

*Dedicated to academician Margareta Giurgea
on her 90th anniversary*

CONFIGURATION MIXING ACCORDING TO LEVEL MATRIX

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This work does approach the Configuration Mixing in terms of Multilevel Matrix Formalism, previously developed for description of Nuclear Reactions. It is proved that, in addition to multilevel couplings, there are also another sources of mixing as Boundary Conditions effects and coupling of Scattering States. The effect of the levels' spectroscopic factors on Configuration Mixing is discussed.

1. INTRODUCTION

The problem of Configurations Mixing is subject of interest in different fields of Quantum Physics as, Nuclear Physics, Molecular Physics, Quantum Optics. Examples of Configuration Mixing were found in Nuclear Structure, [1], Atomic Collisions, [2], Optical Atoms, [3].

The usual treatments of this problem are either perturbative or numerical; for strong mixing an exact treatment, usual numerical, must be used. According to numerical procedures, the problem is solved in two steps, [4]. In first step the mixing terms are ignored; two independent basis sets are constructed, each for corresponding system. The basis for the whole system is direct sum of the basis for the two 'bare' configurations. The complete Hamiltonian, including the mutual interaction, is diagonalized in the whole basis. The numerical calculations prove that for perturbative interactions the levels are displaced and an eventual degeneracy is lifted. If the configuration mixing parameter is large enough, the levels of the two configurations are strongly mixed and an eigenstate from a given configuration could intrude in spectrum of other one; this phenomenon is called "Intruder State", [5].

In this paper one proves that the Configuration Mixing could be treated in terms of Multilevel Matrix formalism, developed in the Theory of Nuclear Reactions, [6]. In addition to an alternative description of Configuration Mixing, one obtains new physical insights. One proves there are at least two additional sources

of mixing *ie* the effect of Boundary Conditions and the coupling to Scattering States. The primary source of mixing is same as in usual Bound-State calculations, *ie* level-level interactions. It is proved that Boundary Conditions result into a level displacement which depends on spectroscopical factors of the involved levels. This result is not yet mentioned in Nuclear Structure Physics; perhaps it is implicitly obtained in numerical calculations. The coupling of unbound Scattering States to bound states of Configuration could be also significant but perhaps only for near-zero energy bound states.

2. ON TWO LEVELS SYSTEMS

The Configuration Mixing's prototype is the Two-Levels Mixing [7,8]. We expose the usual approach for Two-Levels Mixing in order to evince some mechanisms of the Configuration Mixing.

Let start with the mixing of two independent levels $|\Phi_1\rangle$ and $|\Phi_2\rangle$ which are eigenstates of the Hamiltonians, H_{11}^0 and H_{22}^0 , for the two "configurations" 1 and 2. By mixing the two configurations through "residual" interaction H' , the Hamiltonian becomes $H = H_0 + H'$ with matrix elements $H_{11}, H_{12}, H_{21}, H_{22}$. The eigenvalues resulting from mixing are

$$E_1 = 1/2(H_{11} + H_{22}) - 1/2[(H_{22} - H_{11})^2 + 4 H_{12}^2]^{1/2}$$

$$E_2 = 1/2(H_{11} + H_{22}) + 1/2[(H_{22} - H_{11})^2 + 4 H_{12}^2]^{1/2}$$

One defines a mixing angle α , [7],

$$\sin \alpha = -H_{21} / [(H_{22} - E_1)^2 + 4 H_{12}^2]^{1/2}$$

$$\cos \alpha = + (H_{22} - E_1) / [(H_{22} - E_1)^2 + 4 H_{12}^2]^{1/2}$$

The two mixed eigenstates, $|\psi_1\rangle$ and $|\psi_2\rangle$, are obtained (up to an overall sign) by an orthogonal transformation

$$|\psi_1\rangle = \cos \alpha |\Phi_1\rangle + \sin \alpha |\Phi_2\rangle$$

$$|\psi_2\rangle = \cos \alpha |\Phi_2\rangle - \sin \alpha |\Phi_1\rangle$$

In order to approach the problem of intruder states, one defines the projection operators $P = |\Phi_1\rangle\langle\Phi_1|$ and $Q = |\Phi_2\rangle\langle\Phi_2|$, resulting into

$$P|\psi_1\rangle = \cos \alpha |\Phi_1\rangle, Q|\psi_1\rangle = \sin \alpha |\Phi_2\rangle$$

$$Q|\psi_2\rangle = \cos \alpha |\Phi_2\rangle, P|\psi_2\rangle = -\sin \alpha |\Phi_1\rangle$$

