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Crossing and anticrossing of energies and widths for unbound levels

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Abstract

The crossing and anticrossing properties of the energies and widths of two unbound levels under the influence of a symmetrical complex interaction are investigated. It is found that a sufficiently large variation of the difference of the ‘‘unperturbed’’ energies or of the widths leads always to a crossing of either the energies or the widths of the ‘‘perturbed’’ system. A particularly interesting result is that for a real off diagonal interaction there is a joint crossing of the ‘‘unperturbed’’ energies and of either the ‘‘perturbed’’ energies or the ‘‘perturbed’’ widths. © 1999 Elsevier Science B.V. All rights reserved.

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The two level system is a fruitful tool in physics and has many applications [1–5]. One usually considers, the properties of a system of two bound states. It is of interest to extend this study from bound states to unbound states [6–15]. Interesting examples of unbound two level systems are e.g.:

1. The $I^{\pi}=2^{+}$, $T=1$, $T=0$ doublet in ^{8}Be [16,17].
2. The ρ–ω $T=1$, $T=0$ doublet of mesons [9,18,19].
3. Doublets of resonance’s in cavities [20].

This paper discusses the crossing and anticrossing of energies and widths of the two level system for unbound levels. For the system of two bound states it is known that the difference $\Delta E = E_1 - E_2$ of the energies E_1 and E_2 can not vanish if the off diagonal matrix element of the interaction does not vanish [1–6]. In short: the energies of two bound states, anticross for a non vanishing offdiagonal interaction: $\nu \neq 0$. This statement is a special case of a theorem of Wigner and von Neumann [1].

In the present paper the crossing and anticrossing of unbound levels is studied. The energy ε of an unbound level is in general a complex number:

$$\varepsilon = E - \mathrm{i}/2\,\Gamma \tag{1}$$

Here $E = \mathrm{Re}\ \varepsilon$ is the real energy and $\Gamma = -2\ \mathrm{Im}\ \varepsilon$ is the width of the unbound state. The complex

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energy difference $\varepsilon_1 - \varepsilon_2$ of two unbound states is thus also in general a complex number

$$\varepsilon_1 - \varepsilon_2 = \Delta E - \mathrm{i}/2\,\Delta\Gamma \tag{2}$$

There are different possible cases of crossing and of anticrossing in the unbound two level system depending on the vanishing or non vanishing of the real part ΔE or of the imaginary part $-1/2\Delta\Gamma$ of the complex energy difference $\varepsilon_1 - \varepsilon_2$.

We mention that there have been several works in which the concept of energy repulsion and width attraction was discussed for a system of two unbound states [6–12,17]. This problem is related to but different from the crossing and anticrossing relation which will be discussed here. Furthermore the crossing and anticrossing relations are derived here for the general case of a 2×2 matrix with a symmetrical complex off diagonal interaction whereas the energy repulsion width attraction relations were derived previously only for an off diagonal interaction which was either real or purely imaginary.

Before the crossing problem is discussed in detail, the meaning of the effective Hamiltonian for unbound states will be clarified. A proper description of the unbound system is done in the frame of an $\boldsymbol{S}$-matrix. We can define an effective Hamiltonian $\boldsymbol{H}$ from the propagator of the $\boldsymbol{S}$-matrix. A convenient form of an unitary $\boldsymbol{S}$-matrix which exhibits the propagator has been given by Mahaux and Weidenmüller in their book [21] and was also used by other authors e.g.: [13–15,22–25]. Time reversal invariance is assumed and therefore the $\boldsymbol{S}$-matrix is symmetric. For a system with two unbound states this leads to the following representation of the $\boldsymbol{S}$-matrix [21]:

$$\boldsymbol{S}(E) = \boldsymbol{U}\left\{1 - \mathrm{i}\boldsymbol{W}\left[\boldsymbol{D}^{-1}(E)\right]\boldsymbol{W}^{t}\right\}\boldsymbol{U}^{+}, \tag{3}$$

$$\begin{aligned}\boldsymbol{D}(E)_{nm} &= E\boldsymbol{\delta}_{nm} - \boldsymbol{H}_{nm}\\ &= E\boldsymbol{\delta}_{nm} - \boldsymbol{h}_{nm} + 1/2\mathrm{i}(\boldsymbol{W}^{t}\boldsymbol{W})_{nm},\end{aligned} \tag{4}$$

with

$$\boldsymbol{h}^{*}_{nm} = \boldsymbol{h}_{nm}, \boldsymbol{W}_{cn} = \boldsymbol{W}^{*}_{cn} \text{ and } n,m \in [1,2] \tag{5}$$

