Multiple poles of the $S(E)$ matrix and the geometric phase of resonant states

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ABSTRACT. We show that, in striking contrast with the case of bound states, accidental degeneracies of resonant states give rise to multiple poles in the scattering matrix as function of complex energy. We also show that, close to a crossing of resonances, the topology of the energy surfaces is different from that at a crossing of bound states. We discuss some consequences of these differences for such physical properties as the Berry phase of resonant states, the distribution of resonance spacings in the spectrum of a quantum chaotic system and the phenomenon of level width attraction.

RESUMEN. Demostramos que en marcado contraste con el caso de los estados ligados, las degeneraciones accidentales de los estados resonantes dan lugar a polos múltiples en la matriz de dispersión como función de la energía compleja. También demostramos que cerca de un cruce de resonancias la topología de las superficies de la energía es diferente de la de un cruce de estados ligados. Discutimos algunas consecuencias de estas diferencias en algunas propiedades físicas tales como la fase de Berry de un estado resonante, la distribución de espaciamientos entre resonancias en el espectro de un sistema cuántico caótico y el fenómeno de atracción de anchuras de niveles.

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1. INTRODUCTION

The phenomenon of avoided level crossings and energy level repulsion observed in the spectra of closed quantum systems driven by Hermitian Hamiltonians was explained in terms of the impossibility or at least improbability of the occurrence of an accidental degeneracy when the number of external control parameters that may be varied is too small or the range of variation of these parameters is too restricted [1,2]. These properties are important for the understanding of a wide variety of quantum phenomena, such as the Landau-Zener effect [3], the Berry phase [4], the statistical distribution of energy level spacings in nuclei [5] and other quantum chaotic systems [6]. Accidental degeneracies have also been linked to the onset and properties of quantum chaos [7].

Accidental degeneracies of resonances produced by the variation of the external parameters of an open quantum system were observed by McVoy [8] as “collisions” of resonance poles of the scattering matrix in the complex energy plane. This author noticed that degeneracies of resonances differ markedly from degeneracies of bound states. The occurrence of multiple poles of the scattering matrix at the “collision” energy, that is, at an accidental degeneracy of resonances, had already been mentioned by Goldberger and Watson in

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their well known text book on Collision Theory [9]. Two nice examples of double poles of the scattering matrix in potential scattering are given by Bell and Goebel [10] and Huestis [11]. More recently, Friedrich and Wintgen [12] and von Brentano [13] investigated the behaviour of two resonances mixed by a Hermitian interaction and found that increasing the strength of the mixing interaction sometimes produces level width attraction instead of the energy level repulsion observed in bound state accidental degeneracy. But, although most of the information on statistical properties of nuclear spectra as well as the effects due to interference of nuclear states is obtained from resonances [14], virtually all the existing literature has been concerned with accidental degeneracies of stable closed systems driven by Hermitian Hamiltonians [15]. It was only recently that we started a systematic investigation of the accidental degeneracy of resonances in relation with the study of the geometric phase of resonant states [16]. Later, we obtained the codimension of a degeneracy of an n-tuplet of resonances and also found the topology of the energy surfaces in parameter space close to a crossing of two resonances [17]. A numerical analysis of the 2+ doublet in 8Be allowed us to show, in a realistic example, that accidental degeneracies of two resonant states mixed by a Hermitian interaction give rise to one simple and one double pole of the scattering matrix in the complex energy plane, and that a true crossing may be brought about by the variation of only two real independent parameters [18]. In this paper we give a short review of some of our results, the reader is referred to the original papers for the demonstrations.

2. ACCIDENTAL DEGENERACY OF RESONANCES

Let us consider a highly excited atomic nucleus near an excitation energy \( E \), with \( n \) resonances and \( m \) open reaction channels in the given energy region. A general phenomenological expression for the \( S \)-matrix is [19]

\[
S(E) = U \left[ 1 - i W \{ E - H \}^{-1} W^\dagger \right] U^\dagger
\]

(1)

The \( n \times n \) complex matrix \( H \) plays the role of an effective non-Hermitian Hamiltonian in the internal space, \( H = H - i \frac{1}{2} W^\dagger W \). The Hermitian matrix \( H \) consists of the energy matrix of the levels and the shift functions. The \( m \times n \) matrix \( W \) is the matrix of the decay amplitudes. The unitarity of \( S \) is ensured by the form of the anti-Hermitian part of \( H \). When the system is driven by non-time reversal invariant interactions, \( H \) is, in general, non-symmetric, but when the interactions are time reversal invariant \( H \) is symmetric. If the mean spacing between resonances is small compared with the mean spacing between channel thresholds and \( E \) is far from any threshold, both matrices, \( H \) and \( W \), are smooth functions of the energy. In a small region in the complex energy plane the regular variation of these quantities with energy is negligible and they may be taken as constants. The poles of the \( S \)-matrix are the eigenvalues of the complex matrix \( H \), provided \( W \) does not vanish at that point.

