

# *Astérisque*

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*Astérisque*, tome 210 (1992), p. 115-134

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# Classification and Normal Forms for Quantum Mechanical Eigenvalue Crossings

*George A. Hagedorn*

In the study of molecular dynamics, it is often useful to consider the quantum mechanics of the electrons with the nuclei in fixed positions. When this is done, the positions of the nuclei are described by a nuclear configuration vector  $X \in \mathbb{R}^n$ , and the Hamiltonian for the electrons is a self-adjoint operator-valued function  $h(X)$  of the nuclear configurations. A discrete eigenvalue  $E(X)$  of  $h(X)$  is called an electron energy level.

Electron energy levels play a major role in the time-dependent Born-Oppenheimer approximation [1, 2]. In this approximation the electrons propagate adiabatically and the nuclei obey a semiclassical approximation. In this context, adiabatic means that if the electrons are initially in an eigenstate associated with a level  $E(X)$ , then at a later time, they will be again be found in an eigenstate associated with  $E(X)$ . The eigenvalue  $E(X)$  also acts an effective potential for the semiclassical propagation of the nuclei.

This approximation breaks down when the electron energy level  $E(X)$  crosses any other part of the spectrum of  $h(X)$ , and the simplest such breakdown occurs when  $E(X)$  crosses another eigenvalue of  $h(X)$ . In this paper we describe the first step in the study of what happens when a Born-Oppenheimer state encounters such a crossing. This first step is the classification of generic minimal degeneracy quantum eigenvalue crossings and determination of normal forms for  $h(X)$  near each type of crossing. The various different types of crossings arise from different symmetry situations. We prove below that eleven distinct situations can occur.

\* Partially supported by National Science Foundation Grant DMS-9001635.

Throughout the paper we assume  $h(X)$  is a  $C^2$  function of  $X \in \mathbb{R}^n$  in the sense that its resolvent is  $C^2$ . In the various different situations, we assume the dimension  $n$  of the nuclear configuration space is large enough so that the appropriate type of crossing can occur generically. We show below that in each generic crossing situation, the two eigenvalues coincide on a submanifold  $\Gamma$  of some specific codimension. If  $n$  is less than this codimension, then that type of crossing generically does not occur.

We let  $G$  denote the symmetry group of  $h(X)$ . That is,  $G$  is the group of all unitary and antiunitary operators that are  $X$ -independent in some representation of the electronic Hilbert space, and that commute with all the operators  $h(X)$ . We let  $H$  denote the subgroup of unitary elements of  $G$ , and note that antiunitary elements of  $G$  reverse time.

Since the product of unitary and antiunitary operators is antiunitary, there are clearly two cases: Either  $G = H$  or  $H$  is a subgroup of  $G$  of index 2.

When  $G = H$ , standard group representation theory applies, and each distinct eigenvalue of  $h(X)$  is associated with a unique representation of  $G$ . Minimal multiplicity eigenvalues correspond to 1-dimensional representations, and if two simple eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  cross, then there are two possibilities:

**Type A Crossings:** The two irreducible representations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are not unitarily equivalent to one another.

**Type B Crossings:** The two irreducible representations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are unitarily equivalent to one another.

When  $H$  is a subgroup of index 2, standard group representation theory does not apply. Instead of representations, the basic objects of interest are called corepresentations. A general theory of corepresentations was first developed by Wigner [6]. A more modern, non-basis-dependent treatment can be found in [5]. This general theory shows that any corepresentation can be decomposed as a direct sum of irreducible corepresentations. Furthermore, there are three distinct types of irreducible corepresentations which are called *Types I, II, and III*.

To describe these three types, we first note that  $G$  can be decomposed

as  $G = H \cup \mathcal{K}H$ , where  $\mathcal{K}$  is an arbitrary, but fixed, antiunitary element of  $G$ . Then, if  $U$  is an irreducible corepresentation of  $G$ , we let  $U_H$  denote the restriction of  $U$  to  $H$ . Then the three types are described as follows [5]:

*Type I Corepresentations:*  $U_H$  is an irreducible representation.

*Type II Corepresentations:*  $U_H$  decomposes into a direct sum of two equivalent irreducible representations,  $U_H = D \oplus D$ . Furthermore,  $U$  may be cast in the form

$$U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & D(h) \end{pmatrix}, \quad U(\mathcal{K}) = \begin{pmatrix} 0 & -K \\ K & 0 \end{pmatrix}, \quad \text{and} \quad U(\mathcal{K}h) = U(\mathcal{K})U(h),$$

for all  $h \in H$ . Here  $K$  is an antiunitary operator that satisfies  $K^2 = -D(\mathcal{K}^2)$  and  $K D(\mathcal{K}^{-1}h\mathcal{K}) K^{-1} = D(h)$  for all  $h \in H$ .

*Type III Corepresentations:*  $U_H$  decomposes into a direct sum of two inequivalent irreducible representations,  $U_H = D \oplus C$ . Furthermore,  $U$  may be cast in the form

$$U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & C(h) \end{pmatrix}, \quad U(a) = \begin{pmatrix} 0 & D(\mathcal{K}^2)K^{-1} \\ K & 0 \end{pmatrix}, \quad \text{and} \quad U(\mathcal{K}h) = U(\mathcal{K})U(h),$$

for all  $h \in H$ . Here  $K : \mathcal{H}_D \rightarrow \mathcal{H}_C$  is an antiunitary operator that satisfies  $K D(\mathcal{K}^{-1}h\mathcal{K}) K^{-1} = C(h)$  for all  $h \in H$ .

When  $G \neq H$ , each distinct eigenvalue of  $h(X)$  is associated with a unique corepresentation of  $G$ . From the structure theory outlined above, it is clear that minimal multiplicity eigenvalues associated with Type I corepresentations have multiplicity 1. Minimal multiplicity eigenvalues associated with Type II or Type III corepresentations have multiplicity 2. In the minimal multiplicity situations, the antiunitary operators  $K$  that occur in Type II corepresentations map a one dimensional space to itself. A simple calculation shows that such operators satisfy  $K^2 = 1$ . Thus, in the minimal multiplicity situation,  $K$  is a conjugation, and  $D(\mathcal{K}^2) = -1$ .