Here $\boldsymbol{W}_{cn}$ is the $M\times 2$ matrix of the decay amplitudes which couple the M channels to the 2 levels. U is a unitary matrix, which describes the background. From time reversal invariance one obtains further that the width matrix $\boldsymbol{\Gamma}_{nm} = (\boldsymbol{W}^{t}\boldsymbol{W})_{nm}$ and the energy matrix $\boldsymbol{h}_{nm}$ are real and symmetric 2×2 matrices. The width matrix $\boldsymbol{\Gamma} = \boldsymbol{W}^{t}\boldsymbol{W}$ is a positive semidefinite matrix. Combining the energy matrix $\boldsymbol{h}_{nm}$ with the width matrix $\boldsymbol{\Gamma}_{nm}$ one obtains the effective Hamiltonian matrix: $\boldsymbol{H} = h - \mathrm{i}/2\ \boldsymbol{\Gamma}$.

One can write the effective symmetric Hamiltonian $\boldsymbol{H}$ in the form of Eq. (6).

$$\begin{aligned}\boldsymbol{H} &= \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22}\end{pmatrix}\\ &= \begin{pmatrix} E^0_1 - \mathrm{i}/2\,\Gamma^0_1 & \nu - \mathrm{i}/2\,\omega \\ \nu - \mathrm{i}/2\,\omega & \Delta E^0_1 - \mathrm{i}/2\,\Gamma^0_1\end{pmatrix}\end{aligned} \tag{6}$$

It is further assumed for simplicity that the effective Hamiltonian $\boldsymbol{H}$ is energy independent. This is a reasonable assumption far from thresholds.

This form allows the standard decomposition of $\boldsymbol{H}$ into an ''unperturbed'' effective Hamiltonian $\boldsymbol{H}^0$ and a complex off diagonal interaction V:

$$\boldsymbol{H}^0 = \begin{pmatrix} \varepsilon_{01} & 0 \\ 0 & \varepsilon_{02}\end{pmatrix} = \begin{pmatrix} 0 & \nu - \mathrm{i}/2\,\omega \\ \nu - \mathrm{i}/2\,\omega & 0\end{pmatrix} \tag{7}$$

The special form $\nu - \mathrm{i}/2\ \ \omega$ of writing the off diagonal complex interaction matrix element is used in order to simplify the relations below. The poles ε_1 and ε_2 of the $\boldsymbol{S}$-matrix are identical with the complex eigenenergies of the effective Hamiltonian and are given by the solutions of Eq. (8):

$$\det(\varepsilon\boldsymbol{\delta}_{nm} - \boldsymbol{H}_{nm}) = 0 \tag{8}$$

from which the well-known expressions for the complex energies of the two level system are obtained [1–6]:

$$\begin{aligned}\varepsilon_{1,2} &= 1/2(H_{11} + H_{22})\\ &\pm 1/2\left[(H_{11} - H_{22})^2 + 4H_{12}H_{21}\right]^{1/2}\end{aligned} \tag{9}$$

From Eq. (9) one obtains the square of the difference of the complex energies $(\varepsilon_1 - \varepsilon_2)^2$:

$$(\varepsilon_1 - \varepsilon_2)^2 = (\varepsilon_1^0 - \varepsilon_2^0)^2 + 4(\nu - \mathrm{i}/2\,\omega)^2 = A - \mathrm{i}B \tag{10}$$

