Siegert State Approach to Quantum Defect Theory

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Abstract

The Siegert states are approached in framework of Bloch-Lane-Robson formalism for quantum collisions. The Siegert state is not described by a pole of Wigner $R$- matrix but rather by the equation $1 - R_{nn} L_n = 0$, relating $R$- matrix element $R_{nn}$ to decay channel logarithmic derivative $L_n$. Extension of Siegert state equation to multichannel system results into replacement of channel $R$- matrix element $R_{nn}$ by its reduced counterpart $R_{nn}$. One proves the Siegert state is a pole, $(1 - R_{nn} L_n)^{-1}$, of multichannel collision matrix. The Siegert equation $1 - R_{nn} L_n = 0$, ($n$ - Rydberg channel), implies basic results of Quantum Defect Theory as Seaton’s theorem, complex quantum defect, channel resonances and threshold continuity of averaged multichannel collision matrix elements.
1 Introduction

Quasistationary states with complex eigenenergies have been introduced as an important concept in theories of quantum collisions and decay. They were firstly introduced by Gamow as complex-energy eigenstates in order to describe radioactive decay, associating the lifetime of a quasistationary state with the imaginary part of its energy. Thereafter Kapur and Peierls introduced a discrete set of complex energy eigenstates depending on the scattering energy. Siegert [1] introduced a class of solutions of the Schrödinger equation satisfying regularity conditions at the origin and an outgoing-wave boundary conditions at infinity. The Siegert solution is given as a discrete set of complex momenta \( k_\lambda \) which are the poles of the collision matrix in the complex \( k \)-plane. Pure positive imaginary momenta represent bound states, pure negative imaginary ones virtual states, and poles lying close but below the real positive \( k \)-axis quasistationary or resonant states. The Siegert states provide a unified description of bound and resonant states.

Gamow-Siegert states were and are an important ingredient in quasistationary formalisms, e.g. [2], in Green function formalisms, e.g. [3], or in the Rigged Hilbert Space formulation, e.g. [4, 5].

The present approach to Siegert state is developed in framework of Bloch-Lane-Robson formalism for quantum collisions, [6, 7], using Bloch boundary condition operator \( \mathcal{L} \), [8]. The boundary condition should be congruent with outgoing behaviour at infinity of the Siegert state. The usual Schrödinger equation and Bloch out wave operator result into an eigenvalue equation for Siegert state. The Schrödinger equation for Siegert state is rewritten in channel space in terms of scattering operators; it will result into an equation, \( 1 - R_{nn}L_n = 0 \), relating \( R \)-matrix element to logarithmic derivative of decay channel. Implication of (bound or quasistationary) Siegert state equation in multichannel collisions results into a pole, \( (1 - R_{nn}L_n)^{-1} \), of collision matrix. The Siegert state equation, in its \( R \)-matrix parametrization, is applied to electron scattering on atoms resulting in a new approach to Multichannel Quantum Defect Theory.

2 Siegert State in Collision Theory

In this section we follow the formalism of Lane and Thomas [9] and Lane and Robson [6, 7]. The Bloch outgoing-wave boundary condition operator,
for short the Bloch operator, is defined by

\[ L = \sum_c |c > \frac{\hbar^2}{2m_c} \delta(r_c - a_c) \left[ \frac{d}{dr_c} - \frac{b_c - 1}{a_c} \right] < c| \] (1)

\[ b_c = a_c \frac{dO_c}{dr} / O_c \] (2)

where \( |c > \) and \( O_c \) denote a channel state and the channel outgoing wave, \( r_c \) and \( m_c \) the channel coordinate and reduced mass, and \( a_c \) the channel radius, respectively. This Bloch operator \( L \) projects out outgoing-waves states in all channels provided the set \( |c > \) is orthogonal.