Usually the description of a collision or reaction process is made in terms of well defined kinematic and dynamic laws, and a number of real, linearly independent "external" parameters whose numerical values are not given by the theory. Therefore, we may consider
the $S$-matrix embedded in a population of $S$-matrices smoothly parametrized by a set of $N$ external parameters which take values in some domain of a manifold or parameter space. To each point in this domain corresponds an $S-$matrix. This implies that, in the representation of (1), we may consider the matrix $H$ embedded in a population of complex matrices smoothly parametrized by a set of $N$ real external free parameters. When the numerical values of the external parameters change, the poles of $S(E)$ move in the complex energy plane.

An accidental degeneracy of $v$ resonances occurs when $v$ resonance poles of $S$ coincide, that is when $v$ ($v \geq 2$) eigenvalues of $H$ coincide. We may now ask: How many parameters must one vary, in general, to obtain a coincidence of $v$ resonance poles of $S$? It may be shown that this number is given in terms of the number $k$ and lengths $\ell_1(E^*) \geq \ell_2(E^*) \geq \ldots \geq \ell_k(E^*)$ of the cycles of generalized eigenvectors belonging to the $(v-1)$-fold repeated complex eigenvalue $E^*$ of $H$.

In effect, we have shown that the minimum number of real parameters that should be varied to bring about a coincidence of $v$ resonance poles of the $S$-matrix is

$$C_t = 2 \left\{ v - 1 + \sum_{s=1}^{k} (s - 1) \ell_s(E^*) \right\} \quad (2)$$

when the interactions are time reversal invariant, and

$$C_{nt} = 2 \left\{ v - 1 + 2 \sum_{s=1}^{k} (s - 1) \ell_s(E^*) \right\} \quad (3)$$

in the case of non time reversal invariant interactions. A detailed proof may be found in Mondragón and Hernández [17].

3. DEGENERACY OF TWO RESONANCES

If we are interested in the particular case of a degeneracy of two resonances, all other eigenvalues of $H$ being non-degenerate, we may suppose that we already know the correct eigenvectors of $H$ for all the complex eigenenergies except for the two the crossing of which we want to investigate. Using for these two, two vectors which are not eigenvectors but which are orthogonal to each other and to all other eigenvectors, we obtain a complete basis to represent $H$. In this basis $H$ will be diagonal except for a $2 \times 2$ non-diagonal block which may conveniently be written in terms of the Pauli matrices as

$$\mathcal{H} = \mathcal{E}1_{2 \times 2} + \left( \vec{R} - i \frac{1}{2} \vec{F} \right) \cdot \vec{\sigma} \quad (4)$$

$\vec{R}$ and $\vec{F}$ are real vectors with cartesian components $(X, Y, Z)$ and $(\Gamma_x, \Gamma_y, \Gamma_z)$ (when the system is driven by time reversal invariant interactions $Y$ and $\Gamma_z$ vanish). Therefore, the corresponding poles of the $S$-matrix are $E_{1,2} = \mathcal{E} \mp \epsilon$ with

$$\epsilon = \sqrt{\left( \vec{R} - i \frac{1}{2} \vec{F} \right)^2} \quad (5)$$
The condition for accidental degeneracy of the two resonances is \( \epsilon = 0 \). Since real and imaginary parts should vanish, we get

\[
R_d^2 - \frac{1}{4} \Gamma_d^2 = 0, \\
\bar{R}_d \cdot \bar{\Gamma}_d = 0.
\]

