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MULTICHANNEL QUANTUM DEFECT AND REDUCED R-MATRIX

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This work demonstrates that 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 Quantum Defect Theory is, according to present approach, a general framework relating collision matrices of two reaction systems which differ only in dynamics of eliminated channels.

Key words: Quantum Defect, 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 (*e.g.* Seaton 1983). 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 a simple field as *e.g.* the Coulomb one), are treated analytically by extensive use of Coulomb wavefunctions; this fact resulted into perception that the MQDT is a specific theory for atomic collisions. On the other hand the general assumptions of the MQDT are similar to those of R-Matrix Theory, (*e.g.* Lane and Thomas 1958). Developing this idea and by using only basic properties of Whittaker and Coulomb functions, Lane (1986) 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. At this level of derivation, the role of single particle states (from eliminated closed channel) for producing resonances in the competing open reaction channels of the multichannel system is proved; this is done by relating the above approach to the R-Matrix bound state condition. 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 parameterized (Lane and Thomas 1958) in terms of the R-Matrix, the Coulombian hard-sphere phase shifts Φ, the logarithmic derivative L and its imaginary part, penetration factor P,

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

Another form suitable for the present purpose is

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

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, ($a,b = 1,2,\ldots,N$); 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 collision U (W)

square matrices 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

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

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

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

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 $(\Delta L_n)/(\Delta L_n)^{*}$ allows to define a "defect scattering phase shift" δ_n, a corresponding "K-Matrix element" $\tau_{nn}=\tan\delta_n$, and a "collision matrix element" $U_{nn}^{\delta}(W_{nn}^{\delta})$

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

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

The collision matrix form of the MQDT

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

results into a corresponding K-matrix form, (Hategan and Ionescu 1995)

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

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

One can prove, by evaluating ΔL_n near threshold for Coulomb field, (*e.g.* Baz *et al* 1971; Landau and Lifshitz 1980), that the δ_n phase shift is related to effective quantum number of MQDT, $\delta_n=\pi|\eta|$.

It is worthy of mention another result which can be obtained from collision matrix formula (6) of MQDT

$$U_N^{<}U_{Nn}^{>+}=e^{-2i\delta_n}\frac{(U_{nn}^{>}-e^{-2i\delta_n})^{*}}{(U_{nn}^{>}-e^{-2i\delta_n})}U_{Nn}^{>} \tag{8}$$

In zero energy limit, for scattering on a short range potential, $U_{nn}^{>}\to 1$, it reduces to $U_N^{<}U_{Nn}^{>+}=-U_{Nn}^{>}$, a result of R-Matrix Theory, (Lane and Thomas 1958).

Obtaining the U-Matrix and standard K-Matrix forms of MQDT, we have, in next step, to relate them 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), one uses the R-Matrix parameterization of the collision matrix below threshold

$$W_N^{<} = 1 - 2iP_N^{1/2} L_N^{-1} P_N^{1/2} + 2iP_N^{1/2} L_N^{-1} (L_N^{-1} - \mathsf{R}_N^{<})^{-1} L_N^{-1} P_N^{1/2} \tag{9}$$

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

$$(\Delta L_n)/(\Delta L_n)^* = 1 - 2iP_n L_n^{-1} + 2iP_n L_n^{-2} (L_n^{-1} - \rho_n)^{-1} \tag{10}$$

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

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

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

$$\mathsf{R}_N^{<} = R_N - R_{Nn} \frac{1}{R_n - \rho_n} R_{nN} \tag{11}$$

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 parameterization of the MQDT is just Wigner reduced R-Matrix, as defined in Lane and Thomas (1958). The physical basis for this equivalence is following 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" resonances corresponding, respectively, to multielectron excitations and to Rydberg states. Both describe not only the internal dynamics but also the interaction of eliminated closed channels.

The next step is to exploit the physics contained in U (W) matrix form (4) of the MQDT, (Hategan, Ionescu and Wolter, work in progress). The collision matrix dependence on eliminated channel is contained in the product $R_{Nn}(L_n^{-1} - \mathsf{R}_{nn})^{-1} R_{nN}$, where R_{nn} is the reduced R-Matrix element of the n channel. The inner multichannel resonances are described by R-Matrix while the channel resonances are represented by L_n^{-1} logarithmic derivative. In the R-Matrix theory, usually, one considers only multichannel resonances described by poles of all its elements; in Lane's approach to MQDT, (Lane 1986), the Rydberg resonances are described by a meromorphic term added to genuine R-Matrix. There are also multichannel resonances originating in single particle (bound or quasistationary) states as proved in following two paragraphs.

Below threshold a pole in $U_N^{<}$ collision matrix elements could be obtained from the condition $\mathsf{R}_{nn}^{-1} = L_n^{<} = S_n^{(-)}$, ($S_n^{(-)}$ - shift function). In non-coupling limit, R_{nn} reduces to single channel R-Matrix element R_{nn}. Or this is just bound state condition of the R-Matrix Theory, (Lane and Thomas 1958); 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 channel state of a closed channel does induce resonance in competing open channels of the multichannel system. The above result is known in a different framework of the Collision Theory, (*e.g.* Drukarev 1978); but this is the first R-Matrix demonstration of the relation of a multichannel resonance to a bound single particle state. The above result transcends the MQDT framework, being a general result in R-Matrix theory too.

The standard form of the MQDT was derived only for (bound states in) eliminated closed channels; extended (see next paragraph) 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, $\mathsf{R}_{nn}^{-1} = L_n$; 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 $|1 - R(H_\lambda)L| = 0$, (Lane and Thomas 1958). A quasistationary state originating in an eliminated channel induces a quasiresonant structure in other open competing channels. Apparently, (see, for example, Kukulin *et al* 1989), this situation (multichannel resonance originating in a quasistationary state from an unobserved channel) was not reported until now. In the literature (Badalyan *et al* 1982) 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.

To complete this R-Matrix approach one has to remark that, according to present derivation, MQDT does provide a relation connecting collision matrices of two multichannel systems which differ only in interaction from the eliminated channel, (3). Therefore the derivation can be extended also to the case when the eliminated channel n of both reaction systems is open; both logarithmic derivatives $L_n^>$ and $L_n^<$ refer now to positive energy but they will correspond to different interactions in unobserved (eliminated) n-channel. The "defect" scattering phase shift δ_n becomes complex, $\mathrm{Im}\,\delta_n > 0$, and U_{nn}^δ is not more unitary. This form of 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 (*e.g.*, monotone- and resonant-logarithmic derivatives for the same n-channel of the two reaction systems). If the logarithmic derivatives of the eliminated n channel do coincide, $\Delta L_n = 0$, ($U_{nn}^\delta = 0$), then the collision matrices of the two multichannel systems are identical, as it should be. If the n-channel logarithmic derivative of one reaction system is zero (decoupling n-channel from that multichannel system), one obtains the reduced collision matrix (analogue of reduced R-Matrix) which includes generalization of the threshold Cusp Theory.

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