40 years of the Berggren representation

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Plan of the talk

- Berggren completeness
- Influence of the Berggren completeness
- Interpretation problemes
- Berggren completeness in complex potential

Berggren completeness

40 years ago in 1967 Tore Berggren submitted:
On the use of resonant states in eigenfunction expansions of scattering and reaction amplitudes
to Nuclear Physics A. New completeness realtion, or basis, now is called Berggren representation.
Composed of bound states and Gamow resonances and complex energy continuum.

$$\delta(r-r') = \sum_n w_n(r,E_n)w_n(r',E_n) + \int_L dE u(r,E)u(r',E) \ , \quad (1)$$

$$E \sim k^2$$

Discrete states belong to poles of $S(k_n)$

$$w_n(r,E_n) \sim O_l(k_n r) \sim e^{ik_n r} \ .$$

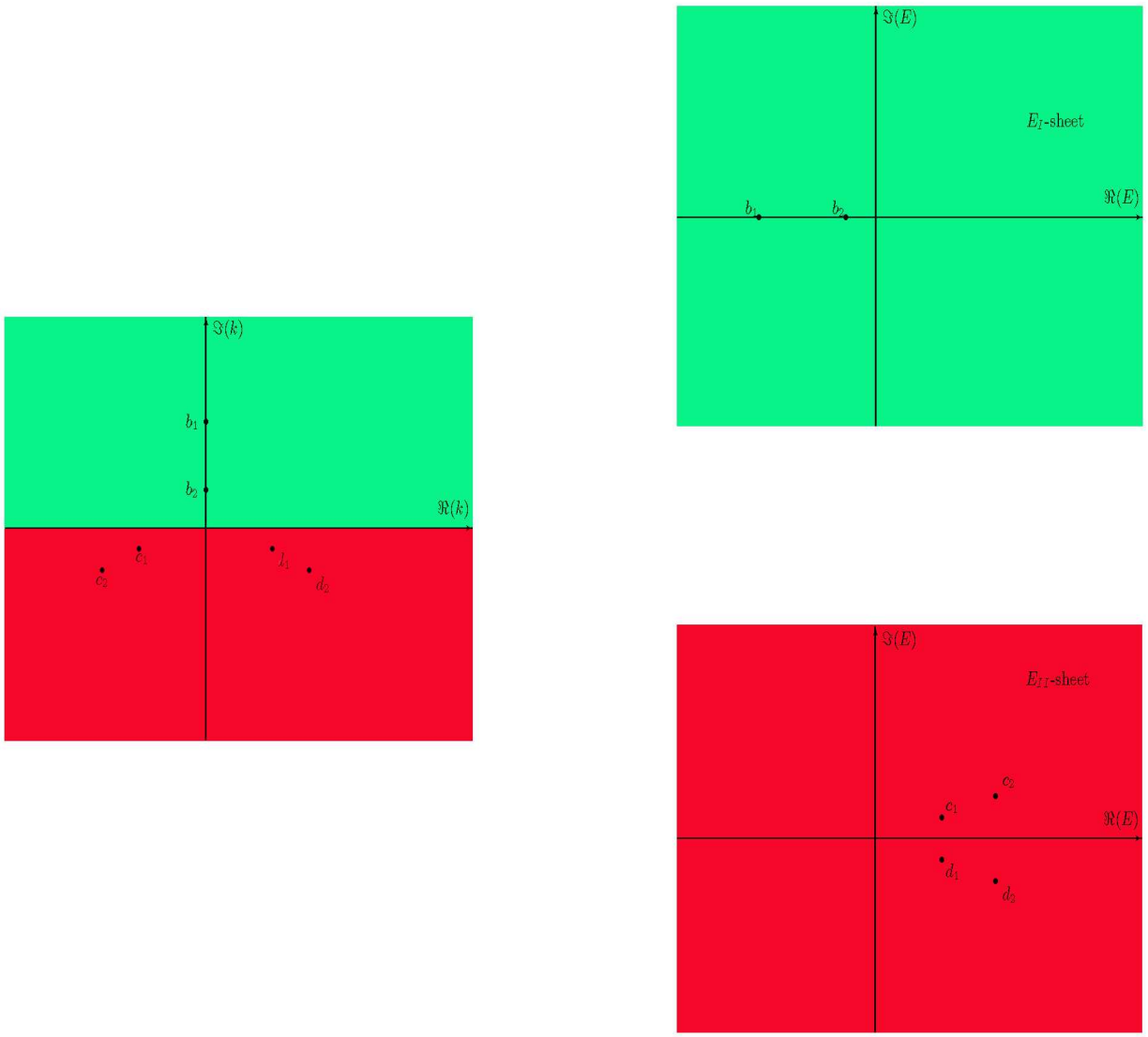


Figure 1: Poles of S-matrix on the complex k and E-sheets. Traditional basis expands functions with asymptotics e^{ikr} taken from the green region.