These equations admit two kinds of solutions depending on \( H_{2 \times 2} \) being or not being diagonal at the degeneracy. i) When both \( \bar{R}_d \) and \( \bar{\Gamma}_d \) vanish, Eqs. (6) and (7) define a point in parameter space. \( \mathbf{H} \) is diagonal at the degeneracy, its first Jordan block has two cycles of length one \( (k = 2, \ell_1 = \ell_2 = 1) \) all other Jordan blocks have one cycle of length one. In this case the two simple poles of \( S \) migrate to the real axis where they fuse into one real positive energy eigenvalue embedded in the continuum which is not a pole of the \( S \)-matrix. Hence from Eqs. (2) and (3): The minimum number of external parameters that should be varied to produce a degeneracy of two resonances into bound states embedded in the continuum (BIC) is four or six depending on the quantum system being or not being time reversal invariant.

ii) When Eqs. (6) and (7) are satisfied for non-vanishing \( \bar{R}_d \) and \( \bar{\Gamma}_d \) they define a circle in parameter space. \( \mathbf{H} \) is non-diagonal at the degeneracy, its first Jordan block has one cycle of length two \( (k = 1, \ell = 2) \), all other Jordan blocks have one cycle of length one. In this case the two poles of \( S \) which become degenerate fuse into one simple and one double poles at \( \mathcal{E} \). From these properties and Eqs. (2) and (3) it follows that: The minimum number of external parameters that should be varied to produce a degeneracy of two resonances leading to one simple and one double poles of the \( S \)-matrix is two independently of the time reversal invariant character of the interactions.

4. ENERGY SURFACES IN PARAMETER SPACE

In the absence of more specific information about the external parameters, we may parametrize \( \mathbf{H} \) and \( \mathbf{S} \) in terms of \( \bar{R} \) and \( \bar{\Gamma} \). In the case of a degeneracy of two resonances leading to one simple and one double pole of the \( S \) matrix, we may bring about the degeneracy varying only two parameters. Therefore, we may keep the matrix \( \mathbf{W} \) of the transition amplitudes constant, that is \( \bar{\Gamma} \) fixed, and let the parameters \( \bar{R} \) of the internal interaction vary. To simplify the notation we choose the \( OZ \) axis parallel to the fixed vector \( \bar{\Gamma} \).

Then, from Eq. (5), the real and imaginary parts of the energy difference \( \epsilon \) are given by

\[
X^2 + Y^2 - (\text{Re} \, \epsilon)^2 = \frac{1}{4} \Gamma^2, \quad \text{Im} \, \epsilon = 0,
\]

when \( R^2 \geq \frac{1}{4} \Gamma^2 \). When \( R^2 \leq \frac{1}{4} \Gamma^2 \),

\[
(\text{Re} \, \epsilon) = 0, \quad X^2 + Y^2 + (\text{Im} \, \epsilon)^2 = \frac{1}{4} \Gamma^2,
\]

It is apparent that close to the degeneracy the hypersurface which represents the complex energy in parameter space has two pieces: a) The surface representing the real part of the
5. LEVEL WIDTH ATTRACTION

The level repulsion theorem does not always hold for this kind of degeneracy of resonances. From (5), the distance between the interacting resonance poles in the complex energy plane is

\[ |\epsilon|^2 = \left[ \left( R^2 - \frac{1}{4} \Gamma^2 \right)^2 + (\vec{R} \cdot \vec{\Gamma})^2 \right]^{\frac{1}{2}}. \]  

The first term under the square root is the difference of two positive quantities. Therefore it is not always an increasing function of the strength \( R^2 \) of the mixing interaction. If \( R^2 < \frac{1}{4} \Gamma^2 \) and \( (\vec{R} \cdot \vec{\Gamma})^2 \ll R^2 \Gamma^2 \), the distance \(|\epsilon|\) between the two interacting poles in the complex energy plane decreases when \( R^2 \) increases. This is to be contrasted with the well known level repulsion phenomenon observed in the case of bound state mixing, in which case the absolute value of the difference of the energies always increases when the strength \( R^2 \) of the mixing interaction increases. Hernández and Mondragón [18] have made a numerical analysis of the \( 2^+ \) doublet in \(^{18}\text{Be} \) where this and other properties of a second rank degeneracy of resonances are made explicit.