Given a hamiltonian \( H \), we define an ideal state \( |\lambda > \) by, [7],

\[ (H - E_\lambda)|\lambda > = 0 \] (3)

e.g an R-matrix state, subject to mixing with complementary states due to changes in boundary conditions and interactions. The Siegert state \( |g_\lambda > \), on the other hand, as a purely outgoing one, is an eigenstate of the Bloch operator with zero eigenvalue, \( L|g_\lambda > = 0, [10] \). It obeys a modified Schrödinger equation, [7],

\[ (H + L - E)|g_\lambda > = (E_\lambda + \Phi_\lambda - E)|\lambda >, \] (4)

with \( \Phi_\lambda \) a quantity defining a complex level shift. Inserting it into the usual Schrödinger equation

\[ (H + L(E') - E')|g_\lambda > = L(E')|g_\lambda > = 0 \] (5)

one obtains a constraint for the energy of the quasistationary state \( |g_\lambda > \), namely \( E' = E_\lambda = E_\lambda + \Phi_\lambda \).

We also define the corresponding Green operator for the Hamiltonian \( H \) and boundary condition \( L \) as, [11]

\[ G = (H + L - E)^{-1}. \] (6)

The Siegert state equation \( G^{-1}|g_\lambda > = 0 \) is rewritten in channel space by projecting on the adjunct state \( < \tilde{g}_\lambda c \) and by inserting the channel projector \( \sum_c |c >< c| \), assuming that the channels \( c \) exhaust the decay of Siegert state,

\[ \sum_{c\tilde{c}} \tilde{\omega}_{\lambda c} < c|G^{-1}(E_\lambda)|\tilde{c} > \omega_{\tilde{c}' \lambda} = 0 \]
with \( \omega \) as the Siegert state reduced widths.

The Green operator \( \mathcal{G} \) defines the \( \mathcal{R} \) matrix, \[11\],

\[
\mathcal{R}_{cc'} = \langle c' | \mathcal{G} | c \rangle
\]

(7)

associated with collision matrix \( U \),

\[
U = \Omega W \Omega = \Omega (1 + 2 i P^\dagger \mathcal{R} P^\dagger) \Omega
\]

(8)

where \( \Omega \) and \( P \) are the phase and penetration factor diagonal matrices \[9\].

The Siegert state equation in terms of the \( \mathcal{R} \) matrix becomes

\[
\sum_{cc'} \tilde{\omega}_{\lambda c} \mathcal{R}_{cc'}^{-1} \omega_{c' \lambda} = 0
\]

(9)

The Green operator is related to the \( R \)-matrix, as, \[6\],

\[
\mathcal{R}_{cc'} = [(1 - RL)^{-1} R]_{cc'}
\]

(10)

with \( L \) as the channel logarithmic derivative. The Siegert state equation in \( R \)-matrix terms becomes

\[
\sum_{c'} (1 - RL)_{cc'} \omega_{c' \lambda} = 0
\]

(11)

The poles \( \mathcal{E}_\lambda \) are the complex roots of the determinant equation

\[
|1 - R(\mathcal{E}_\lambda)L(\mathcal{E}_\lambda)| = 0
\]

(12)

Both \( R \) and \( L \) are energy dependent and are assumed to be analytically continuable to complex \( \mathcal{E}_\lambda \).

We now consider the case of Siegert state \( g_\lambda \) in a particular channel \( c = n \). Coupling to other channels is taken into account in terms of the multi-channel reduced \( R \)-matrix element \( \mathcal{R} \),

\[
\mathcal{R}_{nn} = [(1 - RL)^{-1} R]_{nn} = (1 - \mathcal{R}_{nn} L_n)^{-1} \mathcal{R}_{nn}
\]

(13)

It is a complex quantity due to implication of open channels logarithmic derivatives in its very definition \[9\]. Accordingly, the single channel equation for the quasistationary level \( g_\lambda \) in channel \( n \) becomes

\[
|1 - \mathcal{R}_{nn}(\mathcal{E}_\lambda)L_n(\mathcal{E}_\lambda)|\omega_{n\lambda} = 0
\]

(14)
The complex energy pole $\mathcal{E}_\lambda$ is again given by the implicit equation $1 - \mathcal{R}_{nn}(\mathcal{E}_\lambda) L_n(\mathcal{E}_\lambda) = 0$.

