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NUCLEAR THRESHOLD CUSP AND ATOMIC QUANTUM DEFECT - UNITARY APPROACH -

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This work relates the theories of Nuclear Threshold Cusp and Atomic Multichannel Quantum Defect to the Reduced Scattering/Collision Matrix. The Reduced Scattering Matrix accounts for the effect of the eliminated (invisible or unobserved) channels on the retained (observed) ones. The Cusp Theory does emerge in zero-energy limit of the Reduced Scattering Matrix approach. The Multichannel Quantum Defect Theory, according to present approach, does relate the Scattering Matrices of same reaction system which differ only in Reaction Dynamics of the eliminated channel.

1. INTRODUCTION

The Threshold Cusp and Multichannel Quantum Defect are cardinal concepts in Atomic and Nuclear Scattering Physics. Both concepts were devised to describe phenomena which occur near thresholds delimiting the bound and scattering states. The traditional fields of Nuclear and Atomic Physics are the Spectroscopy (study of bound states) and Reactions/Collisions (study of continuum). The transition zone discrete-continuum is of current interest for many problems of Atomic and Nuclear Physics, *e.g*. Rydberg Atoms or Halo Nuclei and Threshold Effects.

The Threshold Cusp was devised by Wigner [1] in order to describe the "breaking" in energy derivative of cross-section for a nuclear reaction due to opening of a neutron threshold channel. The Nuclear Threshold Cusp is the effect induced in open reaction channels by the opening of an *s*-wave neutron channel provided the reaction mechanism is potential scattering. The Threshold Physics field appears to be more rich in phenomena than in Cusp Theory, (see [2]). The threshold effects variety can be described in an unitary approach, [3], according to Reduced Scattering Matrix.

The Atomic Quantum Defect, [4], is a global parameter describing the effect of the inner electronic core on the peripherical electrons of Hydrogen-like atoms. The Atomic Quantum Defect does simulate the effect of the inner electron core on both spectra and scattering phase shift of outer electrons. This concept was initially devised in order to describe the modified Balmer spectra; later on it was extended to electron collision processes, involving resonances. The resonances in electron multichannel scattering on atoms or ions originate either in multielectron excitations of inner electronic core or from excitation of Rydberg far-away located states; these are called "inner" and "channel" resonances", respectively. The excitation of the inner electronic core results in multichannel scattering; the corresponding theoretical frame is Multichannel Quantum Defect Theory.

This work embodies the two theories devoted to the phenomena occurring below and above threshold in the frame of Reduced Scattering/Collision Matrix. The Reduced Scattering Matrix, [5], is a concept similar to that of Reduced *R*- (*K*-) Matrix, taking into account the effect of eliminated channels on the retained (observed) ones. The Scattering Matrix is primary object of Scattering Theory and it describes the complete Dynamics of reaction processes. The Reduced *S*- Matrix approach to scattering problems has the major physical advantage to use only effective physical quantities.

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2. NUCLEAR THRESHOLD CUSP

The threshold effects in a multichannel reaction system originate in conservation of the flux. The opening of a new (threshold) reaction channel results into redistribution of flux in old open channels, *i.e.* changes of their reaction cross-sections. The modification of reaction cross-sections of open channels, due to opening of a threshold one, is called threshold effect.

The threshold effect's magnitude should be proportional to the amount of the flux absorbed by the threshold channel. If the threshold channel has no barriers, *i.e.* it is an *s*- wave neutron one, a sudden transfer of flux is produced, resulting in a specific threshold effect, called Threshold Cusp. Because the flux in *s*-wave neutron threshold channel is proportional to channel wave number, (*i.e.* $\sim\sqrt{E}$), one obtains that the Threshold Cusp has an infinite energy derivative just at zero (threshold) energy; actually, here comes from the Cusp denomination. The Threshold Cusp should be an universal phenomenon, appearing with every new *s*-wave neutron channel. For higher partial waves, the centrifugal barrier should inhibit flux transfer between the neutron threshold channel and the observed open ones and, accordingly, should result in a smaller threshold effect.

