THE PUBLISHING HOUSE
OF THE ROMANIAN ACADEMY

PROCEEDINGS OF THE ROMANIAN ACADEMY, Series A
Volume 24, Number 1/2023, pp. 43–50
DOI: 10.59277/PRA-SER.A.24.1.06

ON SINGLE PARTICLE STATES AND RESONANCES IN MULTICHANNEL REACTIONS

H. COMISEL[1], C. HATEGAN[1], R.A. IONESCU[1], H.H. WOLTER[2]

[1] Institute of Atomic Physics, Bucharest, Romania
[2] Universität München, Fakultät für Physik, Germany

Abstract. The Multichannel Quantum Defect Theory and the Reduced R-Matrix are formally related and physically equivalent; both theories describe not only the internal dynamics but also the interactions in space of eliminated channels. One proves the Multichannel Quantum Defect Theory is Reduced Collision Matrix describing effect of eliminated channel on observed ones.

The multichannel resonances originating in bound or quasistationary single particle states are described in terms of Reduced Collision Matrix. The single particle states are defined by Bound- or Quasistationary- State equation in the eliminated channel, relating channel logarithmic derivative to R-Matrix.

Key words: Multichannel Quantum Defect Theory (MQDT), R-Matrix Theory, Rydberg states.

1. INTRODUCTION

The collision of an electron with the atomic electronic core or the scattering of a nucleon on the atomic nucleus, usually, results into multiparticle excitations producing a resonance of a compound system, followed by its decay in reaction channels. Both in the electron-atom collisions and in nucleon-nucleus reactions, these multichannel resonances are described by poles of R-Matrix elements.

The resonances originating in single particle states, either in electron- atom collision or in nucleon-nucleus scattering, are approached in quite different descriptions. For example, the single-particle resonance in nuclear scattering is described, in R-Matrix Theory, by a perturbative method (Lane and Thomas [1]). By perturbative residual interactions, the single particle state is subject to transitions to actual states of compound system and to couplings to other reaction channels. The R-matrix becomes a series of resonant terms, collected, with statistical assumptions, into giant single particle resonance formula. The electron, involving single particle Rydberg state in an atomic collision, “avoids” its wave function mixing with that of inner multielectron core, because it is spatially located far-away from that core. In the electron-atom scattering the effect of inner multielectron core on Rydberg electrons is rather studied by means of a global parameter, historically called “Quantum Defect”; the electron-atom scattering is described by the Multichannel Quantum Defect Theory (MQDT), (Seaton [2]). Both these (electron or nucleon) types of resonances have in common the persistence of the single-particle motion in a complex system with multiparticle excitations.

In this work the single- particle (electron or nucleon) state in a multichannel system. are not more described by a R-Matrix pole (specific for resonances originating in multiparticle excitations) but rather by a natural method for incorporating a single particle state in R-Matrix Theory. Firstly, one establishes a formal relation and a physical equivalence of the MQDT and the Reduced R-Matrix; both concepts describe, in addition to internal dynamics, the interactions in space of eliminated channels. The electron Rydberg state or the nucleon single particle state, both from an eliminated (invisible or unobserved) channel, are described by R-Matrix bound or quasistationary state condition. The coupling of single particle (electron or nucleon) bound or quasistationary state from eliminated channel to the observed open channels results into a multichannel resonance. The zero-energy single particle states result, by coupling to open observed channels, into threshold effects with corresponding spectroscopic strengths.

2. MULTICHANNEL QUANTUM DEFECT AND REDUCED R-MATRIX

The Multichannel Quantum Defect Theory (MQDT) is based on possibility of separating the effects of long and short range interactions between an electron and an atomic core [2]. 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. The long range interactions, (represented by simple fields as *e.g.* the Coulomb or dipolar ones), are treated analitically by extensive use of Coulomb or other Special Functions. On the other hand the general assumptions of the MQDT are similar to those of R-Matrix Theory, [3]. Developing this idea and by using only basic properties of Whittaker and Coulomb functions, Lane [3] has extracted MQDT from Wigner's R-Matrix Theory. A relationship between K-Matrix, on one side, and R-Matrix, boundary condition parameters and Coulomb functions, on other side, was established. This relation was then rewritten, by using specific boundary conditions, in a K-Matrix form of MQDT.