In order to discuss Eq. (10) it is useful to consider the differences of the energies ΔE and of the widths $\Delta\Gamma$ of the two ''perturbed'' states and of ΔE^0 and $\Delta\Gamma^0$ of the ''unperturbed'' states. By decomposing Eq. (10) into its real part: A and its imaginary part: $-B$ one obtains Eqs. (11a) and (11b):

$$(\Delta E)^2 - 1/4(\Delta\Gamma)^2 = (\Delta E^0)^2 - 1/4(\Delta\Gamma^0)^2 + 4(\nu^2 - 1/4\omega^2) = A \tag{11a}$$

$$(\Delta E \Delta\Gamma) = (\Delta E^0 \Delta\Gamma^0) + 4\nu\omega = B \tag{11b}$$

These equations are the basis of the following discussions of the crossing and anticrossing of the levels. One notes that the functional dependence of the quantities A and B on the parameters of the Hamiltonian H of Eqs. (2) and (6) are given by Eqs. (11a) and (11b).

To begin the discussion we first consider the full complex energy crossing i.e. the case: $\varepsilon_1 = \varepsilon_2$. One finds the Eq. (12):

$$\varepsilon_1 = \varepsilon_2 \Leftrightarrow A = 0 \text{ and } B = 0 \tag{12}$$

Eq. (12) gives the conditions for full complex energy crossing. Such crossing is possible in the case of unbound levels also for a nonvanishing interaction $\nu - \mathrm{i}/2\,\omega \neq 0$. This was noted before [8–12]. The reason is, that a complex symmetrical 2×2 matrix has more parameters than the real symmetrical 2×2 matrix and these many parameters make it possible to fulfil the two relations $A = 0$ and $B = 0$ also for a non vanishing off diagonal interaction. The complex energy crossing has been discussed in great detail by Mondragón and Hernández [11].

We now discuss the partial crossing which is particularly interesting for the unbound system. Namely we consider that either the energy difference ΔE, or the width difference $\Delta\Gamma$ vanish. One finds in both cases that the parameter B must vanish. One obtains Eq. (13):

$$B = 0 \Leftrightarrow (\Delta E \Delta\Gamma) = 0 \Leftrightarrow \Delta E = 0 \text{ or } \Delta\Gamma = 0 \tag{13}$$

Eq. (13) contains the logical ''or'', which includes of course the possibility that ΔE and $\Delta\Gamma$ vanish simultaneously as was discussed above. Eq. (13) is a crossing anticrossing relation. One finds further that the sign of A specifies whether there is energy crossing ($\Delta E = 0$) or width crossing ($\Delta\Gamma = 0$) as is shown in Eqs. (14a) and (14b):

$$A > 0 \text{ and } B = 0 \Leftrightarrow \Delta E \neq 0 \text{ and } \Delta\Gamma = 0 \tag{14a}$$

$$A < 0 \text{ and } B = 0 \Leftrightarrow \Delta E = 0 \text{ and } \Delta\Gamma \neq 0 \tag{14b}$$

Relation (14a) is interesting. It states that for $B = 0$ energy anticrossing implies width crossing. For bound states the relation is trivial because the widths vanish everywhere. The relation is nontrivial for unbound states, however. Eq. (11b) implies that by varying ΔE^0 or $\Delta\Gamma^0$ in a sufficiently large range while keeping the other parameters of H constant one can make $B = 0$. Thus in cases where ΔE^0 or $\Delta\Gamma^0$ can be varied in the experiment in a sufficiently large range one finds either energy or width crossing. The width crossing relation is a rather general, somewhat surprising and interesting result. The conditions under which it holds can be realized in experiments.

Particularly simple and strong results are obtained for a special off diagonal interaction for which $\nu\omega = 0$. That is for either a real or a purely imaginary off diagonal interaction. One finds:

$$\nu\omega = 0 \text{ and } B = 0 \Leftrightarrow (\Delta E \Delta\Gamma) = (\Delta E^0 \Delta\Gamma^0) = 0 \tag{15}$$