The Cusp Theory, [6], does assume the Scattering Matrix elements, near *s*-wave neutron channel threshold, depend on neutron energy, E_n, or its wave number, k_n, only via (monotone) penetration factors, ($k_n \to 0$),

$$S_{nn} = 1 - N_{nn} k_n \; ; \; S_{an} = M_{an} k_n^{1/2}$$

$$S_{ab} = S_{ab}^0 + \Delta S_{ab} = S_{ab}^0 + A_{ab} k_n$$

The unitary S^0 - Scattering Matrix describes the N open channels, ($a, b = 1,2,\cdots, N$), system in absence of threshold channel, $n = N+1$. The matrices N, M, A are supposed constant ones. The Scattering Matrix Unitarity results into evaluation, in zero energy limit, $k_n \to 0$, of the Cusp term for open channels; it is related to transitions to and from threshold channel.

$$\Delta S_{ab} = (1/2) S_{an} S_{nb} = (1/2) M_{an} M_{nb} k_n$$

In order to deal explicitly with neutron penetration factor one has to work with Collision Matrix U, parameterized in terms of R-Matrix and Logarithmic Derivative, $L = S + iP$, (S- Shift factor, P- Penetration factor), [7],

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

The R- Matrix approach to Threshold Cusp has to evaluate the difference, $\Delta U_{ab} = U_{ab} - U_{ab}^0$, where U_{ab}^0 is Collision Matrix for "bare" N- open channels, (parameterized with R- Matrix block of N open channels), and U_{ab} is evaluated in terms of complete R- Matrix, for both open and threshold channels. The Cusp term of Collision Matrix is, in zero-energy limit,

$$\Delta U_{ab} = (1/2) U_{an} U_{nb} (L_n / iP_n)$$

(L_n - n channel logarithmic derivative, P_n - penetration factor), which for s-wave neutron scattering, $L_n = iP_n$, reduces to the S- Matrix one. A similar formula was obtained, up to a phase, by Abramovich, Baz and Guzhovskii [8],

$$\Delta U_{ab} = L_n M_{an} M_{nb}$$

with M_{an}, M_{nb}, considered as constants.

Below threshold k_n and P_n become pure imaginary and consequently the Cusp effect in open channels, below ($<$) and above ($>$) threshold, are linked by a simple relation, $\Delta S^{<} = i\Delta S^{>}$ and

$\Delta U^{<} = i\Delta U^{>}$. In this paper one proves that the Cusp Theory is obtained in zero-energy limit of Reduced Scattering Matrix, provided the reaction mechanism is the potential scattering.

3. ATOMIC QUANTUM DEFECT

The spectra of a Hydrogen-like atom is described by formula, $E_n = I - \mathrm{R}/(n^*)^2$, where R is Rydberg energy, I is the continuum threshold, n^* is effective quantum number, $n^* = n - \mu_n$, n - principal quantum number and μ_n - quantum defect describing the effect of the inner electronic core on peripherical electrons, [4]. The inner electronic core provides an additional short range potential, (deviation from pure Coulomb potential), resulting in shifts of electronic spectra, below threshold, and in scattering phase shifts $\delta(E)$, above threshold, (Seaton's Theorem), $\delta(E = I) = \pi\mu(E = I)$. For long range Coulomb potential there exist a specific connection between a quasi-continuum of bound states just below threshold and the genuine continuum of scattering states above threshold. The One-Channel Quantum Defect Theory describes both phenomena, below and above threshold, through the equation, ($K = \tan\pi\mu$), [9],

$$\tan\pi\nu + K = 0$$

where the effective quantum number $\nu = n^*$ is defined either by spectra $E = I - \mathrm{R}/\nu^2$ or by scattering phase shift $\nu(E) = \delta(E)/\pi$.

The excitation of the electrons in the inner core results in scattering channels; the corresponding theoretical frame becomes now the Multichannel Quantum Defect Theory. The Multichannel Quantum Defect Theory (MQDT) is based on possibility of separating the effects of long and short range interactions between an electron and the atomic core (*e.g.* [4]). The effect of short range interactions, within the core, are very complex but 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 analytically by extensive use of Coulomb or other special functions. The general assumptions of the MQDT are similar to those of R-Matrix Theory, (*e.g.* [7]). Developing this idea and by using only basic properties of Whittaker and Coulomb functions, Lane [10] 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.