To summarize this section, the matching of the R-matrix element $R_{nn}$ to the channel logarithmic derivative $L_n$ is expressed by the channel equation $1 - R_{nn} L_n = 0$. Below threshold, with $L_n = S_n$ ($S_n$ - shift function), this is the R-matrix equation for bound states, $1 - R_{nn} S_n = 0$ or $R_{nn}^{-1} = S_n$: a bound state appears at that energy at which the internal $R_{nn}^{-1}$ and the external $S_n$ logarithmic derivatives match. At positive energy it is the logarithmic derivative $L_n$ of the outgoing wave which has to match the logarithmic derivative of internal wave function $R_{nn}^{-1}$ at the channel radius. This condition defines the quasistationary state. The root of the implicit equation $1 - R_{nn}(\mathcal{E}_\lambda) L_n(\mathcal{E}_\lambda) = 0$ is a complex energy pole $\mathcal{E}_\lambda$. As in the case of bound states, the equation yields a set of eigenenergies which now are complex. Thus the channel equation $1 - R_{nn} L_n = 0$ defines both the bound state (below threshold) or quasistationary state (above threshold).

The R-matrix Siegert equation in case of multichannel systems becomes $1 - \mathcal{R}_{nn}(\mathcal{E}_\lambda) L_n(\mathcal{E}_\lambda) = 0$ where $\mathcal{R}_{nn}$ is reduced R-matrix element. The essential term in the collision matrix, describing effect of the eliminated channels on channel $n$, is $(1 - \mathcal{R}_{nn} L_n)^{-1}$, both below and above $n$-channel threshold. The collision matrix formalism, expresses here in the R-matrix approach in terms of Siegert states, is applied in the next chapter to electron scattering on atoms.

3 Siegert State and Quantum Defect Theory

The Siegert R-matrix equation, $L_n^{-1} - \mathcal{R}_{nn} = 0$, can be discussed in two different aspects, either with respect to the R-matrix element or to the logarithmic derivative. The logarithmic derivative can have a resonant form, eg as proposed by Abramovich et al [12], resulting in a generalization of the Wigner-Breit-Baz threshold cusp theory. In atomic physics an energy-dependent logarithmic derivative with poles on the real axis is used for studying Rydberg states, at negative energy. By applying the Siegert equation to electron Rydberg states, we derive in a new way basic results of Quantum Defect Theory.

This approach to QDT, based essentially on Siegert equation, is an alternative to classical variant. It follows the spirit of previous approaches to MQDT based on R-Matrix [13] or on Level-matrix. The Siegert equa-
tion implies Seaton’s theorem both for one-channel and multichannel problems, relating the complex quantum defect to complex scattering phase-shift. Thereafter the Level- matrix approach is reformulated in order to relate (multichannel) collision matrix to Siegert equation. The MQDT collision matrix, in its relation to Siegert equation, is applied to derivation of channel resonances and to prove the Threshold Continuity Theorem. This theorem relates the collision matrix elements above threshold to the averaged ones below threshold; it is an alternative to Gailitis’ theorem.

3.1 Quantum Defect and Siegert Equation

The logarithmic derivative of a purely Coulombic electron state \( n \equiv e; e \) Rydberg channel label) for energy \( E \) below the threshold energy \( E_\pi \) is given by, [14] p. 408, [15], [16] p. 708, \( L_e^< = -\cot \pi \sqrt{e_1^2 e_2^2 m/2h^2 (E_\pi - E)} \) \( (e_1, e_2, \) and \( m \) are the particles electric charges and the reduced mass, respectively). The pure Coulomb states, i.e. in the absence of an inner core, are defined by the level equation \( (L_e^<)^{-1} = 0 \). It yields the eigenenergies \( E_\pi - E_n = (1/n^2) e_1^2 e_2^2 m/2h^2 \), with \( n \) an integer number, the principal quantum number.

We now consider an inner electron core, characterized by a finite R-matrix element \( R_{ee} \), and a level equation \( (L_e^<)^{-1} - R_{ee} = 0 \). We are interested in Rydberg states, which have a very large spatial extent relative to the core. Thus we are allowed to use the same form of the logarithmic derivative as above. Then the effect of the inner core on the electron spectrum (resulting into a level-shift) is expressed by replacing the principal quantum number \( n \) by an effective non-integral quantum number \( \nu \), or a so-called quantum defect \( \mu \) defined by the relation \( \nu = n - \mu \). The logarithmic derivative below threshold then is written as \( L_e^< = -\cot \pi \nu = \cot \pi \mu \) and the relation between the eigenenergies and the effective quantum number is \( E_\pi - E_\nu \propto 1/\nu^2 \). The condition for a single electron bound Rydberg state is now \( \tan \pi \mu = R_{ee} \). It constitutes a relation between the one-channel quantum defect \( \mu \) to the Rydberg channel R-matrix element \( R_{ee} \). Let proceed with Siegert equation to Seaton’s theorem and to complex quantum defect.