In the present work one proves that the MQDT is rather equivalent to the Wigner Reduced R-Matrix. The K-Matrix form of the MQDT is obtained from R-Matrix Theory by a procedure for relating the collision matrices defined for the multichannel system both above and below threshold. This approach proves that the essential aspects of the MQDT originate in variation across threshold of the logarithmic derivative of the eliminated channels. According to this approach, the MQDT provides a relationship between the collision matrices of two multichannel reaction systems with the same inner core but differing only in interactions of the eliminated channels.

The Collision Matrix U is parametrized [1] in terms of the R-Matrix, the Coulombian hard-sphere phase shifts Φ, the logarithmic derivative L and its imaginary part, penetration factor P,

$$U = e^{-i\Phi} W e^{-i\Phi} \quad = \quad e^{-i\Phi}[1 + 2iP^{1/2}(R^{-1} - L)^{-1}P^{1/2}]e^{-i\Phi} \tag{1}$$

Another form suitable for the present purpose is

$$W \quad = \quad 1 - 2iP^{1/2}L^{-1}P^{1/2} + 2iP^{1/2}L^{-1}(L^{-1} - R)^{-1}L^{-1}P^{1/2} \tag{2}$$

The penetration factor matrix P is a diagonal matrix with dimension equal to number of open channels. Below threshold, $P = ||P_a\delta_{ab}|| = P_N$ for N open channels, $(a, b = 1, 2, \cdots, N)$; it will select the corresponding $N \times N$ submatrix of the whole $(R^{-1} - L)^{-1}$ matrix. Above threshold, a new open channel $n = N + 1$ is added to the reaction system. The dimension of penetration factor P and of U (W) square Collision Matrix rises by one. The R-Matrix and the logarithmic derivative L, corresponding to whole reaction system, are represented both below and above threshold by square matrices of dimension $(N + 1)$.

The Collision Matrix elements are constructed, both below $(<)$ and above $(>)$ n-threshold, by assuming that the only changing parameter across threshold is the logarithmic derivative of the channel n (or a group n of degenerate channels)

$$(L^{-1} - R)_> = \begin{pmatrix} L_N^{-1} - R_N & -R_{Nn} \\ -R_{nN} & L_{n>}^{-1} - R_n \end{pmatrix} = (L_>^{-1} - R) \tag{3a}$$

$$(L^{-1} - R)_< = \begin{pmatrix} L_N^{-1} - R_N & -R_{Nn} \\ -R_{nN} & L_{n<}^{-1} - R_n \end{pmatrix} = (L_<^{-1} - R) \tag{3b}$$

Relating $(L_<^{-1} - R)^{-1}$ to $(L_>^{-1} - R)^{-1}$ by an identity for sub-matrix blocks

$$(L_<^{-1} - R)_N^{-1} \quad = \quad (L_>^{-1} - R)_N^{-1} - (L_>^{-1} - R)_{Nn}^{-1} \frac{1}{-(L_{n>}^{-1} - L_{n<}^{-1})^{-1} + (L_{n>}^{-1} - R)_{nn}^{-1}} (L_>^{-1} - R)_{nN}^{-1}$$

it results into a formula connecting Collision Matrices defined above $W^{>}$ and below $W^{<}$, n-threshold

$$W_N^{<} \quad = \quad W_N^{>} - W_{Nn}^{>} \frac{1}{-(\Delta L_n)^{\star}/(\Delta L_n) + W_{nn}^{>}} W_{nN}^{>} \tag{4}$$

In this derivation it is assumed that $L_{n<}$ is real and $\Delta L_n = L_{n>} - L_{n<}$ is logarithmic derivative variation across threshold of the n-channel. The modulus one quantity $(\Delta L_n)^{\star}/(\Delta L_n)$ allows to define a "defect scattering phase shift" δ_n, a "Collision Matrix element" U_{nn}^{δ} and a corresponding "K-Matrix element" $\tau_{nn} = \tan\delta_n, \tan(\delta_n - \phi_n) = Im\Delta L_n/Re\Delta L_n$,