This structure theory of corepresentations shows that if two minimal multiplicity eigenvalues  $E_A(X)$  and  $E_B(X)$  cross, then there are nine possibilities:

**Type C Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_A(X)$  and  $E_B(X)$  are both of Type I, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 1 away from the crossing.

**Type D Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are both of Type *II*, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 2 away from the crossing.

**Type E Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are both of Type *III*, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 2 away from the crossing.

**Type F Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are of Types *I* and *II*. Away from the crossing, the eigenvalue associated with the Type *I* corepresentation has multiplicity 1 and the other eigenvalue has multiplicity 2 away from the crossing.

**Type G Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are of Types *I* and *III*. Away from the crossing, the eigenvalue associated with the Type *I* corepresentation has simple multiplicity and the other eigenvalue has multiplicity 2.

**Type H Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are of Types *II* and *III*. Both eigenvalues have multiplicity 2 away from the crossing.

**Type I Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are both of Type *I* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 1 away from the crossing.

**Type J Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are both of Type *II* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 2 away from the crossing.

**Type K Crossings:** The two irreducible corepresentations of  $G$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are both of Type *III* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 2 away from the crossing.

**REMARK:** One can easily find simple quantum systems that provide examples of the various types of crossings.

We now turn to the detailed structure of the electron Hamiltonian function

$h(X)$  near a generic crossing of each type. In our applications [3, 4] we assume that the nuclear wave packets propagate non-tangentially through the manifold  $\Gamma$ , where  $E_{\mathcal{A}}(X) = E_{\mathcal{B}}(X)$ . As these packets propagate through the crossing, their mean momentum is approximately given by a fixed vector  $\eta_0$ . This vector determines a special direction in the nuclear configuration space that is not tangent to  $\Gamma$ . In some cases, the normal forms we derive for  $h(X)$  depend on this special direction.

STRUCTURE OF CROSSINGS OF TYPES A AND C. Suppose two eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  of a  $C^2$  electron Hamiltonian function  $h(X)$  have a crossing of Type A or Type C at  $X = 0$ . By properly labeling the eigenvalues, we may assume that  $E_{\mathcal{A}}(X)$  corresponds to one irreducible representation or corepresentation  $U_1$  of  $G$  for all  $X$ , and that  $E_{\mathcal{B}}(X)$  corresponds to  $U_2$  for all  $X$ . Since  $h(X)$  commutes with the action of  $G$ , it follows that  $h(X)$  commutes with the orthogonal projections  $P_1$  and  $P_2$  onto the mutually orthogonal carrier subspaces associated with  $U_1$  and  $U_2$ , respectively.

For  $X$  in a neighborhood of the origin, one can write the spectral projection  $P(X)$  for  $h(X)$  associated with both the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  as

$$P(X) = \frac{1}{2\pi i} \int_C (z - h(X))^{-1} dz,$$

where  $C$  is a contour that encloses  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  but no other parts of the spectrum of  $h(X)$ . From this it follows that  $P(X)$  is a  $C^2$ , rank 2 operator valued function of  $X$  near  $X = 0$  that commutes with  $P_1$  and  $P_2$ . Since  $U_1$  and  $U_2$  are inequivalent, it follows that  $P_{\mathcal{A}}(X) = P_1 P(X)$  and  $P_{\mathcal{B}}(X) = P_2 P(X)$  are  $C^2$ , rank one orthogonal projections that project onto mutually orthogonal subspaces.

For Type A crossings, we arbitrarily choose  $\Phi_{\mathcal{A}}(0)$  and  $\Phi_{\mathcal{B}}(0)$  to be unit vectors in the ranges of  $P_{\mathcal{A}}(0)$  and  $P_{\mathcal{B}}(0)$ , respectively. We then define

$$\Phi_{\mathcal{A}}(X) = \frac{P_{\mathcal{A}}(X)\Phi_{\mathcal{A}}(0)}{\sqrt{\langle \Phi_{\mathcal{A}}(0), P_{\mathcal{A}}(X)\Phi_{\mathcal{A}}(0) \rangle}}$$

and

$$\Phi_{\mathcal{B}}(X) = \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B}}(0)}{\sqrt{\langle \Phi_{\mathcal{B}}(0), P_{\mathcal{B}}(X)\Phi_{\mathcal{B}}(0) \rangle}}.$$

By standard perturbation theory, these unit-vector valued functions are  $C^2$  in a neighborhood of the origin and belong to the ranges of  $P_{\mathcal{A}}(X)$  and  $P_{\mathcal{B}}(X)$ , respectively, for each  $X$ . Furthermore,  $\Phi_{\mathcal{A}}(X)$  and  $\Phi_{\mathcal{B}}(X)$  are eigenvectors of  $h(X)$  that correspond to  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$ , respectively. Standard arguments also show that  $E_{\mathcal{A}}(\cdot)$  and  $E_{\mathcal{B}}(\cdot)$  are  $C^2$  functions in a neighborhood of the origin.

For Type C crossings, we perform the same construction, but impose an additional constraint. By decomposing  $G = H \cup \mathcal{K}H$ , we have selected a special antiunitary element  $\mathcal{K}$  of  $G$ . A simple calculation shows that we may choose the phases of the vectors  $\Phi_{\mathcal{A}}(0)$  and  $\Phi_{\mathcal{B}}(0)$  so that  $\mathcal{K}\Phi_{\mathcal{A}}(0) = \Phi_{\mathcal{A}}(0)$  and  $\mathcal{K}\Phi_{\mathcal{B}}(0) = \Phi_{\mathcal{B}}(0)$ . By making such choices we obtain vectors  $\Phi_{\mathcal{A}}(X)$  and  $\Phi_{\mathcal{B}}(X)$  that satisfy  $\mathcal{K}\Phi_{\mathcal{A}}(X) = \Phi_{\mathcal{A}}(X)$  and  $\mathcal{K}\Phi_{\mathcal{B}}(X) = \Phi_{\mathcal{B}}(X)$ .