The MQDT equation, in terms of K - Matrix reads as, ($\beta = \pi\nu$), [11],

$$S = -1 + 2i(K + i)^{-1}$$

$$\mathrm{K}_{\mathrm{N}}^{<} = K_N - K_{Nn}[\tan\beta + K_{nn}]^{-1} K_{nN}.$$

One can prove, [12], that K- Matrix form of MQDT can be obtained from Reduced R- Matrix for eliminated closed channel n

$$\mathrm{R}_{N}^{<} = R_N - R_{Nn} \frac{1}{R_n - 1/L_n^{<}} R_{nN}$$

The formal equivalence, [13], of K- and R- Matrix with natural boundary conditions, $K = P^{1/2} R P^{1/2}$, results into

$$\mathrm{K}_{N}^{<} = K_N - K_{Nn}[\tau_{nn} + K_{nn}]^{-1} K_{nN}.$$

where $\tau_{nn} = \tau_n = \operatorname{Im}\Delta L_n / \operatorname{Re}\Delta L_n$, and $\Delta L_n = L_n^> - L_n^<$ is jump across threshold of the eliminated channel logarithmic derivative, (above threshold, $\mathrm{K}_N^>$, $\tau_n = i$). The Coulomb (bound states) case corresponds to $\tau_n = \tan \pi\nu$ as discussed by Hategan and Ionescu [14].

One obtains that the R-Matrix parameterization $\mathrm{R}_N^<$, of the MQDT is just Wigner Reduced R-Matrix, as defined in Lane and Thomas [7]. The basis for this equivalence is physical analogy between the two concepts; both describe not only the internal dynamics but also the interaction from eliminated closed channels.

4. REDUCED SCATTERING MATRIX

Consider the multichannel system of N open (retained) channels, decoupled from the threshold (unobserved, eliminated) channel n. The "bare" independent open channels are described by unitary Scattering Matrix $S_N^0 = \left\| S_{ab}^0 \right\|$. By coupling the threshold channel $n = N+1$, to N open ones, via S_{na} matrix elements, one obtains the Reduced Scattering Matrix $S_N = \left\| S_{ab} \right\|$ for retained channels, [13]; it includes both bare S_N^0 Scattering Matrix and the effect ΔS, of eliminated channel

$$S_{ab} = S_{ab}^0 + \Delta S_{ab} = S_{ab}^0 + S_{an} \frac{1}{1 + S_{nn}} S_{nb}$$

The Reduced Scattering Matrix does include, as limit case, the Cusp Theory, $S_{nn} \to 1$.

The Reduced Collision Matrix U_N is referring to retained (N) channels, but including the effect of eliminated (n)-one. It consists from Collision Matrix U_N^0 which describes the "bare" retained channels (N), uncoupled to eliminated (n) channel, and from an effective term ΔU_N describing this coupling. The Reduced Collision Matrix evaluated above (n), $(>)$, is, [14],

$$U_N^> = U_N^0 + \Delta U_N^>$$

$$\Delta U_N^> = U_{Nn}^> \frac{1}{-L_n^* / L_n + U_{nn}^>} U_{nN}^>$$

For neutron s-wave, $L_n = iP_n$, or for natural boundary conditions or for Teichmann-Wigner-Lane boundary conditions one obtains the Reduced S - Matrix result,

$$S_N^> = S_N^0 + S_{Nn}^> \frac{1}{1 + S_{nn}^>} S_{nN}^>$$

By Reduced Collision Matrix procedures one can relate two reactions systems with same internal dynamics, (R - Matrix), differing only in interactions in eliminated threshold channel, ($L_n^>$ and $L_n^<$).

$$U_N^< = U_N^0 + \Delta U_N^<$$

$$\Delta U_N^< = \Delta U_N^> \frac{1/L_n^> - \mathrm{R}_{nn}}{1/L_n^< - \mathrm{R}_{nn}}$$

$$\mathrm{R}_{nn} = R_{nn} - R_{nN}(R_{NN} - L_N^{-1})^{-1} R_{Nn}$$

$$U_{nn}^{>} = 1 + 2iP_n(\mathrm{R}_{nn}^{-1} - L_n^{>})^{-1}$$

For example the Reduced Collision Matrix for negative energies (closed channel, $<$) is expressed in terms of positive energy quantities ($U^{>}$, $L^{>}$) and also of quantities specifying eliminated closed channel (logarithmic derivative $L_n^{<}$ and Reduced R-Matrix element R_{nn}). We remark, the last equations contain basic formulae of the Cusp Theory, both above and below n-threshold. For nuclear s-wave scattering, the logarithmic derivatives are $L_n^{>} = i\rho$ and $L_n^{<} = -\rho$, ($\rho = k_n \cdot a$; k_n \$ - channel wave number, a - channel radius). The Cusp Theory result, below threshold, $\Delta U_N^{<} = i\Delta U_N^{>}$, is obtained, in zero energy limit ($\rho \to 0$), of above formulae.