$$(\Delta L_n)^{\star}/(\Delta L_n) = e^{2i\Phi_n} e^{-2i\delta_n} \tag{5a}$$

$$U_{nn}^{\delta} = e^{2i\delta_n} = -1 + 2i(\tau_{nn} + i)^{-1} \tag{5b}$$

The Collision Matrix form of the MQDT

$$U_N^{<} \quad = \quad U_N^{>} - U_{Nn}^{>} \frac{1}{U_{nn}^{>} - (U_{nn}^{\delta})^{-1}} U_{nN}^{>} \tag{6}$$

results into a corresponding K-Matrix form, [4]

$$U = -1 + 2i(K + i)^{-1} \tag{7a}$$

$$K_N^{<} = K_N - K_{Nn}[\tau_{nn} + K_{nn}]^{-1} K_{nN} \tag{7b}$$

One can prove, by evaluating ΔL_n near threshold for Coulomb field [5, 6], that the δ_n phase shift is related to effective quantum number of MQDT, $\delta_n = \pi|\eta|$. For s-wave scattering on external (outside inner core) neutral fields, ΔL_n is proportional to $(1+i)$ and $\delta_n = \pi/4$. [7].

Obtaining the U-Matrix form of MQDT, we have, in next step, to relate it to the Reduced R-Matrix. In general theory the R-Matrix has a dimension equal to total number of channels, whether open or closed. The Reduced R-Matrix has (in our case) dimension equal to number of open channels; it takes into account the eliminated closed channel through an additional term. For obtaining a compact R-Matrix form of the MQDT, (analogous to the K-Matrix one (7b)), one uses the R-Matrix parametrization of the Collision Matrix below threshold

$$W_N^{<} \quad = \quad 1 - 2iP_N^{1/2} L_N^{-1} P_N^{1/2} + 2iP_N^{1/2} L_N^{-1} (L_N^{-1} - \mathscr{R}_N^{<})^{-1} L_N^{-1} P_N^{1/2} \tag{8}$$

the explicit form of the $\mathscr{R}_N^{<}$ term has to be determined. One defines a similar R-Matrix parametrization for the diagonal matrix $(\Delta L_n)/(\Delta L_n)^{\star}$, with $L_n = L_n^{>}$

$$(\Delta L_n)/(\Delta L_n)^{\star} \quad = \quad 1 - 2iP_n L_n^{-1} + 2iP_n L_n^{-2} (L_n^{-1} - \rho_n)^{-1} \tag{9}$$

One can remark that $(W_N^{<} - L_N^{\star} L_N^{-1})^{-1}$ can be regarded (up to diagonal matrices $P_N^{1/2} L_N^{-1}$) as a linear function of $\mathscr{R}_N^{<}$ while the right side of MQDT form of W, (4), as a submatrix (corresponding to the system of N open channels) of the difference

$$\left[(W^{>} - L^{\star} L^{-1})_{N+1} - (W^{\delta\star} - L_{\delta}^{\star} L_{\delta}^{-1})_{N+1} \right]_N^{-1}$$

The Collision Matrix $(W^{>})_{N+1}$ describes both open (a,b) and threshold (n) channels while $(W^{\delta\star} - L_{\delta}^{\star} L_{\delta}^{-1})_{N+1}$ has only a non zero element refering to $n = N+1$ channel, defined by (9). By this remark and by using (4) one obtains the explicit form of $\mathscr{R}_N^{<}$ matrix defined below threshold

$$\mathscr{R}_N^{<} \quad = \quad R_N - R_{Nn} \frac{1}{R_n - \rho_n} R_{nN} \tag{10}$$

As from (10) the term ρ_n is identified to be $(L_n^<)^{-1}$, ($\rho_n = 1/L_n^<$), one obtains that the R-Matrix parametrization of the MQDT, $\mathscr{R}_N^<$, is just Wigner Reduced R-Matrix, as defined in Lane and Thomas [1]. The physical basis for this equivalence is analogy between the two concepts; both describe not only the internal dynamics but also the interaction from eliminated closed channels.

3. ON SINGLE PARTICLE STATES IN MULTICHANNEL REACTIONS

The resonances in electron multichannel scattering on atoms or ions originate either in multielectron excitations of electronic inner core or from excitation of Rydberg far-away located states. According to Lane R-Matrix terminology [3] they are called "inner resonances" and "channel resonances", respectively. Adopting this terminology we could have in mind another processes in Scattering Physics, as e.g. nucleon scattering on nuclei. The "inner" and "channel" resonances do correspond to "compound nucleus"- and to "single particle"-resonances, respectively.