Let  $h^{\perp}(X)$  denote the restriction of  $h(X)$  to the subspace orthogonal to the range of  $P(X)$ . By using  $\Phi_{\mathcal{A}}(X)$  and  $\Phi_{\mathcal{B}}(X)$  as a basis for the range of  $P(X)$  and identifying  $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C} \oplus \text{Ran}(1 - P(X))$ , we can locally represent  $h(X)$  by the matrix

$$\tilde{h}(X) = \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 \\ 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & h^{\perp}(X) \end{pmatrix}.$$

Throughout our discussion, no restrictions have been imposed on the functions  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$ , except that they take the same value at the origin. Thus, they could be any two  $C^2$  functions whose values coincide at the origin. Generically the values of two such functions coincide on a submanifold  $\Gamma$  of codimension 1.

STRUCTURE OF CROSSINGS OF TYPES F AND G. Suppose two eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  of a  $C^2$  electron Hamiltonian function  $h(X)$  have a crossing of Type F or Type G at  $X = 0$ . We may assume the eigenvalues are labeled so that the corepresentation associated with  $E_{\mathcal{A}}(X)$  is of type *I* and the corepresentation associated with  $E_{\mathcal{B}}(X)$  is of type *II* or *III*. Let  $U_1$  and  $U_2$  denote the irreducible corepresentations of  $G$  associated with  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$ , respectively, and note that the dimension of the  $U_2$  is 2. As in the case of Type A or C crossings,  $h(X)$  commutes with the orthogonal projections  $P_1$

and  $P_2$  onto the mutually orthogonal carrier subspaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$  associated with  $U_1$  and  $U_2$ , respectively.

For  $X$  in a neighborhood of the origin, one can write the spectral projection  $P(X)$  for  $h(X)$  associated with the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  as an integral of the resolvent of  $h(X)$ . From this it follows that  $P(X)$  is a  $C^2$ , rank 3 operator valued function of  $X$  near  $X = 0$  that commutes with  $P_1$  and  $P_2$ . Since  $U_1$  and  $U_2$  are inequivalent, it follows that  $P_{\mathcal{A}}(X) = P_1 P(X)$  and  $P_{\mathcal{B}}(X) = P_2 P(X)$  are  $C^2$ , rank one and (respectively) rank two orthogonal projections that project onto mutually orthogonal subspaces.

We construct a  $C^2$  unit-vector valued function  $\Phi_{\mathcal{A}}(\cdot)$  exactly as in the case of a Type C crossing, so that  $\mathcal{K} \Phi_{\mathcal{A}}(X) = \Phi_{\mathcal{A}}(X)$ . For a Type F crossing we choose  $\Phi_{\mathcal{B},1}(0)$  to be an arbitrary unit vector in the range of  $P_{\mathcal{B}}(0)$ . We then let

$$\Phi_{\mathcal{B},1}(X) = \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)}{\sqrt{\langle \Phi_{\mathcal{B},1}(0), P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0) \rangle}}$$

and

$$\Phi_{\mathcal{B},2}(X) = \mathcal{K} \Phi_{\mathcal{B},1}(X).$$

Because  $\mathcal{K}$  is antiunitary and  $D(\mathcal{K}^2) = -1$ , it follows that  $\Phi_{\mathcal{B},1}(X)$  and  $\Phi_{\mathcal{B},2}(X)$  comprise an orthonormal basis for the range of  $P_{\mathcal{B}}(X)$ .

For Type G crossings, we let  $P_C$  and  $P_D$  denote the orthogonal projections onto the carrier subspaces for the two representations C and D of the subgroup  $H$  that are involved. These projections commute with  $P_{\mathcal{B}}(X)$  and project onto mutually orthogonal subspaces. Furthermore,  $P_C P_{\mathcal{B}}(X)$  and  $P_D P_{\mathcal{B}}(X)$  are rank one projections. We choose  $\Phi_{\mathcal{B},1}(0)$  to be a unit vector in the range of  $P_D P_{\mathcal{B}}(0)$ . We then let

$$\Phi_{\mathcal{B},1}(X) = \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)}{\sqrt{\langle \Phi_{\mathcal{B},1}(0), P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0) \rangle}}$$

and

$$\Phi_{\mathcal{B},2}(X) = \mathcal{K} \Phi_{\mathcal{B},1}(X).$$

From the structure theory of type III corepresentations, we see that  $\Phi_{\mathcal{B},2}(X)$  belongs to the range of  $P_C P_{\mathcal{B}}(X)$ , and that  $\Phi_{\mathcal{B},1}(X)$  and  $\Phi_{\mathcal{B},2}(X)$  comprise a  $C^2$  orthonormal basis for the range of  $P_{\mathcal{B}}(X)$ .



Let  $h^\perp(X)$  denote the restriction of  $h(X)$  to the subspace orthogonal to the range of  $P(X)$ . By using  $\Phi_{\mathcal{A}}(X)$ ,  $\Phi_{\mathcal{B},1}(X)$  and  $\Phi_{\mathcal{B},2}(X)$  as a basis for the range of  $P(X)$  and identifying  $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C}^2 \oplus \text{Ran}(1 - P(X))$ , we can locally represent  $h(X)$  by the matrix

$$\tilde{h}(X) = \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 & 0 \\ 0 & E_{\mathcal{B}}(X) & 0 & 0 \\ 0 & 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & 0 & h^\perp(X) \end{pmatrix}.$$

As in the case of Type A and C crossings, no restrictions are imposed on  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$ . Thus, they generically cross on a codimension 1 submanifold  $\Gamma$ .

STRUCTURE OF CROSSINGS OF TYPES D, E, AND H. Suppose two eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  of an electron Hamiltonian function  $h(X)$  have a crossing of type D, E, or H at  $X = 0$ . By mimicking the constructions used for Type F and G crossings, we see that we can choose four smooth, mutually orthogonal unit-vector valued functions  $\Phi_{\mathcal{A},1}(X)$ ,  $\Phi_{\mathcal{A},2}(X) = \mathcal{K} \Phi_{\mathcal{A},1}(X)$ ,  $\Phi_{\mathcal{B},1}(X)$ , and  $\Phi_{\mathcal{B},2}(X) = \mathcal{K} \Phi_{\mathcal{B},1}(X)$ , such that  $\Phi_{\mathcal{A},1}(X)$ , and  $\Phi_{\mathcal{A},2}(X)$  are eigenvectors of  $h(X)$  with eigenvalue  $E_{\mathcal{A}}(X)$ , and  $\Phi_{\mathcal{B},1}(X)$ , and  $\Phi_{\mathcal{B},2}(X)$  are eigenvectors of  $h(X)$  with eigenvalue  $E_{\mathcal{B}}(X)$ . Furthermore, whenever a type III corepresentation is involved, the eigenvector with second subscript 1 belongs to one representation of the subgroup  $H$  and the eigenvector with the second subscript 2 belongs to the other representation of the subgroup.