In the limit $\alpha \rightarrow 0$, the two states become uncoupled

$$P|\psi_1\rangle = \cos \alpha |\Phi_1\rangle \rightarrow |\Phi_1\rangle, Q|\psi_2\rangle = \cos \alpha |\Phi_2\rangle \rightarrow |\Phi_2\rangle$$

In the limit $\alpha \rightarrow \pi/2$, one obtains the intruder phenomenon

$$Q|\psi_1\rangle = \sin \alpha |\Phi_2\rangle \rightarrow |\Phi_2\rangle, P|\psi_2\rangle = -\sin \alpha |\Phi_1\rangle \rightarrow -|\Phi_1\rangle$$

In this limit the state $|\Phi_2\rangle$ intrudes the space $|1\rangle$ and the state $|\Phi_1\rangle$ becomes intruder in the space $|2\rangle$.

The energy difference of the two mixed states is larger than energy difference of the two unmixed states

$$E_2 - E_1 = [(H_{22} - H_{11})^2 + 4 H_{12}^2]^{1/2} > |H_{22} - H_{11}|$$

This relation is known as “Level Repulsion” phenomenon and it is a special case of the Non-Crossing Theorem of Wigner and von Neumann. However, if the mixing term is a complex quantity, the crossing of eigenvalues is possible [5].

During recent times the non-crossing problem has been approached for resonant levels too, [9,10]. In Brentano’s approach one evaluates the Scattering Matrix in terms of the Effective Hamiltonian, which is split into an unperturbed diagonal Hamiltonian and a pure off-diagonal interaction. If the pure off-diagonal mixing matrix is hermitian (“internal mixing”) then the (real) energies of two levels repel each other and their imaginary widths attract each other. For a pure imaginary mixing matrix (“external mixing”) the above results are interchanged: a crossing of the real parts of energies and the corresponding imaginary parts (resonances’ widths) avoid each other. These results were obtained for two resonant levels in a single channel system.

The Configuration Mixing, either for bound or unbound levels, is usually approached in terms of Effective Hamiltonian; this effective operator is acting only on retained levels but by taking into account the eliminated ones via Effective Interactions. The coupling of retained states to the (eliminated) scattering states is either simulated or disregarded. Moreover, it is difficult to study, in terms of Effective Hamiltonian, the implication of Boundary Conditions; an appropriate frame could be done in terms of Reaction Operators (R-Matrix, K-Matrix, Level-Matrix, etc) [11].

3. CONFIGURATION MIXING ACCORDING TO LEVEL-MATRIX

The problem of two levels mixing could be incorporated into Level-Matrix Formalism of Quantum Scattering, [6]. The Level-Matrix does contain both specific level parameters (energies, spectroscopic factors, decay widths, non-diagonal coupling terms) as well as Boundary Conditions terms and “Background” Scattering Matrix originating in distant (eliminated) levels. By this approach one takes into account, at least in principle, the eliminated distant levels and also multichannel effects. (One has to recall that the unbound two-level system was studied only for one channel.) An Unitarity Separation of Background effects on retained Multilevel system can be developed, [12].

The Scattering or Collision Matrix, up to (diagonal) coulombian and hard-sphere phase-shifts, is parametrized in terms of R-Matrix and of (channels) L-Logarithmic Derivative Matrix, [6],

$$U = 1 + 2iP^{1/2} (R^{-1} - L)^{-1} P^{1/2}$$

The Logarithmic Derivative Matrix, $L = S + iP$, is related to external (out of channel radius) part of configuration space (*ie* reaction channels). Its real and imaginary components, S and P , are respectively referred as Shift-and Penetration-Factors. The inner configuration space is described in terms of R-Matrix; it describes both unbound and bound levels λ of system

$$R = \sum_{\lambda} (\gamma_{\lambda} * \gamma_{\lambda}) / (E_{\lambda} - E)$$

The R-Matrix labels, R_{ab} , refer to reaction channels, closed or open. The quantity $\gamma_{\lambda c}$ is reduced width *ie* preformation amplitude of the particle c in the state λ ; it is a spectroscopic quantity, *ie* a measure of single particle or cluster c component in wave function of the level λ .