In Lane's approach to MQDT, [3], both the inner and Rydberg resonances are described in similar ways; the Rydberg resonances are represented by a meromorphic term added to inner resonances genuine R-Matrix. The meromorphic function χ, describing Rydberg states, is constructed in terms of Whittaker function and specific boundary condition for n-closed channel. The matrix sum $(R+\chi)$ is then inverted, by retaining only block sub-matrix refering to open channels.

In the present approach the inner multichannel resonances are described by R-Matrix while the channel resonances are related to L_n logarithmic derivative and to n-channel Reduced R-Matrix. The multichannel resonances originating in single particle (bound or quasistationary) states are approached here within the MQDT/Reduced R-Matrix framework.

The MQDT description of (n)-channel resonances results into a formal constraint on denominator in formula (4), namely $-(\Delta L_n)^\star/(\Delta L_n) + W_{nn}^> = 0$. This condition, implicitly, contains assumption the other Collision Matrix terms $W_N^>$, $W_{Nn}^>$, $W_{nN}^>$ are monotone energy dependent near (or across) n-channel threshold. This is questionable, the only quantity which does not feel threshold energy dependance is the R-Matrix. The Collision Matrix $W^>$ terms are dependent on n-channel logarithmic derivative $L_n^>$ which, in principle, could exhibit a strong energy dependance near threshold or a non-monotone one for shape resonances. Moreover these Collision Matrix terms have an implicit dependance on R_{nn}-Matrix element and this implies that effects originating in eliminated n-channel are present not only in denominator of (4) but also in the other $W^>$ Collision Matrix terms.

In Lane's approach [3] this aspect is avoided; the description of resonances is done in terms of R-Matrix (for inner resonances) and of a meromorphic function χ (for channel resonances). This way the inner and channel resonances become mixed in the Collision Matrix.

In the present framework the approach is quite opposite; one has to separe the effects originating in the two groups of channels in order to have a physical insight on phenomena developing in n-closed channel. The MQDT formulae for Collision Matrix have to be recast in forms in which this separation is explicit; this goal could be realized in terms of the Reduced Collision Matrix, a concept similar to Reduced R- or K- Matrix.

The Reduced Collision Matrix is the submatrix $W_N(U_N)$ of the Collision Matrix which refers to retained (N) channels, but by taking into account the effect of eliminated (n)-channel. It consists from Collision Matrix $W_N^0(U_N^0)$ which describes the "bare" retained channels (N), uncoupled to eliminated (n) channel,

$$W_N^0 \quad = \quad 1 - 2iP_N^{1/2}L_N^{-1}P_N^{1/2} + 2iP_N^{1/2}L_N^{-1}(L_N^{-1} - R_N)^{-1}L_N^{-1}P_N^{1/2} \tag{11}$$

and from a term ΔW_N describing this coupling. The Reduced Collision Matrix evaluated above $(>)$ n-threshold is [4]

$$\begin{aligned} W_N^> &= W_N^0 + \Delta W_N^> \\ \Delta W_N^> &= W_{Nn}^>(-L_n^{>*}/L_n^> + W_{nn}^>)^{-1}W_{nN}^> \end{aligned} \tag{12}$$

$$
\begin{aligned}
W^{>}_{nn} &= 1-2iP_nL_n^{-1}+2iP_nL_n^{-2}(L_n^{-1}-\mathscr{R}_{nn})^{-1} \\
\mathscr{R}_{nn} &= R_{nn}-R_{nN}(R_{NN}-L_N^{-1})^{-1}R_{Nn}
\end{aligned}
\tag{13}
$$