As in the earlier constructions, by using these vectors as part of a basis, and identifying  $\mathcal{H} \cong \mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \text{Ran}(1 - P(X))$ , we can locally represent  $h(X)$  by the matrix

$$\tilde{h}(X) = \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 & 0 & 0 \\ 0 & E_{\mathcal{A}}(X) & 0 & 0 & 0 \\ 0 & 0 & E_{\mathcal{B}}(X) & 0 & 0 \\ 0 & 0 & 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & 0 & 0 & h^\perp(X) \end{pmatrix}.$$

As in the earlier cases,  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  generically cross on a submanifold  $\Gamma$  of codimension 1.

STRUCTURE OF TYPE I CROSSINGS Suppose a  $C^2$  electron Hamiltonian function  $h(X)$  has a type I crossing of two simple eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  at  $X = 0$ . As in the earlier cases, the projection  $P(X)$  for  $h(X)$  associated with the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  is a  $C^2$ , rank 2 operator valued function of  $X$  near  $X = 0$ . It follows that  $E_{\mathcal{A}}(X) + E_{\mathcal{B}}(X) = \text{trace}(h(X)P(X))$  is also  $C^2$ . Thus,

$$h_1(X) = h(X) - \frac{1}{2}(E_{\mathcal{A}}(X) + E_{\mathcal{B}}(X))$$

is a  $C^2$  operator-valued function whose restriction to the range of  $P(X)$  is traceless.

Let  $\{\psi_1, \psi_2\}$  be a basis for the range of  $P(0)$ . By altering the phases of these two vectors, we may assume that  $\mathcal{K}\psi_1 = \psi_1$  and  $\mathcal{K}\psi_2 = \psi_2$ , where  $\mathcal{K}$  is the antiunitary operator chosen for the decomposition  $G = H \cup \mathcal{K}H$ . Define  $\psi_1(X)$  for  $X$  by

$$\psi_1(X) = \frac{P(X)\psi_1}{\sqrt{\langle \psi_1, P(X)\psi_1 \rangle}}.$$

Since  $P(X)$  is  $C^2$  and commutes with the action of  $G$ ,  $\psi_1(X)$  is well defined and  $C^2$  in some neighborhood of the origin and satisfies  $\mathcal{K}\psi_1(X) = \psi_1(X)$ . Let  $P_1(X)$  denote the projection onto the subspace spanned by  $\psi_1(X)$ . It is a  $C^2$  operator-valued function in a neighborhood of  $X$  that commutes with  $P(X)$  and the action of  $G$ . We define

$$\psi_2(X) = \frac{P(X)(1 - P_1(X))\psi_2}{\sqrt{\langle \psi_2, P(X)(1 - P_1(X))\psi_2 \rangle}}.$$

This vector valued function is also  $C^2$  in a neighborhood of the origin;  $\mathcal{K}\psi_2(X) = \psi_2(X)$ ; and  $\{\psi_1(X), \psi_2(X)\}$  is an orthonormal basis for the range of  $P(X)$ , for  $X$  in a neighborhood of the origin.

In the basis  $\{\psi_1(X), \psi_2(X)\}$ , the restriction of  $h_1(X)$  to the range of  $P(X)$  is represented by a real symmetric, traceless  $2 \times 2$  matrix valued function  $M(X)$  whose entries are  $C^2$  functions that all vanish when  $X = 0$ . That is,

$$M(X) = \begin{pmatrix} \alpha(X) & \beta(X) \\ \beta(X) & -\alpha(X) \end{pmatrix},$$

where  $\alpha$  and  $\beta$  are real valued  $C^2$  functions. The eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  cross precisely at those points  $X$  where  $\alpha(X) = \beta(X) = 0$ . Generi-

cally this defines a codimension 2 submanifold  $\Gamma$ . Furthermore, the difference between  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  is the same as the difference between the eigenvalues of  $M(X)$ . By direct computation, the eigenvalues of  $M(X)$  are

$$\pm \sqrt{\alpha(X)^2 + \beta(X)^2}.$$

Generically this function is continuous, but not differentiable near  $\Gamma$ . One can easily show that the eigenvectors are not even continuous near  $\Gamma$ .

By standard Taylor series results,  $M(X)$  has the form  $M(X) = N(X) + O(\|X\|^2)$ , where

$$N(X) = \begin{pmatrix} a \cdot X & b \cdot X \\ b \cdot X & -a \cdot X \end{pmatrix},$$

for some vectors  $a$  and  $b$ . Generically  $a$  and  $b$  are linearly independent. By a rotation of the coordinate system we may assume that only the first two components of  $a$  and  $b$  are non-zero.

If  $\eta_0$  is a vector not tangent to  $\Gamma$  at  $X = 0$ , then we can rotate the first two coordinate axes so that the projection of  $\eta_0$  into the two dimensional subspace spanned by  $a$  and  $b$  lies along the positive  $X_1$  axis.

At this point, the  $X_j$  coordinates for  $j > 2$  no longer play a role in the structure of  $N(X)$ . Furthermore, the form of  $N(X)$  is not altered if we do  $X$ -independent orthogonal transformations of the two dimensional space spanned by the basic electronic wave functions  $\psi_1(X)$  and  $\psi_2(X)$ . We replace  $\psi_1(X)$  by  $\cos(\theta)\psi_1(X) + \sin(\theta)\psi_2(X)$  and  $\psi_2(X)$  by  $-\sin(\theta)\psi_1(X) + \cos(\theta)\psi_2(X)$ . A simple calculation shows that we can choose  $\theta$  so that the  $X_1$ -component of  $b$  is zero. Finally, by possibly interchanging the order of  $\psi_1(X)$  and  $\psi_2(X)$  or multiplying one of them by  $-1$ , we can assume that the  $X_1$ -component of  $a$  and the  $X_2$ -component of  $b$  are both positive.