The Level-Matrix A is defined by formula

$$(R^{-1} - L)_{ab}^{-1} = \sum_{\lambda\mu} \gamma_{a\lambda} A_{\lambda\mu} \gamma_{\mu b} = (\gamma^T A \gamma)_{ab}$$

The Level-Matrix is the corresponding of the Effective Hamiltonian Matrix $\|H - E\|$ of previous approach for two resonant levels, (one channel case). The elements of the Level Matrix are

$$(A^{-1})_{\lambda\mu} = (E_{\lambda} - E) \delta_{\lambda\mu} - \zeta_{\lambda\mu} = (e - E - \zeta)_{\lambda\mu}$$

$$e_{\lambda\mu} = E_{\lambda} \delta_{\lambda\mu}; \quad \zeta_{\lambda\mu} = (\gamma L \gamma^T)_{\lambda\mu} = \sum_{ab} \gamma_{\lambda a} L_{ab} \gamma_{b\mu}$$

One remarks the similarities between Hamiltonian Matrix and Level Matrix $E_{\lambda} \leftrightarrow H_{\lambda\mu}^0$, $E_{\lambda} - \zeta_{\lambda\lambda} \leftrightarrow H_{\lambda\lambda}$, $\zeta_{\lambda\mu} \leftrightarrow H_{\lambda\mu}$, ($\lambda \neq \mu$). Proceeding further one can identify formally the Configurations Mixing as transformation from $\|H_0 - E\|$ to $\|H - E\| = \|H_0 - E + H\|$, or in terms of Level Matrix as transformation from “bare” Level Matrix $A_0^{-1} = \|(E_{\lambda}^0 - E) \delta_{\lambda\mu} - \zeta_{\lambda\mu}^0\|$ to the actual Level Matrix $A^{-1} = \|(E_{\lambda} - E) \delta_{\lambda\mu} - \zeta_{\lambda\mu}\|$

$$A^{-1} = A_0^{-1} - \omega$$

$$\omega_{\lambda\mu} = - (E_{\lambda} - E_{\lambda}^0) \delta_{\lambda\mu} + (\zeta_{\lambda\mu} - \zeta_{\lambda\mu}^0)$$

It is obvious that $\omega_{\lambda\mu}$ and $(\zeta_{\lambda\mu} - \zeta_{\lambda\mu}^0)$ play role of configuration mixing potential $H_{\lambda\mu}$, ($\lambda \neq \mu$).

The problem of Configuration Mixing, including that of Intruder States, is to establish relations between the Level Matrices A and A_0 . New relations in Level Matrix formalism have been established [12,13],

$$A = A_0 + A_0 (\omega^{-1} - A_0)^{-1} A_0$$

$$A = A_0 + A (\omega^{-1} + A)^{-1} A$$

For separable interactions, $\omega_{\lambda\mu} = \xi_{\lambda} \xi_{\mu}$, [14], one obtains

$$A = A_0 + A_0 (\xi \times \xi) / [1 - (\xi, A_0 \xi)] A_0$$

$$A = A_0 + A (\xi \times \xi) / [1 + (\xi, A \xi)] A$$

These relations are formal generalizations of Configuration Mixing problem in terms of Level Matrix. At this stage we can proceed further to take into account far-away eliminated levels, resulting into a renormalization of Level-Matrix parameters.