For boundary conditions used by Lane [3], the L_n^*/L_n modulus one quantity is expressed in terms of coulombian hard-sphere phase-shifts, $-L_n^*/L_n=\exp(2i\Phi_n)$, and

$$
U_N^{>}=U_N^0+U_{Nn}^{>}(1+U_{nn}^{>})^{-1}U_{nN}^{>}
\tag{14}
$$

By Reduced Collision Matrix procedure, the MQDT Collision Matrix (4) becomes

$$
\begin{aligned}
W_N^{<} &= W_N^0+\Delta W_N^{<} \\
\Delta W_N^{<} &= W_{Nn}^{>}\frac{1}{-(L_n^{>})^*/(L_n^{>})+W_{nn}^{>}}W_{nN}^{>}\frac{1/L_n^{>}-\mathscr{R}_{nn}}{1/L_n^{<}-\mathscr{R}_{nn}}
\end{aligned}
\tag{15}
$$

i.e. the MQDT is Reduced Collision Matrix for negative energies (closed channel) expressed in terms of positive energy quantities ($W^{>}$, $L^{>}$) and also of quantities specifying eliminated closed channel (logarithmic derivative $L_n^{<}$ and Reduced R-Matrix element $\mathscr{R}_{nn}$) The effective term ΔW_N of Reduced Collision Matrix, valid both below and above n-threshold, is

$$
\begin{aligned}
\Delta W_N = & \frac{1}{2i}(W_N^0-L_N^*L_N^{-1})P_N^{-1/2}L_N \\
& R_{Nn}(L_n^{-1}-\mathscr{R}_{nn})^{-1}R_{nN} \\
& L_NP_N^{-1/2}(W_N^0-L_N^*L_N^{-1})
\end{aligned}
\tag{16}
$$

where for ΔW_N superscripts $>$ or $<$ one has to insert the corresponding logarithmic derivatives $L_n^{>}$ or $L_n^{<}$, respectively.

In next paragraphs we will discuss single particle resonances of multichannel (electron or nucleon) scattering in terms of Reduced Collision Matrix (16), which describes the two groups of channels by well-separated terms.

Below threshold, a pole in $U_N^{<}$ Collision Matrix elements could be obtained from the condition $\mathscr{R}_{nn}^{-1}=L_n^{<}=S_n^{(-)}$, ($S_n^{(-)}$ - shift function). In non-coupling limit, $\mathscr{R}_{nn}$ reduces to single channel R-Matrix element R_{nn}. Or this is just bound state condition of the R-Matrix Theory, [1]; a bound state appears at that energy at which the internal (R_{nn}^{-1}) and external $S_n^{(-)}$ logarithmic derivatives do match. This result is a R-Matrix proof that the single particle state from a closed channel does induce resonance in competing open channels of the multichannel system.

The standard form of the MQDT was derived only for (bound states in) eliminated closed channels; extended to positive energy eliminated channels the corresponding states should be quasistationary ones. A pole in U_N is now obtained by a condition which is analog to the bound state one, $\mathscr{R}_{nn}^{-1}=L_n$; the logarithmic derivative L_n is the corresponding, at positive energy, of the shift function $S_n^{(-)}$ defined for negative energy. According to R-Matrix theory, the quasistationary (Siegert) state is defined by condition $|1-RL|=0$ (Lane and Thomas [1], p. 297). The outgoing wave at infinity corresponds to quasistationary state decay. This condition yields a set of complex eigenenergies which determines the level's energy and width [8]. A quasistationary state originating in an eliminated channel induces a quasiresonant structure in other open competing channels. Apparently (see, for example, [9]), this situation (multichannel resonance originating in a quasistationary single particle state from an unobserved channel) was not discussed until now. In the literature [10] one reports on the "channel coupling pole" observed in numerical experiments for multichannel scattering; a single channel pole may be driven to physical region of the complex energy plane when channel coupling becomes effective. It could be of interest to relate the "channel coupling resonances" and the multichannel resonances originating in quasistationary states.

The n-channel related effects in retained channels (N) are represented by the product $R_{Nn}(L_n^{-1}-\mathscr{R}_{nn})^{-1}R_{nN}$, resembling to additional term of $\mathscr{R}_N$ Reduced R-Matrix, eq. (13). The only difference is the 'bare' R-Matrix element R_{nn} of eliminated n-channel is here replaced by its effective counterpart $\mathscr{R}_{nn}$; the n-channel Reduced $\mathscr{R}_{nn}$ - Matrix element does include also rescattering effects from complementary open channels. The physical implication of the Reduced R-Matrix element $\mathscr{R}_{nn}$, instead of uncoupled n-channel R-matrix R_{nn}, is obtained by writting the open retained channels component $(R_{NN}-L_N^{-1})^{-1}$ in terms of the T_N^0 transition matrix for open uncoupled channels, $W_N^0 = 1+2iT_N^0$. By using natural boundary conditions, $L_N = iP_N$, one obtains $(R_{NN}-L_N^{-1})^{-1}$ = $P_N^{1/2}(T_N^0 - i)P_N^{1/2}$. The Reduced $\mathscr{R}_{nn}$ - Matrix element of the eliminated channel becomes