The logarithmic derivative for an attractive Coulomb channel above threshold is \([14, 15, 16] L_e^> = i; \) in zero-energy limit the channel penetration factor is \( P_e = 1 \) and its shift-factor is \( S_e = 0 \). The equation for the scattering phase-shift \( \delta_e \) in an open electron channel given in R-matrix theory by \( \tan \delta_e = R_{ee} P_e/(1 - R_{ee} S_e) \), reduces to \( \tan \delta_e = R_{ee} \). Comparing to the above
relation for a Rydberg state we obtain Seaton theorem, $\delta_e = \pi \mu$, relating the scattering phase shift above threshold to the quantum defect of the spectrum below threshold. For a single channel the quantum defect and the phase shift are real.

In a multi-channel situation with a coupling of the closed channel $e$ to other closed and open channels the reduced $R$-matrix element $R_{ee}$ is complex. Thus the Siegert equation becomes

$$R_{ee} = \tan \pi \tilde{\mu} = \tan \tilde{\delta}_e,$$

with complex quantum defect, $\tilde{\mu}$, and scattering phase shift, $\tilde{\delta}_e$. The imaginary part of complex quantum defect $\pi Im \tilde{\mu} = Im (\arctan R_{ee})$ is positive, provided $Im R_{ee}$ is positive too. Actually for a multichannel system $Im R_{ee} > 0$; resulting from relation of reduced $R$-matrix element, $R_{ee}$, to subunitary value of collision matrix one, $|W_{ee}| < 1$. The change $\Delta \mu = \tilde{\mu} - \mu$ of the quantum defect in the limit when $\tan \pi \mu \simeq \pi \mu$ becomes $\pi \Delta \mu = R_{ee} - R_{ee}$; it proves $\Delta \mu$ originates in effective term of reduced $R$-matrix element (i.e. coupling of Rydberg channel to complementary ones).

### 3.2 Multi-Channel Quantum Defect Equations

The one-channel Quantum Defect Theory assumes the inner multielectron core is inert. The only 'active' state is the Rydberg one, defining the 'Rydberg channel'. The Rydberg state is a highly excited bound state, located just below the ionization threshold and its eigenenergy is given by the quantum defect. When its energy rises above the threshold it is transformed into a scattering state characterized by a scattering phase shift. (As long as it is closely above threshold we will refer to it as a Rydberg state at positive energy.) The quantum defect below threshold is related to the scattering phase shift above threshold by Seaton’s theorem. In the following we will denote the situation when the Rydberg state is below threshold by the superscript $<$, and the one above threshold by $>$.

In the Multi-Channel Quantum Defect Theory (MQDT) we consider that the multielectron core can be excited, which generates several excited states, lower in energy than the Rydberg state. As the Rydberg state is very close to threshold, we assume that these excited states all form open channels. These then define the scattering channels, labelled by $N$, to which the Rydberg state is coupled. Above the Rydberg channel threshold the open channels
thus consist both of the $N$ core-excited channels and the Rydberg channel $n$. The $N + 1$ channel reaction system is described by the collision matrix $W^>$ with components $W^>_{NN}, W^>_{nn}$ and coupling terms $W^>_{Nn}$ and $W^>_{nN}$. Below threshold only the $N$ core-excited channels are open and the reaction system is described by the collision matrix $W^<_N$, which, of course, depends also on the closed Rydberg channel. But the essential difference between the situations of a closed and an open Rydberg channel is the change in the logarithmic derivatives $L^<_n$ and $L^>_n$. Thus MQDT relates collision matrix below threshold $W^<_N$ to the change across the threshold of the channel logarithmic derivative, $\Delta L^<_n = L^>_n - L^<_n$ and to the collision matrix elements above threshold $W^>_N$, $W^>_{nn}$, $W^>_{nN}$.