Let divide the set of levels in two parts: retained (π) and eliminated ones (β); accordingly the R-Matrix and U-Matrix become,

$$\begin{aligned} R &= R_\pi + R_\beta, \quad U = U_\pi + U_\beta \\ U_\beta &= 1 + 2iP^{1/2} (R_\beta^{-1} - L)^{-1} P^{1/2} \\ U_\pi &= 2iP^{1/2} \sum_{\lambda\mu} \alpha_\lambda^T A_{\lambda\mu} \alpha_\mu P^{1/2} \\ \alpha_\lambda &= \gamma_\lambda (1 - R_\beta L)^{-1} \end{aligned}$$

with renormalized reduced widths α , taking into account effect of far-away eliminated levels denoted by β . The Level Matrix becomes,

$$A = (e - E - \xi)^{-1}; \quad e_{\lambda\mu} = E_\lambda \delta_{\lambda\mu}; \quad \xi_{\lambda\mu} = (\beta, \gamma^T)_{\lambda\mu} = \sum_{ab} \beta_{\lambda a} \gamma_{b\mu}, \quad \beta_\lambda = \gamma_\lambda (L^{-1} - R_\beta)^{-1}$$

The renormalized parameters of Level Matrix are rewritten in terms of background $U\beta$ matrix,

$$\begin{aligned} U_\beta &= 1 + 2iP^{1/2} W P^{1/2} = 1 + 2iT_\beta \\ \alpha_\lambda &= \gamma_\lambda (1 + WL); \quad \beta_\lambda = \gamma_\lambda L(1 + WL) \\ \xi_{\lambda\mu} &= (\beta_\lambda, \gamma_\mu) = (\gamma_\lambda, L \gamma_\mu) + (\gamma_\lambda, LWL \gamma_\mu) \\ \text{For natural boundary conditions, } L &= iP, \text{ one obtains} \\ \alpha_\lambda &= \gamma_\lambda + \gamma_\lambda iP^{-1/2} T_\beta P^{1/2} \\ \beta_\lambda &= \alpha_\lambda iP = \gamma_\lambda iP - \gamma_\lambda P^{1/2} T_\beta P^{1/2} \\ \xi_{\lambda\mu} &= i(\gamma_\lambda, P_{\lambda\mu}) - (\gamma_\lambda, P^{1/2} T_\beta P^{1/2} \gamma_\mu) \end{aligned}$$

Observe that the non-diagonal terms $\xi_{\lambda\mu}$, describing the coupling of different levels, depend on spectroscopic quantities γ and also on distant levels and scattering states via background Collision Matrix U_β .

Let study the effect of background scattering on Multilevel Matrix for one channel case. The one channel background scattering is described in terms of scattering phase-shifts, $U_\beta = \exp(2i\delta)$. The decay of resonances λ and μ in an one channel system a is described by their total/partial decay widths $\Gamma_\lambda = \Gamma_{\lambda a} = \gamma_{\lambda a} P_a^{1/2}$ and Γ_μ . The Multilevel Matrix, in new terms, is

$$\| (E_\lambda^0 - E) \delta_{\lambda\mu} + \Gamma_\lambda^{1/2} \sin\delta \cos\delta \Gamma_\mu^{1/2} - i \Gamma_\lambda^{1/2} \cos^2\delta \Gamma_\mu^{1/2} \|$$

The Level-Matrix elements are obvious dependent on spectroscopic reduced widths and background scattering phase-shifts. Observe that the level-shift, (second term of above matrix element), is dependent on background scattering phase-shift. Another remark does concern the compression of the resonance's width, namely $\cos^2\delta$ instead of unity; this property was previously established as Direct Compression of Resonances in Multichannel Systems, [12]. The energy difference of the two resonant levels, (similar to bound states case), is now complex

$$(E_\lambda^0 - E_\mu)^2 = [(E_\lambda^0 - i \Gamma_\lambda e^{i\delta} \cos\delta) - (E_\mu^0 - i \Gamma_\mu e^{i\delta} \cos\delta)]^2 + 4i \Gamma_\lambda i \Gamma_\mu \cos^2\delta$$

For non-background scattering, $\delta = 0$, one obtains the two-levels formula for complex energies; the decay widths play role of level-coupling terms. For "echo"-scattering, $\delta = \pi/2$, one concludes on the width-extinction, [15].