Thus,  $N(X)$  has the form

$$N(X) = \begin{pmatrix} a_1X_1 + a_2X_2 & b_2X_2 \\ b_2X_2 & -a_1X_1 - a_2X_2 \end{pmatrix},$$

where  $a_1$  and  $b_2$  have the same sign. So, by identifying  $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C} \oplus \text{Ran}(1 - P(X))$ , we can locally approximate  $h_1(X)$  by the matrix

$$\tilde{h}_1(X) = \begin{pmatrix} a_1X_1 + a_2X_2 & b_2X_2 & 0 \\ b_2X_2 & -a_1X_1 - a_2X_2 & 0 \\ 0 & 0 & h_1^\perp(X) \end{pmatrix}.$$

STRUCTURE OF TYPE B CROSSINGS Suppose a  $C^2$  electron Hamiltonian function  $h(X)$  has a type B crossing of two simple eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  at  $X = 0$ . In this situation we mimic the construction of the vectors  $\psi_1(X)$  and  $\psi_2(X)$  in the case of a Type I crossing. Since there is no anitunitary operator  $\mathcal{K} \in G$ , we choose arbitrary orthogonal unit vectors  $\psi_1(0)$  and  $\psi_2(0)$  from the range of  $P(X)$ , and then proceed with the construction. This yields an orthonormal basis  $\{\psi_1(X), \psi_2(X)\}$  for the range of  $P(X)$ .

In this basis, the restriction of

$$h_1(X) = h(X) - \frac{1}{2}(E_{\mathcal{A}}(X) + E_{\mathcal{B}}(X))$$

to the range of  $P(X)$  is represented by a self-adjoint traceless  $2 \times 2$  matrix valued function  $M(X)$  whose entries are  $C^2$  functions that all vanish when  $X = 0$ . That is,

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

where  $\alpha, \beta$ , and  $\gamma$  are  $C^2$  real valued functions. The difference between  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  is the same as the difference between the eigenvalues of  $M(X)$ . By direct computation, the eigenvalues of  $M(X)$  are

$$\pm \sqrt{\alpha(X)^2 + \beta(X)^2 + \gamma(X)^2}.$$

Thus, the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  cross precisely at those points  $X$  where  $\alpha(X) = \beta(X) = \gamma(X) = 0$ . Generically this defines a codimension 3 submanifold  $\Gamma$ . Furthermore, it is clear that the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  are continuous, but generically not differentiable near  $\Gamma$ .

By standard Taylor series results,  $M(X)$  has the form  $M(X) = N(X) + O(\|X\|^2)$ , where

$$N(X) = \begin{pmatrix} a \cdot X & b \cdot X + ic \cdot X \\ b \cdot X - ic \cdot X & -a \cdot X \end{pmatrix},$$

for some vectors  $a, b$ , and  $c$ . Generically  $a, b$ , and  $c$  are linearly independent. By a rotation of the coordinate system we may assume that only the first three components of  $a, b$ , and  $c$  are non-zero.

If  $\eta_0$  is a vector not tangent to  $\Gamma$  at  $X = 0$ , then we can rotate the first three coordinate axes so that the projection of  $\eta_0$  into the three dimensional subspace spanned by  $a$ ,  $b$ , and  $c$  lies along the positive  $X_1$  axis.

At this point, the  $X_j$  coordinates for  $j > 3$  no longer play a role in the structure of  $N(X)$ . Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the  $X_2$  and  $X_3$  coordinate directions, and we can perform  $X$ -independent unitary transformations of the two dimensional space spanned by  $\psi_1(X)$  and  $\psi_2(X)$ . By doing both of these in a special way, we claim that we may assume the following:

1. The first component of  $a$  is non-zero.
2. The first and third components of  $b$  are zero, but its second component is positive.
3. The first and second components of  $c$  are zero, but its third component is positive.

Thus, we may assume that  $N(X)$  has the form

$$N(X) = \begin{pmatrix} a_1X_1 + a_2X_2 + a_3X_3 & b_2X_2 + ic_3X_3 \\ b_2X_2 - ic_3X_3 & -a_1X_1 - a_2X_2 - a_3X_3 \end{pmatrix}.$$

To prove these claims we first do a unitary transformation of the span of  $\psi_1(X)$  and  $\psi_2(X)$  so that when  $X_2 = X_3 = \dots = X_N = 0$ , the matrix  $M(X)$  is diagonal. Standard one variable perturbation theory shows that this can always be done. Thus, we may assume that  $b_1 = c_1 = 0$ .

Next, we show that we can do another unitary transformation of the span of  $\psi_1(X)$  and  $\psi_2(X)$  so that  $b_1$  and  $c_1$  are unchanged, but  $b$  and  $c$  are transformed into perpendicular vectors. The unitary transformation we use simply multiplies  $\psi_2(X)$  by a phase factor  $e^{i\theta}$ . This diagonal transformation leaves  $M(X)$  diagonal when  $X_2 = X_3 = \dots = X_N = 0$ , so  $b_1$  and  $c_1$  are not altered. However, the similarity transformation replaces

$$\begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix}$$

by

$$\begin{pmatrix} \tilde{b}_2 & \tilde{c}_2 \\ \tilde{b}_3 & \tilde{c}_3 \end{pmatrix} = \begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

We need only show that by a proper choice of  $\theta$ , the columns of  $\begin{pmatrix} \tilde{b}_2 & \tilde{c}_2 \\ \tilde{b}_3 & \tilde{c}_3 \end{pmatrix}$  can be forced to be orthogonal. We choose  $\theta$  so that  $\begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}$  and  $\begin{pmatrix} -\sin \theta \\ \cos \theta \end{pmatrix}$  are an orthonormal basis of eigenvectors for the real symmetric matrix  $A^t A$ , where  $A = \begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix}$ . A simple computation then shows that  $\begin{pmatrix} \tilde{b}_2 \\ \tilde{b}_3 \end{pmatrix}$  and  $\begin{pmatrix} \tilde{c}_2 \\ \tilde{c}_3 \end{pmatrix}$  are orthogonal to one another.

