j X_j\right] + b_5\delta\right)^2 + (\tilde{c}_2 X_2 + \tilde{c}_5\delta)^2 + (\tilde{d}_3 X_3 + \tilde{d}_5\delta)^2 + (\tilde{e}_4 X_4 + e_5\delta)^2 + (\tilde{f}_5\delta)^2\right\}^{1/2} + \mathrm{O}(X^2 + \delta^2).$$

8. Completion of the classification

So far we have classified all possible generic, minimal multiplicity avoided crossings that have codimension$(\Gamma) \leqslant 4$. We now conclude our classification theory by showing that no generic, minimal multiplicity avoided crossings can occur when codimension$(\Gamma) \geqslant 5$.

Assume codimension$(\Gamma) \geqslant 5$. As argued in the type 5 situation, the symmetry group G must contain anti-unitary operators and the corepresentation for the eigenvalues must be of *type II*. Under these circumstances, the level crossing of $h(X, \delta)$ must be of type J in the classification given in [1, 2]. Furthermore, the restriction of $h(X, \delta)$ to the spectral subspace associated with $E_{\mathcal{A}}(X, \delta)$ and $E_{\mathcal{B}}(X, \delta)$ is unitarily equivalent to a 4×4 matrix that is an (X, δ)-dependent multiple of the identity plus a matrix whose entries are linear combinations of five real-valued functions of X and δ. $E_{\mathcal{A}}(X, \delta) = E_{\mathcal{B}}(X, \delta)$ if and only if all five of these functions simultaneously vanish.

We now mimic our earlier implicit-function theorem arguments to see that on generic five-dimensional subspaces through any generic point of Γ, there are points $X(\delta)$ near Γ for small δ, such that these five functions simultaneously vanish at $(X(\delta), \delta)$.

Thus, when codimension$(\Gamma) \geqslant 5$, generic, minimal multiplicity level crossings are stable under generic perturbations and do not give rise to avoided crossings.

9. Concluding remark

One might wonder if it is possible to simplify our normal-form matrices further by somehow forcing additional parameters to vanish. To see that this cannot be done, one needs only count the number of independent parameters that describe each type of avoided crossing and see that it is the same as the number of parameters in our normal forms.

In type 1 avoided crossings, for example, one parameter is the minimum eigenvalue gap divided by δ. A second independent parameter is the scaling factor for the leading-order dependence on δ of the location in X of closest approach of the eigenvalues. A third independent parameter is a scaling factor for the X_1 dependence of the eigenvalues. So, the normal form cannot contain fewer than three parameters. Our form contains b_1, b_2, and $\tilde{c}_2$.

Similar counting can be done for the other types of avoided crossings. A listing of independent parameters can be obtained by considering: (1) the number of parameters to specify the X_1 scale factor and the location of the minimum eigenvalue gap, (2) rotations of principal axes of the Hessianat the minimum eigenvalue gap, (3) magnitudes of the Hessian eigenvalues, and (4) the minimum gap divided by δ. In the type 5 and 6 situations, we reduced the number of parameters by 1 and 3, respectively, by rotating certain X axes. In each case, we obtain the number of parameters that appear in our normal forms.

For type 6 avoided crossings, one obtains:

4 for the X_1 scale factor and location of the minimum,

6 for principal axis rotations of the Hessian (dim $SO(4) = 6$),

4 for Hessian eigenvalues,

1 for the δ scale parameter,

-3 for rotating X_2, X_3, and X_4 coordinates.

This yields 12 parameters, which is the number of free parameters in equation (6), figure 6.

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