6. RESONANCE SPACING DISTRIBUTION IN THE ENERGY SPECTRA OF EXCITED NUCLEI

The statistical distribution of energy level spacings \( P(s) \) was introduced by Wigner [5] who investigated the spacings of the real eigenvalues of a large Hermitian Hamiltonian matrix with random coefficients. Here, we will try to extend Wigner’s reasoning to resonances. The statistical distribution of spacings, \( P(s) \, ds \), is defined as the probability that the spacing of a randomly chosen pair of neighbouring resonances will be between \( s \) and \( s + ds \), where the distance \( s \) between resonances is measured as a fraction of the mean resonance spacing \([d(E)]^{-1}\) at the energy considered. Then

\[ P(s) = \delta \left( s - s_n (X,Y,Z) \right), \]  

the bar means energy average. For small \( s \) the only contributions to the energy average come from spacings \( s_n \) for which the point \((X,Y,Z)\) is very close to those points...
\((X^*, Y^*, Z^*)\) in parameter space for which there is a resonance degeneracy. The corresponding \(s_n\) takes the form (10). Now, we will assume that there is nothing special about the system with parameters \((X, Y, Z)\), and that the positions of accidental degeneracies of resonances are randomly distributed in parameter space. Hence, we may replace the energy average by an ensemble average over the matrix elements of \(H\) in a region in parameter space containing the point \((\hat{R}, \hat{\Gamma})\), with probability density \(P(H)\) given by

\[
P(H) = N e^{-\alpha \text{tr}(H^*H)}
\]

(12)

Then, we must evaluate the integral

\[
P(s) = N \int d^3 \Gamma \int d^3 R e^{-\alpha(R^2 + \frac{1}{4} \Gamma^2)} \delta \left( s - \left[ (R^2 - \frac{1}{4} \Gamma^2)^2 + R^2 \Gamma^2 \cos^2 \omega \right]^{\frac{1}{2}} \right)
\]

(13)

for the two kinds of resonance degeneracies with the appropriate constraints to each case. For a degeneracy resulting in bound states embedded in the continuum \(R = s \rho\) and \(\Gamma = s \gamma\) with \(\rho\) and \(\gamma\) independent of \(s\). For a double plus simple pole degeneracy, \(\cos \omega = 0\). The results are shown in the following table,

<table>
<thead>
<tr>
<th>Type of degeneracy</th>
<th>T-invariant character</th>
<th>Codimension of degeneracy</th>
<th>(P(s))</th>
<th>Small separation behaviour of (P(s))</th>
</tr>
</thead>
<tbody>
<tr>
<td>BIC</td>
<td>T-invariant</td>
<td>4</td>
<td>(2 \alpha^2 s^3 K_0(\alpha s^2))</td>
<td>(s^2(-s \ln s))</td>
</tr>
<tr>
<td>BIC</td>
<td>non T-invariant</td>
<td>6</td>
<td>(\alpha^2 s^3 e^{-\alpha s^2})</td>
<td>(s^3)</td>
</tr>
<tr>
<td>Simple plus</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Double pole</td>
<td>T-invariant</td>
<td>2</td>
<td>(2 \alpha s e^{-\alpha s^2})</td>
<td>(s)</td>
</tr>
<tr>
<td>Simple plus</td>
<td>non T-invariant</td>
<td>2</td>
<td>(\frac{4}{5} \alpha^2 s^3 K_1(\alpha s^2))</td>
<td>(s)</td>
</tr>
</tbody>
</table>

In the case of degeneracies leading to one simple and one double poles in the \(S\)-matrix, when the interactions are time reversal invariant the distribution of resonance spacings \(P(s)\) is the same as that calculated from the gaussian orthogonal ensemble (GOE) for bound state level spacings. When the interactions are non-time reversal invariant, for large values of \(s\) our result resembles the spacings distribution obtained from the gaussian unitary ensemble (GUE).

In the case of degeneracies into bound states embedded in the continuum we get a stronger level repulsion which is cubic for non-time reversal invariant interactions, while it goes like \(s^2(-\ln s)\) for time reversal invariant interactions.
7. Topological Phase of a Resonant State