The method of Level Matrix can be extended in order to include the residual interaction, $\langle \lambda | H' | \mu \rangle$, resulting in additional non-diagonal terms,

$$\xi_{\lambda\mu} = (\gamma_\lambda, L \gamma_\mu) + (\gamma_\lambda, LWL \gamma_\mu) - \langle \lambda | H' | \mu \rangle$$

Only the last term of above formula is considered in Nuclear Structure calculations; the other terms are disregarded. The contribution of scattering states is neglected as Nuclear Structure calculations are concerned only with bound states; perhaps such contribution is simulated via effective interactions in Hamiltonian describing retained levels. Another remark does concern the effect of eliminated levels described through $(\gamma_\lambda, LWL \gamma_\mu)$ terms; it takes into account the coupling (via background Collision Matrix) of these levels to those of interest. One has to mention that these two coupling terms depend explicitly on spectroscopic parameters of levels, via reduced widths γ_λ .

One can observe the interplay between multilevel and multichannel effects both in Nuclear Structure and Nuclear Reactions calculations. In absence of background scattering, $W = 0$, the renormalized reduced widths $\beta_{\lambda a}$ reduces to $\gamma_{\lambda a}$ L_a . For negative energies the logarithmic derivative L_a reduces to shift-factor S_a^- only, resulting into a level shift $-\sum_c S_c \gamma_{\lambda c}$, in addition to residual interaction shift $-\langle \lambda | H' | \mu \rangle$. For positive energies, $L_a = S_a + iP_a$ is a complex quantity and the level λ decays in reaction channels with a preformation probability γ ; the level shift, $S_a^+ \gamma_{\lambda a}$, is present too. In both cases the level-shift is strongly dependent on spectroscopic reduced widths. If the two involved levels differ as structure, (ie their spectroscopic factors differ quantitatively), then the relative displacements in the two configurations differ drastically. This could be the case of intruder states; some levels nearly conserve their positions, while the other move in the complementary configuration. One can speculate that the spectroscopic dependence of Configuration Mixing is implicitly contained in standard numerical Nuclear Structure calculations, but this assertion has to be proved only via systematic numerical experiments. Multilevel and multichannel effects on spectroscopic factors have been studied in a recent work, [16].

We conclude the above results in the following statements: the Configuration Mixing has different origins. The first one, usually taken into account in bound state calculations, is the residual interaction mixing. It depends both on transition operator H' and also on nature of involved states. If the states have very different nature then the overlap integral $\langle \lambda | H' | \mu \rangle$ could be small and the level mixing is not significant. A second source of levels coupling and mixing is that of boundary conditions, $S_a \gamma_{\lambda a} \gamma_{\mu a}$. This term depends on boundary shift-factors and on nature of involved states. If the states have nearly same nature, (ie similar spectroscopic reduced widths), then boundary conditions mixing and coupling are enhanced. The coupling via scattering states is another source for Configuration Mixing. The last

two sources result into a conceptual difference on mechanisms of Configuration Mixing as compared to the usual treatment of Nuclear Structure calculations. In usual treatments one diagonalizes a hermitian Hamiltonian, resulting in eigenvalue modifications. The transition probabilities are then calculated as matrix elements of corresponding operators with actual wave functions. According to Level Matrix formalism, the non-diagonal coupling terms are explicitly dependent on boundary conditions and spectroscopic reduced widths. For genuine bound state calculations, the matrix is real resulting in real eigenvalues. For general case, including both bound and unbound states, one obtains an interplay of the both types of states and “bound” states eigenvalues could acquire imaginary components.

Our approach to Level Mixing is related to Theory of Line Broadening, [11]. According to Line Broadening Theory the levels’ mixing has two origins: residual interactions and change of boundary conditions. The boundary conditions mixing mechanism is not under discussion in Nuclear Structure, [1], nor in some approaches to Nuclear Reactions, [17,18]; also, not in Atomic Structure and Collision Physics, [19,20], as well as in Elementary Particle Physics, [21].