The effective term ΔU_N of Reduced Collision Matrix, valid both below and above n-threshold, becomes

$$\Delta U_N = \frac{1}{2i}(U_N^0 - L_N^* L_N^{-1}) P_N^{-1/2} L_N R_{Nn} \frac{1}{L_n^{-1} - \mathrm{R}_{nn}} R_{nN} L_N P_N^{-1/2} (U_N^0 - L_N^* L_N^{-1})$$

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

The n-channel related effects on retained channels (N) are expressed by the product $R_{Nn}(L_n^{-1} - \mathrm{R}_{nn})^{-1} R_{nN}$, resembling to effective term of the Reduced R- Matrix R_N. However there is a difference, namely the "bare" R-Matrix element R_{nn} of eliminated n-channel is here replaced by its effective counterpart R_{nn}; the Reduced R_{nn} - Matrix element does include also rescattering effects from complementary open channels.

The K- Matrix form of effective term in Collision Matrix can be obtained via formal equivalence of K- Matrix and R- Matrix, [13], with natural boundary conditions, $B = S^{>} = \mathrm{Re}\, L^{>}$, *i.e.* $K = P^{1/2} R_S P^{1/2}$, $R_S = (R^{-1} - S)^{-1}$, $L_N = iP_N$, $L_n^{>} = iP_n$, $L_n^{<} = S_n^{<} - B_n = S_n^{<} - S_n^{>} = -\Delta S_n$ and $(L_n^{-1} - \mathrm{R}_{nn})$ transforms into $(\tau_{nn} + \mathrm{K}_{nn})$, with $\tau_{nn}^{>} = i$ and $\tau_{nn}^{<} = \tau_n$. In above 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 $(\Delta L_n)^* / (\Delta L_n)$ allows to define a "phase shift" δ_n, and a "K-Matrix element" $\tau_n = \tan \delta_n = \mathrm{Im}\, \Delta L_n / \mathrm{Re}\, \Delta L_n$. One can prove, by evaluating ΔL_n near threshold for Coulomb field, (*e.g.* [6]; [15]), that the δ_n phase shift is related to effective quantum number of MQDT, [14]. For s-wave scattering on external (outside inner core) neutral fields, ΔL_n is proportional to $(1+i)$ and $\delta_n = \pi/4$, (*e.g.* [16]).

The Reduced S- Matrix, in K- Matrix terms, is now

$$\Delta S_N = \frac{1}{2i}(S_N^0 + 1) K_{Nn} \frac{1}{\tau_{nn} + \mathrm{K}_{nn}} K_{nN} (S_N^0 + 1)$$

$$\Delta S_N^{<} = \Delta S_N^{>} \frac{i + \mathrm{K}_{nn}}{\tau_n + \mathrm{K}_{nn}}$$

$$\mathsf{K}_{nn} = K_{nn} - K_{nN} (K_{NN} + i \cdot 1)^{-1} K_{Nn}$$

The Cusp relations, $\Delta S_N^< = i \Delta S_N^>$, are obtained in zero energy limit ($\mathsf{K}_{nn} \to 0$ and $\tau_n = 1$) for s-wave neutron channel.

Interesting physical results could emerge for study of resonances according to present approach. The resonances are described via condition $\tau_{nn} + \mathsf{K}_{nn} = 0$ for denominator of effective term in Scattering Matrix. The Reduced K- Matrix element K_{nn} takes into account the rescattering effects from complementary channels; the rescattering effects are absent in the usual approaches.

One concludes this paragraph that Reduced Scattering/Collision Matrix does reproduce the Cusp Theory (for positive energy) as well as Multichannel Quantum Defect Theory (for negative energy).

5. CONCLUSIONS

Two Quantum Scattering problems, the Threshold Cusp and Multichannel Quantum Defect, were approached in terms of Reduced Scattering/Collision Matrix. The Reduced S- (U-) Matrix describes effects originating in unobserved channels; they are induced in observed open channels via channel couplings (real or virtual transitions). The Cusp and other types of threshold effects are described in zero-energy limit of Reduced S- Matrix. The Quantum Defect, observed both in atomic spectra and collisions, is described according to Reduced S- Matrix too. It is proved the Multichannel Quantum Defect formalism is a relation of the Reduced S- Matrix at negative energy and its counterpart defined above threshold. The Reduced S- Matrix approach to MQDT does evince the role of rescattering effects (from complementary channels) in producing multichannel resonances originating in single particle states.

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