$$\mathscr{R}_{nn} = R_{nn} + R_{nN}P_N^{1/2}(i-T_N^0)P_N^{1/2}R_{Nn} \tag{17}$$

The single particle level's (real or complex) energy, E_n^0, in absence of coupling to open channels, is defined by bound or quasistationary state condition $L_n^{-1} - R_{nn} = 0$. The actual level's energy implies the level acquires a shifth, $\Delta_n = -R_{nN}P_N^{1/2}\mathrm{Re}T_N^0 P_N^{1/2}R_{Nn}$, and width, $\Gamma_n = R_{nN}P_N^{1/2}(1-\mathrm{Im}T_N^0)P_N^{1/2}R_{Nn}$, due to coupling to open channels. One has to remark that both level's shift and width depend not only on coupling strength R_{Nn} but also on rescattering T_N^0 in open channels. The effect of potential scattering in open channels is more visible for the level's width. The Unitarity Condition, $\mathrm{Im}T_{aa} = (TT^\dagger)_{aa}$ results into $(1-\mathrm{Im}T_{aa}) = (1-\sum_{b=1}^N |T_{ab}|^2) < 1$. The corresponding component of the width is compressed by term $\sum_{a=1}^N R_{na}(1-\sum_{b=1}^N |T_{ab}^0|^2)R_{an}$. A bound or a quasistationary state, originating in an eliminated channel, induces a resonance in open competing channels. Both the width and level shift are determined by channels couplings and by rescattering in open channels; a broad quasistationary state (from eliminated channel) results in a smaller width resonance (in retained channel). Multichannel resonances originating in quasistationary or bound single particle states and 'Channel Coupling Resonances' have similar width property.

4. ON ELECTRON RYDBERG STATES IN MULTICHANNEL SYSTEMS

The single particle resonance equation, $L_n^{-1} - \mathscr{R}_{nn} = 0$, can be approached in two different ways, either refering to Reduced R-Matrix element, as above, or to Logarithmic Derivative. The logaritmic derivative itself could have a resonant form, e.g. as that proposed in Nuclear Physics [11], resulting in a generalization of Cusp Theory. In Atomic Physics an energy-dependent logarithmic derivative, with poles on real axis, is used for studying electron Rydberg states, at negative energy. The (Reduced) R-Matrix element of eliminated channel could be then considered as non-dependent on energy. By applying the resonance equation to electron Rydberg states, one should obtain basic results of Quantum Defect Theory.

The electron (closed channel, $n = e$) logarithmic derivative is given by [5,6]

$$L_e = -\cot\pi\sqrt{e_1^2 e_2^2 m/2\hbar^2(E_\pi - E)}$$

(e_1, e_2 and m – channel particles electric charges and reduced mass). The Rydberg states, in absence of inner core, are defined by equation $L_e^{-1} = 0$. The level equation $L_e^{-1} = 0$ results into energy of Rydberg states, defined with respect to E_π threshold energy, $E_\pi - E_n$= $(1/n^2)\ e_1^2 e_2^2 m/2\hbar^2$, with n an integer number.

If quantum defect, due to inner core, is taken into account then the principal quantum number n is replaced by effective quantum number ν resulting into level-shift, which, at its turn, is related to quantum defect μ by relation $\nu = n - \mu$ (Seaton [2]). The electron logarithmic derivative below threshold becomes $L_{e<} = \cot\pi\mu$. In non-coupling limit, the Reduced R-Matrix becomes the single channel R-Matrix element R_{ee}. The bound state condition, for one electron closed channel, according to $L_{e<}^{-1} - R_{ee} = 0$, is now $\tan\pi\mu = R_{ee}$; it relates one-channel quantum defect, μ, to Rydberg channel R-Matrix element, R_{ee}.