Thus for this special interaction the ''perturbed'' widths or energies will cross at the crossing point of the ''unperturbed'' widths or energies. The question whether the ''perturbed'' widths or energies cross depends again on the sign of A as is shown in Eqs. (11a) and (11b). One finds Eqs. (16a) and (16b):

$$|2\nu| > |1/2\,\Delta\Gamma^0| \text{ and } \Delta E^0 = 0 \text{ and } \omega = 0$$
$$\Rightarrow \Delta\Gamma = 0 \text{ and } \frac{\partial \Delta E}{\partial \Delta E^0} \text{ and } \Delta E \neq 0 \tag{16a}$$

$$|2\nu| < |1/2\,\Delta\Gamma^0| \text{ and } \Delta E^0 = 0 \text{ and } \omega = 0$$
$$\Rightarrow \Delta E = 0 \text{ and } \frac{\partial \Delta\Gamma}{\partial \Delta E^0} \text{ and } \Delta\Gamma \neq 0 \tag{16b}$$

In Eqs. (16a) and (16b) all quantities of the ''perturbed'' system as e.g. ΔE, $\Delta\Gamma$, treated as functions of the parameter ΔE_0 are to be taken at the value $\Delta E^0 = 0$. One can also obtain corresponding relations for a variation of the parameter $\Delta\Gamma_0$. The derivatives $\partial\Delta E/\partial\Delta E^0$ and $\partial\Delta\Gamma/\partial\Delta E^0$ in Eqs. (16a) and (16b) are obtained from Eqs. (11a) and (11b) by keeping all parameters $(\Delta\Gamma_0,\nu,\omega)$ constant except ΔE_0.The relation (16a) implies that for a sufficiently large real interaction with $|2\nu| > |1/2\ \ \Delta\Gamma^0|$ the three quantities ΔE^0, $\Delta\Gamma$ and $\partial\Delta\Gamma/\partial\Delta E^0$ will vanish jointly wheras ΔE does not vanish for $\Delta E^0 = 0$.

Eq. (16b) gives the conditions for a joint vanishing of the three quantities ΔE_0, ΔE and $\partial\Delta\Gamma/\partial\Delta E^0$ whereas $\Delta\Gamma$ does not vanish for $\Delta E^0 = 0$. One notes that Eq. (16a) is well known for boundstates. It shows that the difference of the energies $(\Delta E) = (E_1 - E_2)$ of the two states has an extremal value at the crossing point of the ''unperturbed'' energies ($\Delta E^0 = 0$).

It should be stressed that the joint crossing of the three quantities is found for purely real or imaginary interactions. For a general complex interaction the three quantities will not vanish jointly in general.

It is useful to derive the width crossing relation directly in a simple model. The electromagnetic decay of a system of two interacting bound states ψ_1 and ψ_2 to the groundstate $\psi_{\rm g}$ is considered in perturbation theory. The system is described by the Hamiltonian of Eq. (6) with $\omega = 0$ and vanishing ''unperturbed'' widths: $\Gamma_0^1 = \Gamma_2^0 = 0$. One assumes that the two states ψ_1, ψ_2 decay by electromagnetic E2-transitions to the ''unperturbed'' groundstate $|\psi_{\rm g}^0\rangle = |\psi_{\rm g}\rangle$. Thus one obtains the transition decay widths $\Gamma_1^{\rm t}$ and $\Gamma_2^{\rm t}$ in perturbation theory by Eq. (17):

$$\Gamma_{1g}^t = |\langle\psi_g^0|E2|\psi_1\rangle|^2 a^2\,, \quad \Gamma_{2g}^t = |\langle\psi_g^0|E2|\psi_2\rangle|^2 a^2 \tag{17}$$

where a is a constant. We use the same relations also for the unperturbed case. One assumes in this model for simplicity that in the ''unperturbed'' system H^0 there is only one nonvanishing transition width $\Gamma_{1g}^{t0} \neq 0$, $\Gamma_{2g}^{t0} = 0$. With these assumptions one can calculate the difference of the widths: $\Delta\Gamma^{\rm t} = \left(\Gamma_{1g}^t - \Gamma_{2g}^t\right)$ as a function of the parameters ΔE^0 and ν. $\Delta\Gamma^{\rm t}$ is directly related to the difference of the amplitudes α^2 and β^2 of the expansion of the ''perturbed'' states into the ''unperturbed'' states which is given in Eq. (18):

$$\psi_1 = \alpha\psi_1^0 + \beta\psi_2^0, \quad \psi_2 = -\beta\psi_1^0 + \alpha\psi_2^0 \tag{18}$$

One finds $\Delta\Gamma^{\,t} = (\alpha^2 - \beta^2)$. This shows the origin of width crossing. Namely the amplitudes α^2 and β^2 cross at the parameter value $\Delta E^0 = 0$.