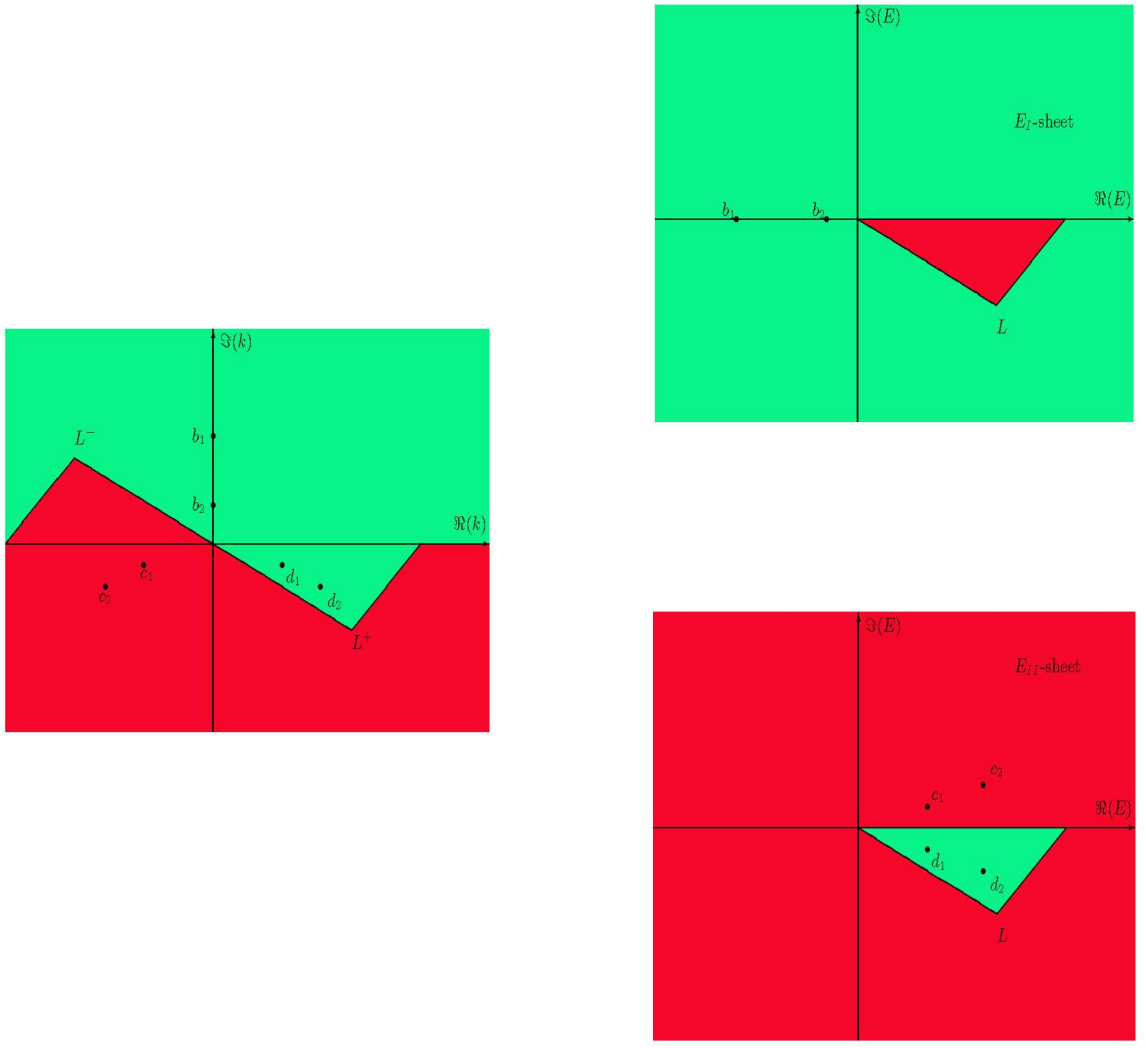


Figure 2: Poles of S-matrix on the complex k and E-sheets. Berggren basis expands functions with asymptotics e^{ikr} taken from the green region.