The resonance equation of Rydberg channel implies basic results of Quantum Defect Theory. The logarithmic derivative above threshold is [5,6] $L_e^> = i$; the electron penetration factor is one $P_e = 1$ and its shift-factor is zero $S_e = 0$. The scattering phase-shift in open electron channel δ_e, defined according to R-Matrix by

$\tan\delta_e = R_{ee}P_e/(1-R_{ee}S_e)$, becomes $\tan\delta_e = R_{ee}$. The two relations involving R_{ee} matrix element results in the Seaton theorem, $\delta_e = \pi\mu$, relating the scattering phase shift above threshold to the quantum defect from spectra below threshold.

The only strong dependent on energy of Reduced Collision Matrix ΔW_N is the closed Rydberg electron channel term $(L_e^{-1} - \mathscr{R}_{ee})$. The energy dependence is contained in logarithmic derivative; below threshold $L_{e<} = -\cot\pi\nu$, above threshold $L_{e>} = i$. The R_{ee} matrix element of multielectron inner core is considered as nearly constant in threshold region. The energy average (over mean spacing of levels D) of the effective term, below threshold, $\overline{\Delta W_N}$ is calculated following [5] One obtains $\overline{(L_{e<}^{-1} - \mathscr{R}_{ee})} = (L_{e>}^{-1} - \mathscr{R}_{ee})$, that the averaged effective term and averaged Collision Matrix, are continous across threshold, $\overline{\Delta W_N^<} = \Delta W_N^>$ and $\overline{W_N^<} = W_N^>$. (Gailitis [12]). The Seaton' and Gailitis' theorems are basic ones in Quantum Defect Theory.

The coupling of the closed channel e to open channel a results in the resonance equation

$$\tan\pi\nu + \mathscr{R}_{ee} = 0. \tag{18}$$

This relation results into definition of 'complex quantum defect' $\tilde{\mu}$ in terms of Reduced R-Matrix element, $\mathscr{R}_{ee}$, of electron Rydberg channel, $\tan\pi\tilde{\mu} = \mathscr{R}_{ee}$. The transition between two channels is represented by the R_{ae} matrix elements; P_a is penetration factor for open elastic channel and T_{aa}^0 is transition amplitude $W_{aa}^0 = 1 + 2iT_{aa}^0$ for elastic channel uncoupled to Rydberg channel. The additional term in the complex quantum defect, $\tilde{\mu} = \mu + \delta + i\gamma$, is in weak coupling limit

$$\delta + i\gamma = R_{ea}P_a^{1/2}[-\mathrm{Re}T_{aa}^0 + i(1 - \mathrm{Im}T_{aa}^0)]P_a^{1/2}R_{ae}\,. \tag{19}$$

The level shift, due to inert inner core, is given by the one-channel quantum deffect μ, $R_{ee} = \tan\pi\mu$. The additional terms, $\delta \sim (\mathrm{Re}T_{aa}^0)$ and $\gamma \sim (1 - \mathrm{Im}T_{aa}^0)$, are related both to interchannel transitions as well as to potential scattering in the electron elastic channel; the last one implies resonance's width diminution, ($\mathrm{Im}T_{aa}^0 > 0$) .

The Rydberg states, with energies $E_n - E_\pi = -\alpha^2/n^2$, from the electron closed channel will induce in the electron (elastic) scattering channel set of resonances shifted to new energy positions $\mathscr{E}_\nu = E_\pi - \alpha^2/\nu^2$. The resonance equation, $\tan\pi(\nu - n) + \mathscr{R}_{ee} = 0$, results, in weak coupling limit, in the complex energy , (see also [13], [2]),

$$\mathscr{E}_\nu = E_\pi - \frac{\alpha^2}{\nu^2} = E_n - \frac{2}{\pi}\frac{\alpha^2}{n^3}(\mathrm{Re}\mathscr{R}_{ee} + i\,\mathrm{Im}\mathscr{R}_{ee}). \tag{20}$$

The open channel level shift and resonance width are determined by reduced R-matrix or complex quantum defect of Rydberg channel. The resonance width is subject to compression due to potential scattering in open channel. The resonance's width compression is a general property of multichannel resonances originating in single particle states.

5. CONCLUSIONS

The Multichannel Quantum Defect Theory and the Reduced R-Matrix are formally related and physically equivalent; both theories describe not only the internal dynamics but also the interactions in space of eliminated channels.