This model gives an intuitive explanation for width crossing in terms of a complete mixing of the two states. This model is valid of course only for very small widths, when perturbation theory applies. We do not know a similarly intuitive explanation for energy crossing.

Summing up the anticrossing relation for the energies in a system of two bound states is extended to crossing–anticrossing relations for the energies and widths of a system of two unbound states. Since the energies of the unbound states are complex numbers there is a rich physical scenario for crossing and anticrossing of the real or imaginary parts of the complex energies.

A particularly interesting result is that in a system of two unbound states with an off diagonal interaction there is a value of the difference of the real ''unperturbed'' energies ΔE_0 for which the ''perturbed'' energies or the ''perturbed'' widths cross. An even stronger result is obtained for a sufficiently strong real interaction. For such an interaction one finds that the three quantities ΔE^0, $\Delta\Gamma$ and $\partial\Delta E/\partial\Delta E^0$ will vanish jointly.

This is a rather general result because the conditions for which it holds are rather weak and can be realized in experiments.

Finally we give an experimental example for which the scenario of joint ''unperturbed'' energy crossing: $\Delta E^0 = 0$ and ''perturbed'' width crossing: $\Delta\Gamma = 0$ is at least approximately fullfilled. This example is the famous doublet of $I^\pi = 2^+$ $T = 0$ and $T = 1$ resonances in ^{8}Be. These resonances were studied both in experiment and in analysis in great detail, e.g. by Hinterberger et.al. [16]. They have become one of the most completely studied examples of resonance doublets in nuclear physics (see also references in [16]). We follow here an analysis [17] which used the same form of the *S*-matrix as is used in the present paper.

The parameters ε_1, ε_2 and ε_1^0, ε_2^0 and ν obtained for the ^{8}Be doublet in Ref. [17] are:

$$\varepsilon_1 = (16722 - \mathrm{i}/2 \cdot 108)\,\mathrm{keV}$$

$$\varepsilon_2 = (17010 - \mathrm{i}/2 \cdot 74)\,\mathrm{keV}$$

$$\varepsilon_1^0 = (16838 - \mathrm{i}/2 \cdot 182)\,\mathrm{keV}$$

$$\varepsilon_2^0 = 16893\,\mathrm{keV}$$

$$\nu = 148\,\mathrm{keV}$$

From these parameters one can find the parameters $\Delta\varepsilon$, $\Delta\varepsilon^0$ and ν. One finds:

$$\Delta\varepsilon^0 = (-55 - \mathrm{i}/2 \cdot 182)\,\mathrm{keV}$$

$$\Delta\varepsilon = (-288 - \mathrm{i}/2 \cdot 35)\,\mathrm{keV}$$

As the interaction $\nu = 148$ keV is real, Eq. (15) holds. This is indeed true: $\cong$ $288 \times 35 = 55 \times 182$. We note that although both ΔE_0 and $\Delta\Gamma$ both do not vanish they are both rather small compared to $|\Delta E|$ and $|\Delta\Gamma_0|$ respectively:

$$|\Delta E_0| = 55\,\mathrm{keV} \ll 288\,\mathrm{keV} = \Delta E$$

$$\text{and } |\Delta\Gamma| = 35\,\mathrm{keV} \ll 182\,\mathrm{keV} = |\Delta\Gamma_0|$$

Thus although there is no true ''perturbed'' width crossing in ^{8}Be the system is near to such a crossing. We also note that the interaction $|\nu|$ is large: $|2\nu| = 298$ keV > 91 keV $= |1/2\ \Delta\Gamma_0|$ and thus Eq. (16a) implies near ''perturbed'' width crossing as found in the experiment. The two resonances in ^{8}Be have also been used as an example of a near complex energy crossing [12].

Other applications may be found in atomic physics or in microwave cavities. One can consider e.g. that the energies of an atom are changed by a magnetic field or one can consider a set of nearly identical coupled microwave cavities in which the energies widths and the interaction ν of the individual cavities can be separately varied [20,26].

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