We can now rotate the  $X_2$  and  $X_3$  coordinate directions so that  $\tilde{b}$  and  $\tilde{c}$  point along the positive  $X_2$  and  $X_3$  directions, respectively. By adding  $\pi$  to our choice of  $\theta$ , we can change the signs of both  $\tilde{b}$  and  $\tilde{c}$ . By interchanging  $\psi_1(X)$  and  $\psi_2(X)$  we can change the sign of  $\tilde{c}$  without altering  $\tilde{b}$ .

Thus, we can arrange for  $b_1 = 0$ ,  $b_2 > 0$ ,  $b_3 = 0$ ,  $c_1 = 0$ ,  $c_2 = 0$ , and  $c_3 > 0$ . This proves our claims.

**STRUCTURE OF CROSSINGS OF TYPE K** Suppose a  $C^2$  electron Hamiltonian function  $h(X)$  has a Type K crossing of two multiplicity 2 eigenvalues  $E_A(X)$  and  $E_B(X)$  at  $X = 0$ . As in the earlier constructions, we let  $P(X)$  be the spectral projection for  $h(X)$  corresponding to both the eigenvalues  $E_A(X)$  and  $E_B(X)$ . This projection has rank 4, and its range is the direct sum of a two dimensional subspace that lies in the carrier subspace for the  $D$  representation of the subgroup  $H \in G$ , and a two dimensional subspace that lies in the carrier subspace for the  $C$  representation. We arbitrarily pick two orthonormal vectors  $\psi_1(0)$  and  $\psi_2(0)$  that lie in the range of  $P(0)$  and in the carrier subspace for the  $D$  representation. We let

$$\psi_1(X) = \frac{P(X)\psi_1(0)}{\sqrt{\langle \psi_1(0), P(X)\psi_1(0) \rangle}}.$$

We let  $P_1(X)$  denote the orthogonal projection onto the span of  $\psi_1(X)$  and define

$$\psi_2(X) = \frac{(1 - P_1(X))P(X)\psi_2(0)}{\sqrt{\langle \psi_2(0), (1 - P_1(X))P(X)\psi_2(0) \rangle}}.$$

In a neighborhood of the origin, these two vectors form an orthonormal basis for the intersection of the range of  $P(X)$  and the carrier subspace for the  $D$

representation. We let  $\psi_3(X) = \mathcal{K}\psi_1(X)$  and  $\psi_4(X) = \mathcal{K}\psi_2(X)$ . Then  $\psi_3(X)$  and  $\psi_4(X)$  form an orthonormal basis for the intersection of the range of  $P(X)$  and the carrier subspace for the  $C$  representation. The set of all four vectors is an orthonormal basis for the range of  $P(X)$ .

In this basis, the restriction of

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

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

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

and

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

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

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

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are  $C^2$  real valued functions. By direct computation, the eigenvalues of  $M(X)$  are

$$\pm \sqrt{\alpha(X)^2 + \beta(X)^2 + \gamma(X)^2}.$$

Thus, the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  cross precisely at those points  $X$  where  $\alpha(X) = \beta(X) = \gamma(X) = 0$ , which generically defines a codimension 3 submanifold  $\Gamma$ .

By standard Taylor series results,  $M(X)$  has the form  $M(X) = N(X) + O(\|X\|^2)$ , where

$$N(X) = \begin{pmatrix} a \cdot X & b \cdot X + ic \cdot X & 0 & 0 \\ b \cdot X - ic \cdot X & -a \cdot X & 0 & 0 \\ 0 & 0 & a \cdot X & b \cdot X - ic \cdot X \\ 0 & 0 & b \cdot X + ic \cdot X & -a \cdot X \end{pmatrix},$$

for some vectors  $a$ ,  $b$ , and  $c$ . Generically  $a$ ,  $b$ , and  $c$  are linearly independent. By a rotation of the coordinate system we may assume that only the first three components of  $a$ ,  $b$ , and  $c$  are non-zero.

If  $\eta_0$  is any vector not tangent to  $\Gamma$  at  $X = 0$ , then we can rotate the first three coordinate axes so that the projection of  $\eta_0$  into the three dimensional subspace spanned by  $a$ ,  $b$ , and  $c$  lies along the positive  $X_1$  axis.

At this point, the  $X_j$  coordinates for  $j > 3$  no longer play a role in the structure of  $N(X)$ . Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the  $X_2$  and  $X_3$  coordinate directions, and we can perform  $X$ -independent unitary transformations of the two dimensional space spanned by the basic electronic wave functions  $\psi_1(X)$  and  $\psi_2(X)$ . If we do such unitary transformations, we also redefine  $\psi_3(X)$  and  $\psi_4(X)$  to preserve the relations  $\psi_3(X) = \mathcal{K} \psi_1(X)$  and  $\psi_4(X) = \mathcal{K} \psi_2(X)$ . We do these operations, mimicking the procedure used in our discussion of Type B crossings, to see that the following three conditions can be satisfied:

1. The first component of  $a$  is non-zero.
2. The first and third components of  $b$  are zero, but its second component is positive.
3. The first and second components of  $c$  are zero, but its third component is positive.