Assuming that the only changing parameter across the threshold is the $n$-channel logarithmic derivative we obtain the following relation connecting the collision matrices below and above threshold, provided $L^<_n$ is real, [17]

$$W^<_N = W^>_N - W^>_{NN} \frac{1}{(\Delta L^<_n)/(\Delta L^>_n) + W^>_{nn} W^>_{nN}}$$

(16)

The collision matrix $W^>_N$ above threshold is

$$W^>_N = W^0_N + W^>_{NN} \frac{1}{L^>_n/L^>_n + W^>_{nn} W^>_{nN}}$$

(17)

$$W^>_{nn} = 1 + 2iP^1/2 \frac{R^{-1}_{nn} - L^>_n}{P^1/2}$$

$$W^>_{nn} = L^>*/L^>_n + 2iP_n(L^>_n)^{-2} (L^>_n - R_{nn})^{-1}$$

$$R_{nn} = R_{nn} - R_{nN} (R_{NN} - L^>_n)^{-1} R_{nN}$$

$$W^0_N = 1 + 2iP^1/2 (R^>_n - L^>_n)^{-1} P^1/2$$

(18)

where $R_{nn}$ is reduced R-matrix element of the $n$ channel and and $W^0_N$ is the collision matrix for the $N$ uncoupled core-excited channels.

All $W^>$ Collision Matrix elements related to $n$-channel, $W^>_n$, $W^>_n$ and $W^>_n - L^>*/L^>_n$ are proportional to $(R_{nn} - L^>_n)^{-1}$ and this results into same dependence for the increment $\Delta W^>_N = W^>_N - W^0_N$.

$$\Delta W^>_N = A_{NN} (L^>_n - R_{nn})^{-1} A_{nN}$$

(19)

The complementary matrix term $A_{NN} = A_N R_{Nn}$ is not dependent on Siegert state paramaters $L_n$ and $R_{nn}$. The increment of collision matrix below...
threshold $\Delta W_N^< = W_N^< - W_N^0$ is proportional to $(R_{nn} - L_n^{<})^{-1}$ and has a similar dependence

$$\Delta W_N^< = A_{Nn}(L_n^{<})^{-1} - R_{nn})^{-1}A_{nN}$$  (20)

The increments of the collision matrix below and above threshold $\Delta W_N^<$ and $\Delta W_N^>$ due to the couplings are related as

$$\Delta W_N^< = \Delta W_N^> L_n^< - R_{nn} L_n^<$$  (21)

This relation involves Siegert equations below and above threshold. It gives rise to a pole of collision matrix below threshold defined by the Siegert equation for the closed channel $1/L_n^< - R_{nn} = 0$.

The above expressions give the MQDT equations for electron-atom collisions provided the logarithmic derivative of the Rydberg channel $n \equiv e$ is explicitly specified in the threshold limit. Using the results for the pure Coulombic case we have $L_e^< = -\cot \pi \nu$, $L_e^> = i$, $\Delta L_e = L_e^> - L_e^< = e^{i\pi \nu}/\sin \pi \nu$, $(\Delta L_e)^*/(\Delta L_e) = e^{-2i\pi \nu}$, $\tau = Im\Delta L_e/Re\Delta L_e = \tan \pi \nu$. Note that the only quantity here, strongly dependent on energy is the Rydberg channel logarithmic derivative $L_e^<$. We then obtain the MQDT result for electron-atom scattering (see [18, 19])

$$W_N^< = W_N^> - W_{Ne}^> - e^{-2i\pi \nu} + W_{ee}^> \quad (22)$$

The poles of collision matrix are related either to R-matrix or to Siegert equation, (eq. 22). The R-matrix poles correspond to “inner resonances”, originating in multielectron excitations of the inner core, [13]. The poles related to Siegert equation, $(1/L_{ee}^< - R_{ee})^{-1}$, describe the ”channel resonances” in electron scattering on atoms and ions. The ”channel resonances” originate in excitation of Rydberg far-away located states. The complex energies of ”channel resonances” are obtained either in terms of reduced R-matrix element or complex quantum defect, (see [18], or transition matrix element (see [20]).