The multichannel resonances originating in bound or quasistationary single particle states are described in terms of Reduced R-Matrix or Reduced Collision Matrix. This last concept is analogue of Reduced R-matrix, describing in terms of Collision Matrix the effect of eliminated channel on observed ones. By effective components of Reduced R-(U-) Matrix one takes into account the coupling and the rescattering from complementary channels. A Single Particle Resonance Equation is obtaind by relating the channel logarithmic derivative to Reduced R-Matrix element. Application of Single Particle Resonance Equation to Multichannel Collisions is illustrated for electron scatterings near threshold.

The single particle state, either bound or quasistationary, is defined in this work by matching the R-matrix to reciprocal of channel logarithmic derivative. A suitable framework for this problem is Reduced Collision Matrix which deals with Reduced R-Matrix. One obtains a singularity in the effective term of the Reduced Collision Matrix, relating the (eliminated) channel logarithmic derivative to corresponding Reduced R-Matrix. By effective component of Reduced R-Matrix one takes into account the coupling of and the rescattering from complementary open channels.

The coupling of single particle channel to complementary channels of reaction system will result into a multichannel resonance, described by a pole of effective collision matrix. This pole is solution of an equation similar to that of single particle state but now R-matrix is replaced by reduced R-matrix, thus taking into account channels couplings and rescattering. The life-time of multichannel resonance increases, as result of open channels couplings and rescattering. Formally this results in compression of decay width.

The resonance equation, defined in terms of reduced R-matrix element and channel logarithmic derivative, can be approached either by parametrization of reduced R-matrix element, as in nuclear case, or by pole parametrization of channel logarithmic derivative, as in case of electrons in Rydberg channels. The study of electron Rydberg states according to Resonance equation results into essentials of Quantum Defect Theory (Seaton and Gailitis theorems). The application of the formalism to atomic multichannel scattering problems aims to evince the extent of this approach to multichannel reactions.

REFERENCES

1. A.M. LANE, R.G. THOMAS, *R-Matrix theory of nuclear reactions*, Rev. Mod. Phys., **30**, pp. 257–353, 1958.
2. M.J. SEATON, *Quantum defect theory*, Rep. Prog. Phys., **46**, pp. 167–257, 1983.
3. A.M. LANE, *The application of Wigner's R-matrix theory to atomic physics*, J. Phys. B: At. Mol. Opt. Phys., **B19**, pp. 253–257, 1986.
4. C. HATEGAN, R.A. IONESCU, *Level-matrix approach to multichannel quantum defect theory*, J. Phys. B: At. Mol. Opt. Phys., **B28**, pp. L681–L684, 1995.
5. A.I. BAZ, I.B. ZELDOVICH, A.M. PERELOMOV, *Rasseianie, Reaktsii i Raspady v Nereliativistskoi Kvantovoi Mekhanike*, Nauka, Moskva, 1971.
6. L.D. LANDAU, E.M. LIFSHITZ, *Mécanique quantique*, Mir, Moscou, 1980.
7. U. FANO, Comm. At. Mol. Phys., **10**, p. 223, 1981.
8. A.G. SITENKO, *Theory of nuclear reactions*, World Scientific, Singapore, 1990.
9. V.I. KUKULIN, V.M. KRASNOPOLSKY, J. HORACEK, *Theory of resonances: principles and applications*, Kluwer Academic Publishers, Prague, 1989.
10. A.M. BADALYAN, L.P. KOK, M.I. POLIKARPOV, Yu.A. SIMONOV, *Resonances in coupled channels in nuclear and particle physics*, Physics Reports, **82**, pp. 31–177, 1982.
11. S.N. ABRAMOVICH, A.I. BAZ, B.Ya. GUZHOVSKII, *Nearthreshold anomaly in the* $^{7}Li\ (t,\ ^{9}Li)\ ^{1}H$ *reaction*, Yad. Fiz., **32**, pp. 402–406, 1980.
12. M. GAILITIS, *Bahavior of cross section near threshold of a new reaction in the case of a Coulomb attraction field*, J.E.T.P., **17**, pp. 1328–1332, 1963.
13. I.I. SOBELMAN, L.A. VAINSHTEIN, E.A. YUKOV, *Excitation of atoms and broadening of spectral lines*, Springer, Berlin, 1981.

Received January 20, 2023