Thus, we may assume that  $N(X)$  has the form

$$\begin{pmatrix} \sum_{j=1}^3 a_j X_j & b_2 X_2 + ic_3 X_3 & 0 & 0 \\ b_2 X_2 - ic_3 X_3 & -\sum_{j=1}^3 a_j X_j & 0 & 0 \\ 0 & 0 & \sum_{j=1}^3 a_j X_j & b_2 X_2 - ic_3 X_3 \\ 0 & 0 & b_2 X_2 + ic_3 X_3 & -\sum_{j=1}^3 a_j X_j \end{pmatrix}.$$

STRUCTURE OF TYPE J CROSSINGS Suppose a  $C^2$  electron Hamiltonian function  $h(X)$  has a Type J crossing of two multiplicity 2 eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  at  $X = 0$ . As in the earlier constructions, we let  $P(X)$  be the rank 4 spectral projection for  $h(X)$  corresponding to both the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$ . We arbitrarily pick a unit vector  $\psi_1(0)$  that lies in the range of  $P(0)$ , and we define  $\psi_2(0) = \mathcal{K} \psi_1(0)$ . We then choose another unit vector  $\psi_3(0)$  that is in the range of  $P(0)$ , but is orthogonal to both  $\psi_1(0)$  and  $\psi_2(0)$ . We then let  $\psi_4(0) = \mathcal{K} \psi_3(0)$ . For Type II corepresentations of minimal multiplicity,  $D(\mathcal{K}^2) = -1$ , and it follows that the four vectors form an orthonormal basis for the range of  $P(0)$ . We define

$$\psi_1(X) = \frac{P(X) \psi_1(0)}{\sqrt{\langle \psi_1(0), P(X) \psi_1(0) \rangle}}.$$

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

$$\psi_3(X) = \frac{(1 - P_{1,2}(X))P(X) \psi_3(0)}{\sqrt{\langle \psi_3(0), (1 - P_{1,2}(X))P(X) \psi_3(0) \rangle}}.$$

We then define  $\psi_4(X) = \mathcal{K} \psi_3(X)$ . For each  $X$  in a neighborhood of the origin, these four vectors form an orthonormal basis for the range of  $P(X)$ .

In this basis, the restriction of

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

to the range of  $P(X)$  is represented by a self-adjoint traceless  $4 \times 4$  matrix valued function  $M(X)$  whose entries are  $C^2$  functions that all vanish when

$X = 0$ . Because  $h(X)$  commutes with the action of  $\mathcal{K}$ ,  $M(X)$  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  $M(X)$  must have the form

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

where  $\alpha, \beta, \gamma, \delta$ , and  $\epsilon$  are  $C^2$  real valued functions. The difference between  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  is the same as the difference between the eigenvalues of  $M(X)$ . By direct computation, the eigenvalues of  $M(X)$  are

$$\pm \sqrt{\alpha(X)^2 + \beta(X)^2 + \gamma(X)^2 + \delta(X)^2 + \epsilon(X)^2}.$$

Thus, the eigenvalues  $E_{\mathcal{A}}(X)$  and  $E_{\mathcal{B}}(X)$  cross precisely at those points  $X$  where  $\alpha(X) = \beta(X) = \gamma(X) = \delta(X) = \epsilon(X) = 0$ , which generically defines a codimension 5 submanifold  $\Gamma$ .

By standard Taylor series results,  $M(X)$  has the form  $M(X) = N(X) + O(\|X\|^2)$ , where

$$\begin{pmatrix} a \cdot X & 0 & b \cdot X + ic \cdot X & d \cdot X + ie \cdot X \\ 0 & a \cdot X & -d \cdot X + ie \cdot X & b \cdot X - ic \cdot X \\ b \cdot X - ic \cdot X & -d \cdot X - ie \cdot X & -a \cdot X & 0 \\ d \cdot X - ie \cdot X & b \cdot X + ic \cdot X & 0 & -a \cdot X \end{pmatrix},$$

for some vectors  $a, b, c, d$ , and  $e$ . Generically  $a, b, c, d$ , and  $e$  are linearly independent. By a rotation of the coordinate system we may assume that only the first five components of  $a, b, c, d$ , and  $e$  are non-zero.

If  $\eta_0$  is any vector not tangent to  $\Gamma$  at  $X = 0$ , then we can rotate the first five coordinate axes so that the projection of  $\eta_0$  into the five dimensional subspace spanned by  $a, b, c, d$ , and  $e$  lies along the positive  $X_1$  axis.

At this point, the  $X_j$  coordinates for  $j > 5$  no longer play a role in the structure of  $N(X)$ . Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the  $X_2, X_3, X_4$ , and  $X_5$  coordinate directions, and we can perform those  $X$ -independent unitary transformations of the four dimensional space spanned by the basic electronic

wave functions  $\psi_1(X)$ ,  $\psi_2(X)$ ,  $\psi_3(X)$ , and  $\psi_4(X)$  that preserve the relations  $\psi_2(X) = \mathcal{K} \psi_1(X)$  and  $\psi_4(X) = \mathcal{K} \psi_3(X)$ . We claim that by doing such operations in generic situations, we can arrange for the following five conditions to be satisfied:

1. The first component of  $a$  is non-zero.
2.  $b_1 = b_3 = b_4 = b_5 = 0$ , but  $b_2 \neq 0$ .
3.  $c_1 = c_2 = c_4 = c_5 = 0$ , but  $c_3 \neq 0$ .
4.  $d_1 = d_2 = d_3 = d_5 = 0$ , but  $d_4 \neq 0$ .
5.  $e_1 = e_2 = e_3 = e_4 = 0$ , but  $e_5 \neq 0$ .

Thus, we may assume that  $N(X)$  has the form

$$\begin{pmatrix} \sum_{j=1}^5 a_j X_j & 0 & b_2 X_2 + ic_3 X_3 & d_4 X_4 + ie_5 X_5 \\ 0 & \sum_{j=1}^5 a_j X_j & -d_4 X_4 + ie_5 X_5 & b_2 X_2 - ic_3 X_3 \\ b_2 X_2 - ic_3 X_3 & -d_4 X_4 - ie_5 X_5 & -\sum_{j=1}^5 a_j X_j & 0 \\ d_4 X_4 - ie_5 X_5 & b_2 X_2 + ic_3 X_3 & 0 & -\sum_{j=1}^5 a_j X_j \end{pmatrix}.$$