For s-wave scattering on external (outside inner core) neutral fields, $L_n^> = iP_n = i\rho$, $L_n^< = S_n^< = -\rho$, $\Delta S_n = \rho$, $(\rho = k_n r)$, $(k_n$ -wave number, $r$-channel radius), one obtains $\tau = P_n/\Delta S_n = 1$ and arctan $\tau = \pi/4$, (see [21]). The increments in this case are related by $\Delta W_N^< = \Delta W_N^>(i + \rho R_{nn})/(1 + \rho R_{nn})$ which in zero-energy limit of potential scattering $(\rho \to 0)$ reduces to Wigner-Breit-Baz threshold cusp theory result $\Delta W_N^< = i\Delta W_N^>$, [14], ch.IX, [15].
3.3 Threshold Continuity Theorem

The collision matrix, both below and above $e$-threshold, is

$$ W_N = W^0_N + \Delta W_N $$

(23)

with $W^0_N$ as collision matrix for $N$ independent channels, (uncoupled to Rydberg one), and $\Delta W_N$ as effective term due to channels couplings. According to (20-21) the dependence on threshold channel of the effective term is

$$ \Delta W_N = A_N e (L^{-1} - R_{ee})^{-1} A_e $$

(24)

where for $\Delta W_N$ superscripts $>$ or $<$ one has to insert the corresponding logarithmic derivatives $L^>_e$ or $L^<_e$ of the channel $e$, respectively. In following $\Delta W_N$ denotes only the term $(L^{-1} - R_{ee})^{-1}$; the complementary matrix term $A_N e$ does not depend significantly on energy.

The only term of collision matrix $\Delta W_N$ strong dependent on energy is the closed Rydberg electron channel term $(L^{-1} - R_{ee})$. 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 for multielectron inner core is considered as nearly constant in threshold region. The energy average of the effective term below threshold $\Delta W^<_N$

$$ \overline{\Delta W^<_N} = \int \rho(E) dE \Delta W^<_N $$

(25)

where averaging weight is $\rho(E)$ - density of states, [14], p. 410, [15],

$$ \rho(E) = \frac{1}{2} e_1 e_2 \sqrt{\frac{m}{2}} \frac{1}{(E_\pi - E)^{3/2}} $$

(26)

Introducing the variable $\lambda = L^<_e$ one obtains

$$ \frac{d\lambda}{1 + \lambda^2} = \pi \rho(E) dE $$

(27)

$$ \overline{\Delta W^<_N} = \int \rho(E) dE \Delta W^<_N = \frac{1}{\pi} \int \frac{d\lambda}{1 + \lambda^2} \Delta W^<_N $$

(28)

The denominator $1 + \lambda^2$ has in upper half plane a pole at $\lambda = i$, implying

$$ \int \rho(E) dE = \frac{1}{\pi} \int \frac{d\lambda}{1 + \lambda^2} = 1 $$

(29)
The term $\Delta W_N^<\geq$ has a pole in lower half plane,

$$\Delta W_N^< = (1/\lambda - R_{ee})^{-1}$$  \hspace{1cm} (30)

at $\lambda = 1/R_{ee} = R_{ee}^*/|R_{ee}|^2$, ie $Im \lambda \sim -Im R_{ee} < 0$, (because $Im R_{ee} > 0$). 

As $\Delta W_N^<\geq$ has no pole in upper half plane, by using the residue’s theorem

$$\overline{\Delta W_N^<} = \frac{1}{\pi} \int \frac{d\lambda}{1 + \lambda^2} \Delta W_N^< = \Delta W_N^<(\lambda = i)$$  \hspace{1cm} (31)

$$\overline{(I_c< - R_{ee})^{-1}} = (1/i - R_{ee})^{-1} = (1/I_c> - R_{ee})^{-1}$$  \hspace{1cm} (32)

one obtains that the averaged effective term and averaged reduced collision 

matrix, are continous across threshold, $\overline{\Delta W_N^<} = \Delta W_N^>\geq$ and $\overline{W_N^<} = W_N^>\geq$. The physical interpretation of this result is: the near-threshold (high excited) bound states in coulombian field are physically similar to scattering 
states (small positive energy) of continuum spectrum, [14], ch. IX, [15]. The energy 
average (over mean spacing of levels) of the reaction total cross section of 
open channel $a \in N$, $\sigma_{aa}^t \sim Re(1 - W_{aa})$, results into Gailitis’ theorem, $\overline{\sigma_{aa}^t} = \sigma_{aa}^t$.