4. ON CONFIGURATION MIXING IN OPTICAL ATOMS AND IN ATOMIC MULTICHANNEL QUANTUM DEFECT THEORY

The two levels problem (either bound or resonant levels) appears in Quantum Optics too, [3]. By an Optical Atom it is understood two coupled optical modes in an optical cavity. The two optical modes are distinguishable by their polarizations or by their directions of propagation *eg* in a ring cavity. For an Optical Atom one defines conservative (hermitian) and dissipative (imaginary) couplings, similar to previous discussion for Quantum Resonances (internal mixing, external mixing). The conservative coupling results into level repulsion. The dissipative coupling tends to pull together the mode frequencies (levels). The damping rates of the modes are given by imaginary parts of eigenvalues. The real eigenvalues denote distinct eigenfrequencies; the imaginary eigenvalues denote distinct loss-rates. The approach to this problem are quite similar to the problem of Quantum Resonances’ repulsion/attraction; the coupling of two modes is realized only in terms of radiation field (“Hamiltonian”’s residual interaction). Apparently the problem of level-shifts in the Optical Atom, due to presence of the cavity boundaries, is not yet approached. This aspect could be of interest for Cavity Quantum Optics.

A basic theory of Atomic Spectra and Collisions is Multichannel Quantum Defect Theory (MQDT), [22,20]. The MQDT is based on possibility of separating the effects of long and short range interactions between an electron and an atomic core. The effect of short range interactions, within the core, are very complex but, nevertheless, can be concisely represented by a global parameter, named Quantum Defect. (For positive energies, above threshold, the Quantum Defect is related, by a

simple relation, to scattering phase shift). The long range interactions, represented by a simple field, as *eg* the Coulomb one, are treated analitically by extensive use of Coulomb wavefunctions; this fact resulted into perception that the MQDT should be a specific Theory for Atomic Collisions.

An alternative description of MQDT, based on Configuration Mixing treatment, has been developed by Fano, [23,24]. The derivation is based on Green's Operator of Scattering Theory; its application to atomic problems is based on "Two-Potential" formula, *ie* the interaction is described by a Model Hamiltonian and a "residual" interaction. Configuration Mixing treatments use to separate the Hamiltonian of the whole system into two terms, $H = H_0 + H'$, and of constructing its eigenfunctions as superposition of eigenfunctions set of H_0 . The MQDT is approached from a Configuration Mixing point of view, *ie* by representing the eigenfunctions of the whole Hamiltonian as superpositions of eigenfunctions of Model Hamiltonian.

The MQDT has to be related also to other approaches to Collision Theory as K-or R-Matrix. One has to remark, the general assumptions of the MQDT are similar to those of R-Matrix Theory, [6]. Developing this idea and by using only basic properties of Whittaker and Coulomb functions, [25] has extracted MQDT from R-Matrix Theory. One can prove that MQDT is rather physically and formally equivalent to Reduced R-Matrix. The physical basis for this equivalence is analogy between the two concepts. The Reduced R-Matrix describes not only the internal dynamics, (as R-Matrix does), but also the interaction in space of eliminated closed channels. The MQDT is dealing also with "inner" and "channel" states corresponding, respectively, to multielectron excitations and to Rydberg states. Both theories describe not only the internal dynamics but also the interaction of eliminated closed channels.

A Level Matrix Approach to MQDT has been developed, [14]; it is based on relations connecting Level Matrices for "bare" and "mixed" systems. Both Configuration Mixing and MQDT can be approached within same formalism of Level Matrix. The Level-Matrix approach to the MQDT does connect two multichannel systems with identical dynamics in the internal regions of the configuration space but having different interactions in the eliminated-channel regions of configuration space.

5. CONCLUSIONS

The problem of Configuration Mixing has been approached in terms of Level-Matrix formalism of Nuclear Reactions Theory and it is, in principle, related to Theory of Line Broadening. The main part of the work is related to Configuration Mixing in Nuclear Structure and Reactions; one discusses also the Configuration Mixing with respect to Atomic Multichannel Defect.

The concept of Reduced Level Matrix is presented; it takes into account the effect of eliminated levels and channels. The level's parameters are renormalized in terms of background Collision Matrix. It is proved that, in addition to multilevel couplings, there are also multichannel sources for Configuration Mixing originating in boundary conditions and couplings to scattering states. Both the levels' shifts and widths are directly dependent on spectroscopic factors; this way the spectroscopic aspects of Configuration Mixing are, for first time, evinced. Additional states could occur in space of retained ones; one has to mention the Intruder States, also another states described as zero of Reduced Level-Matrix similar to R-Matrix bound state condition. These aspects of Interacting Multilevel Systems deserve additional insight.

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