We have seen that the topology of the energy surfaces in the vicinity of a resonance degeneracy differs significantly from the corresponding one of a bound state degeneracy. This difference is reflected in the properties of the geometric phase of the corresponding states. In order to make this difference explicit, we have investigated the adiabatic time evolution of a nuclear state which is a superposition of resonant states and evolves irreversibly due to the spontaneous decay of the unstable states [16]. To have a concrete example in mind, although a very hypothetical one, we may think of the $^8$Be nucleus, which has only unstable energy eigenstates, moving in the field of a heavy doubly magic nucleus, like $^{208}$Pb, in a peripheral collision in which the separation of both nuclei is never smaller than the sum of the nuclear radii. In a semiclassical treatment of the collision the time evolution of the system is governed by a Hamiltonian $H$ which is the sum of a time independent part $H_0$ describing the evolution of the system of unperturbed nuclei plus a time dependent perturbation term $H_1$, parametrized in terms of a set of slow variables $\{X(t), Y(t), Z(t), \ldots\}$. Let us further assume that the system has a pair of unstable states close in energy which are strongly mixed by the interaction $H_1(t)$. In our hypothetical example these could be the two $2^+$ states of $^8$Be with $T = 0, 1$ at $E_0 = 16.7$ MeV and $E_1 = 16.9$ MeV Hernández and Mondragón [18] have shown that the actual physical $2^+$ doublet is close to an accidental degeneracy of resonances to which it is continuously connected by a small variation in the Hermitian mixing interaction.

There seems to be some incompatibility between adiabaticity, that is slow motion, and the relaxation of the system, i.e. vanishing of the signal. It may be shown [16] that if $T$ is some typical time of the driving Hamiltonian, such that

$$\left| \langle \dot{\phi}_s \left| \frac{dH_1}{dt} \right| \phi_m \rangle \right| \simeq \frac{1}{T} \left| \langle \dot{\phi}_s | H_1 | \phi_m \rangle \right|$$

(14)

where $\phi_s$ and $\phi_m$ are two adiabatic eigenstates of the energy, $T$ should not be so long that the signal cannot be measured. Hence, it is reasonable to estimate $T$ from $\Gamma_{\text{max}}$, the largest half width of the two resonances. Therefore, a rough criterion for the validity of the adiabatic approximation for unstable states would be

$$\max \left\{ \left| \langle \phi_s | H_1 | \phi_m \rangle \right| \right\} \frac{\Gamma_{\text{max}}}{(\Delta E)^2} \ll 1$$

(15)

where $\max \left\{ \left| \langle \phi_s | H_1 | \phi_m \rangle \right| \right\}$ indicates the maximum value along the path traced by the system in parameter space.

Assuming that in the course of the time evolution the system makes an excursion in parameter space around the diabolical circle, it acquires a Berry phase given by

$$\gamma = \frac{1}{2} \int_{\Sigma} \int_{\partial \Sigma} \frac{\langle \dot{R} - i\frac{1}{2} \Gamma \rangle \cdot d\Sigma}{R^3}$$

(16)

with $R = \sqrt{(\dot{R} - i\frac{1}{2} \Gamma)^2}$, $d\Sigma$ is the surface element normal to $\Sigma$. 
The expression (16) we have found for $\gamma$ is formally identical to Berry’s result [4]. However there are some important differences:

I) The Berry phase is now complex. This means that, in the adiabatic evolution of the system, besides the change in phase and magnitude of dynamic origin, the wave function of the unstable system suffers a change in phase and magnitude of purely geometric origin.

II) The condition $R = 0$, which defines the singularity in parameter space, is satisfied when the degeneracy conditions, Eqs. (6) and (7) are satisfied. Hence, in this case the singularity is not a point singularity but the extended singularity we have called the diabolical circle. We might say that instead of the “monopole” singularity occurring in the accidental degeneracy of bound states, we have a “string” singularity in the accidental degeneracy of resonances. A detailed discussion of the Berry phase of a resonant state may be found in Mondragón and Hernández [16].

8. Conclusions

We have shown that accidental degeneracies of resonant and bound states differ essentially in some of their mathematical properties such as the codimension of the degeneracy, the singularities of the $S$ matrix associated to them, the topology of the energy surfaces close to the level crossing and others. These differences are reflected in observable differences in some physical properties of the system under study, such as the geometric phase of the state, the phenomenon of level width attraction and the distribution of level spacings in the energy spectrum. Level width attraction in a system with two resonant states mixed by a Hermitian interaction was seen in the calculation of Friedrich and Wintgen [12] and in the phenological analysis of the $2^+$ doublet in $^8$Be made by von Brentano [13] and Hernández and Mondragón [18]. We compared the distribution of resonant spacings for non-time reversal invariant interactions shown in the table and the numerical computation of the distribution of resonance spacings of an excited hydrogen atom in crossed external electric and magnetic fields made by Hegerfeldt and Henneberg [20], and a very good agreement was found.

References