### 3.4 R-matrix approach to MQDT; a remark

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, eg [18, 22, 19]. The effects of short range inter-
actions, 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 the Coulomb or dipolar ones), 
are treated analyitically by extensive use of Coulomb or other special functions 
[18, 23]. On the other hand the general assumptions of the MQDT are simi-
lar to those of R- matrix theory, [13]. Developing this idea and by using only 
basic properties of Whittaker and Coulomb functions, Lane 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 was also derived from the Level- matrix parametrization of the colli-
sion matrix [17]. This last approach proves that the essential aspects of the
MQDT originate in variation across threshold of the logarithmic derivative of the Rydberg channel. In this work the role of Rydberg states (from closed channel) for producing resonant effects in the competing open reaction channels of the multichannel system is pointed out, by relating the Level- matrix approach to the Siegert state equation.

4 Conclusions

The Siegert state, defined as a channel single particle state subject of out wave boundary conditions, is described in terms of Bloch-Lane-Robson formalism for quantum collisions and, thereafter, its equation is related to scattering operators. This way the Siegert state, either bound or quasistationary, is approached in terms of R- matrix and channel logarithmic derivative. It is not described by a Wigner R- matrix pole but rather by an equation relating R- matrix to channel logarithmic derivative. The channel equation

\[ 1 - R_{nn} L_n = 0 \]  

(with \( L_n \) real for bound state and complex for quasistationary states), results into (real or complex energy) poles of the collision matrix. If the channel under question is part of a multichannel system then the channel R- matrix element \( R_{nn} \) is replaced by its reduced counterpart \( R_{nn} \).

The Siegert state is reflected in complementary channels of the reaction system as a pole \((1 - R_{nn} L_n)^{-1}\) in the effective term \(\Delta W_N \sim (1 - R_{nn} L_n)^{-1}\) of collision matrix. The effective term of collision matrix, corresponding of reduced R- matrix, describes the effect of unobserved (eliminated) channel on observed (retained) ones.

The collision matrix for case of electron closed channel is equivalent to QDT equations. The electron channel equation \(L_{ee}^{-1} - R_{ee} = 0\) or \(\tan \pi \mu = R_{ee}\) is equivalent to Seaton’ theorem, relating at zero energy the quantum defect \(\mu\) to scattering phase shift \(\delta_e\). The Seaton’ equation in multichannel system, \(L_{ee}^{-1} - R_{ee} = 0\) or \(\tan \pi \tilde{\mu} = R_{ee}\) results into complex quantum defect, \(\tilde{\mu}\). The equation results also in channel resonances, defining energies in term of complex quantum defect. The Siegert state, formally enviced in effective term \(\Delta W_N^<\) of collision matrix, is origin of the ’channel resonance’, as distinct from ’inner’ R- matrix resonance. The energy averaged collision matrices, evaluated below and above threshold, are related by a threshold continuity equation, \(\overline{W_N^<} = \overline{W_N^>}\), which is alternative to Gailitis’ theorem.
The present approach to Siegert state in multichannel scattering is applied to physics of multichannel electron scattering; it does reproduce some results of Multichannel Quantum Defect Theory, without pretense for substitution of MQDT exhaustive derivation, but rather guided by it.

This work does follow the philosophy of Lane’s paper [13]: a direct derivation of MQDT starting with a basic theory or concept. An interesting problem which does not fit in streamline of the work is comparison of the Siegert state approach to previous theoretical formalisms for multichannel electron scattering (see however Appendix).