To prove these claims we first note that if we replace  $\psi_j(X)$  by  $\tilde{\psi}_j(X)$ , where

$$\begin{aligned} \tilde{\psi}_1(X) &= z_1 \psi_1(X) + z_2 \psi_2(X), & \text{with } |z_1|^2 + |z_2|^2 &= 1, \\ \tilde{\psi}_2(X) &= \mathcal{K} \tilde{\psi}_1(X), \\ \tilde{\psi}_3(X) &= z_3 \psi_3(X) + z_4 \psi_4(X), & \text{with } |z_3|^2 + |z_4|^2 &= 1, & \text{and} \\ \tilde{\psi}_4(X) &= \mathcal{K} \tilde{\psi}_3(X), \end{aligned}$$

then  $N(X)$  is transformed into

$$\begin{pmatrix} \tilde{a} \cdot X & 0 & \tilde{b} \cdot X + i\tilde{c} \cdot X & \tilde{d} \cdot X + i\tilde{e} \cdot X \\ 0 & \tilde{a} \cdot X & -\tilde{d} \cdot X + i\tilde{e} \cdot X & \tilde{b} \cdot X - i\tilde{c} \cdot X \\ \tilde{b} \cdot X - i\tilde{c} \cdot X & -\tilde{d} \cdot X - i\tilde{e} \cdot X & -\tilde{a} \cdot X & 0 \\ \tilde{d} \cdot X - i\tilde{e} \cdot X & \tilde{b} \cdot X + i\tilde{c} \cdot X & 0 & -\tilde{a} \cdot X \end{pmatrix}.$$

We show below that by making an appropriate choice of the  $z_j$ , we can force  $\tilde{b}$ ,  $\tilde{c}$ ,  $\tilde{d}$ , and  $\tilde{e}$  to be mutually orthogonal (and all non-zero in generic situations).

Once this is done, we rotate the  $X_2, X_3, X_4$ , and  $X_5$  coordinate axes, so that  $\tilde{b}, \tilde{c}, \tilde{d}$ , and  $\tilde{e}$  point along the  $X_2, X_3, X_4$ , and  $X_5$ , respectively. This proves the claims.

Arbitrarily choosing the  $z_j$ 's is equivalent to arbitrarily choosing two matrices  $U_1 \in SU(2)$  and  $U_2 \in SU(2)$ , so that

$$\begin{pmatrix} \tilde{\psi}_1(X) \\ \tilde{\psi}_2(X) \end{pmatrix} = U_1 \begin{pmatrix} \psi_1(X) \\ \psi_2(X) \end{pmatrix}$$

and

$$\begin{pmatrix} \tilde{\psi}_3(X) \\ \tilde{\psi}_4(X) \end{pmatrix} = U_2 \begin{pmatrix} \psi_3(X) \\ \psi_4(X) \end{pmatrix}.$$

In this notation,

$$\begin{pmatrix} \tilde{b} \cdot X - i\tilde{c} \cdot X & -\tilde{d} \cdot X - i\tilde{e} \cdot X \\ \tilde{d} \cdot X - i\tilde{e} \cdot X & \tilde{b} \cdot X + i\tilde{c} \cdot X \end{pmatrix} = U_2 \begin{pmatrix} b \cdot X - ic \cdot X & -d \cdot X - ie \cdot X \\ d \cdot X - ie \cdot X & b \cdot X + ic \cdot X \end{pmatrix} U_1^{-1}.$$

The mapping

$$(w_1, w_2, w_3, w_4) \longmapsto W = \begin{pmatrix} w_1 - iw_2 & -w_3 - iw_4 \\ w_3 - iw_4 & w_1 + iw_2 \end{pmatrix}$$

is an isometric isomorphism of standard Euclidean  $\mathbb{R}^4$  into a subspace  $\mathcal{W}$  of the  $4 \times 4$  complex matrices endowed with the inner product  $\langle W_1, W_2 \rangle = \frac{1}{2} \text{trace}(W_1^* W_2)$ . Furthermore, the action of  $SU(2) \times SU(2)$  on  $\mathcal{W}$  given by  $W \longmapsto \tilde{W} = U_2 W U_1^{-1}$  is isometric on this space. Since  $SU(2) \times SU(2)$  is connected, it follows that the corresponding action on Euclidean  $\mathbb{R}^4$  is given by

$$(w_1, w_2, w_3, w_4) \longmapsto (\tilde{w}_1, \tilde{w}_2, \tilde{w}_3, \tilde{w}_4) = (w_1, w_2, w_3, w_4) \mathcal{O}_{U_1, U_2},$$

where  $\mathcal{O}_{U_1, U_2} \in SO(4)$ . The mapping  $(U_1, U_2) \longmapsto \mathcal{O}_{U_1, U_2}$  is a group homomorphism. By explicit calculation, the differential of this map takes the generators of the Lie algebra  $su(2) \times su(2)$  onto the generators of the Lie algebra  $so(4)$ . Thus, the map is a local isomorphism of the Lie groups.  $SU(2) \times SU(2)$  is connected and simply connected, and  $SO(4)$  is connected. It follows that the mapping is a covering map, and therefore is surjective (In fact, it is two-to-one with kernel  $\{(I, I), (-I, -I)\}$ ). If  $(b \ c \ d \ e)$  denotes the  $4 \times 4$  matrix

whose columns are the vectors  $b$ ,  $c$ ,  $d$ , and  $e$ , then we have

$$\begin{pmatrix} \tilde{b} & \tilde{c} & \tilde{d} & \tilde{e} \end{pmatrix} = \begin{pmatrix} b & c & d & e \end{pmatrix} \mathcal{O}_{U_1, U_2},$$

where  $\mathcal{O}_{U_1, U_2}$  can be taken to be any element of  $SO(4)$  if  $U_1$  and  $U_2$  are chosen properly. Our claims are thus proved if we can show that any invertible matrix  $A = \begin{pmatrix} b & c & d & e \end{pmatrix}$  has the property that it maps some orthonormal basis (the columns of  $\mathcal{O}_{U_1, U_2}$ ) into non-zero, mutually orthogonal vectors  $\{\tilde{b}, \tilde{c}, \tilde{d}, \tilde{e}\}$ . To show that this is the case, we choose the orthonormal basis  $\{v_1, v_2, v_3, v_4\}$  to be an orthonormal basis in which the real symmetric matrix  $A^* A$  is diagonal. Such bases always exist, and one can always arrange for  $\mathcal{O}_{U_1, U_2} = \begin{pmatrix} v_1 & v_2 & v_3 & v_4 \end{pmatrix}$  to be in  $SO(4)$ . Then for  $i \neq j$ ,  $\langle Av_i, Av_j \rangle = \langle v_i, A^* Av_j \rangle = \mu_j \langle v_i, v_j \rangle = 0$ . This proves the claim.

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