Appendix

A  The Siegert state approach versus theoretical models for multichannel electron scattering: some remarks

The Collision matrix $W_N^<$, for case of eliminated closed ($<$) $n-$channel, is related to Collision matrix elements $W_N^<$, $W_N^{<n}$, $W_N^{>n}$ of open ($>$) channel system and to jump across threshold of logarithmic derivative $\Delta I_n$. Actually this equation relates two reaction systems (denoted $<$ and $>$) which have same internal dynamics, (R- matrix), but differ in interaction in channel space, ($L_n^<$ and $L_n^>$).

The effective terms $\Delta W_N^<$ and $\Delta W_N^>$ of the Collision matrix are a formal frame for description of threshold effects in quantum collisions. Actually they generalize the Wigner-Breit-Baz threshold cusp theory [14, 15], by relating threshold effects to reaction dynamics. The threshold cusp is obtained in limit of potential scattering, ie no Siegert pole near threshold.

The Collision matrix $W_N^<$ and $\Delta L_n^*/\Delta L_n$ correspond, respectively, to physical Scattering matrix and to long range Scattering matrix defined in [24]. By specializing to Coulomb interaction, $\Delta L_n^*/\Delta L_n = e^{-2i\pi\nu}$, the Collision matrix equation of MQDT is derived [18]. The threshold continuity theorem of energy-averaged Collision matrix for multichannel electron scattering is straightforward derived.

One can prove that the MQDT equation for Collision matrix $W_N^<$ is equivalent to reduced R- matrix, $R_N^< = R_N - R_{Nn}(R_{nn} - 1/L_n^<)^{-1}R_{nN}$. The R-matrix, subject of natural boundary conditions, results in a reduced K- ma-
trix parametrization of $W_N^< \text{Collision- matrix}$ with, $K_N^< = K_N - K_{NN}(K_{nn} + \tau^<)^{-1}K_{nN}$ and $\tau^< = (Im\Delta L_n)/(Re\Delta L_n)$. This formal result for short-range effective $K$- matrix is in common with channel elimination methods in MQD theories [18] or reaction matrix projector method [22] or phase-shifted MQDT [24].

The effective term $\Delta W_N$ of Collision matrix is related to Siegert equation. The Siegert pole describes the 'channel resonances' while R- matrix poles correspond to 'inner resonances'. In this work the two types of resonances are quite separated; however they could be formally mixed as in Lane’s work [13] or in MQD theories.

The Siegert boundary condition is just condition that the Jost function expressing the fact that there is no incoming wave should vanish.

The QD formalism, developed by Greene, Rau and Fano [23], is based on Jost function. The Jost matrices of Eigenchannel formalism [22] involve connections between fragmentation channels and eigenchannels. Eigenchannel method proved its versatility by extension to molecular spectra [25]. This formalism displays explicitly quantum numbers and parameters of atomic dynamics which makes it adequate for theoretical analysis of data.

Zero of Jost function $J^-$ associated with a bound state or resonance is a pole of collision matrix, $U \sim J^+/J^-$, eg [22]. The corresponding of Jost function in R-matrix terms $U \sim (1 - L^*R)/(1 - LR)$ is just the Siegert term $J^- \sim 1 - LR$. A Jost matrix approach to multichannel electron scattering on coulombian fields is presented in [26], ch. 3.5, [27]: the Collision matrix for this problem is $I^*I = (M - \lambda^*)(M - \lambda)^{-1}$. This Jost matrix $I$ is acting in space of fragmentation channels. The matrices $M$ and $\lambda$ are logarithmic derivatives at channel radius of internal and channel wave functions. Observe they can be identified with $R^{-1}$ and $L$ of R- matrix theory. The corresponding Jost matrix for multichannel electron scattering is $I \sim R^{-1} - L$.

All reaction channels, irrespective open or closed, are treated in same way both in above approach as well as in Eigenchannel method. Our MQD approach is based on effective Collision matrix which, at its turn, is related to Siegert equation displaying effect of closed channel on open ones.

The comparison between Siegert state to well established MQD approaches is not an easy matter and it is not in streamline of this work; some of above remarks do touch only possible relationships. One should note that Siegert state approach to MQD, in the present compact form, has no direct application in analysis of experimental data. It is, mainly, a methodological result and a physical demonstration of role of Siegert state concept in MQDT.
Acknowledgements

One of the authors (CH) acknowledges support of A v Humboldt Foundation and hospitality of the Munich University.

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