Radial wave functions with $\Im(k) < 0$ diverge as $r \to \infty$.
Scalar product is generalized.

- Biorthogonal basis is used for the radial wave function, i.e. different basis set for the states in bra: $\langle$ | and ket: | $\rangle$ positions
- for radial integrals regularization is needed.

Generalization of the traditional scalar product, since it reduces for that between bound states. The new completeness reduces to the traditional one if the contour is the real axis.

Bound and resonant states are equally treated by Berggren.

The complex energy behaviour of the Green-function and the scattering matrix was recognized well before Berggren e.g. by Humblet and Rosenfeld but the bound and resonant states thought to be non-ortogonal to each other.
This excluded the posibility of using them in structure calculations.

Berggren applied the regularization method of Zel'dovich (with Gaussian convergence factor) Berggren could normalize Gamow states and proved the completeness of the new basis.

Influence of the Berggren completeness

Berggren's paper opened the door for using Gamow states in nuclear structure calculations.
It caused some excitement.
Romo introduced another regularization and solved a shell model type 2-channels problem.
Bang and Zimányi used a Gamow form factor in stripping reaction to a resonant final state.
The Debrecen group headed by Borbála Gyarmati was very active in following Berggren. Normalization of Gamow function:
In 1972 Gyarmati and Vertse proved that the Zeldovich's and Romo's procedures result the same norm for a neutron resonance.
We proved the existence of the norm for proton resonance.

Introduced a new regularization procedure in which r is rotated to complex beyond r_{max}.
It is still used extensively in numerical calculations.
Gyarmati, Vertse, J. Zimányi, and M. Zimányi used a skeleton Berggren basis for calculating IAR in ^{49}Sc

Gyarmati paid a visit to Lund in 1972.
Mainly the questions of the interpretation of complex physical quantities were discussed.
A major part of the results will be summarized in Borbála Gyarmati's talk: **Decaying states** .
Since she was not able to come I shall present her lecture here.

Now I make a sort of summary from my personal point of view in which the numerical calculations are emphasized.

We with K. F. Pál and Z. Balogh developed the code GAMOW for numerical calculation of the complex resonant energy and the normalized Gamow wave function.
This program is fast and flexible for calculating all outgoing wave solutions: bound, anti-bound states and Gamow resonances.

Debrecen-Stockholm collaboration (1985-...) when I visited AFI and joined to the group headed by Roberto Liotta.
His talk **Influence of the work of Berggren on the Stockholm group** will be heared later. He will speak about the resonant RPA (RRPA) approach for giant resonances.

In RRPA we used a truncated Berggren basis, complex contiuum was neglected.
We contacted Tore Berggren and discussed our results.
We met at the Symposium held at Lertorpet, August 1987.
The interest of the Debrecen group turned to the complex scaling method (CS).
Kruppa presented in Lertorpet the first application of the *complex scaling method* in nuclear RGM calculation.

In the complex scaling method the coordinates are transformed into the complex and the discrete eigen functions of the complex rotated Hamiltonian are square integrable functions.
A common feature of the CS with Berggren's picture is that the resonance energy and the matrix elements of the operators are complex.

In CS matrix elements of the complex scaled operators are calculated between square integrable functions. No regularization needed.

In the Stockholm group we followed the line of Berggren and we explored the wide application field opened by the Berggren representation.
In the first decade the Berggren basis was truncated to the bound and resonant states.
In 1996 we (Liotta, Maglione, Sandulescu, Vertse) used the Berggren representation in its full form with the discretized complex continuum.
We diagonalized the matrix of a Hamiltonian with spherical symmetric potential in a full Berggren basis of a similar Hamiltonian with different potential.

The elements of the Berggren basis have been computed by using the piecewise perturbation method (PPM), introduced by Liviu Ixaru, Bucharest. PPM is good for oscillating solutions.
The method is decribed in the paper
Ixaru, Rizea, Vertse, Comput. Phys. Commun.**85** (1995).
With this program the Stockholm group used the full or the truncated Berggren basis in different type of nuclear structure calculations.
Attempt was made to calculate resonances of deformed potential in diagonalizing the matrix of the deformed Hamiltonian in spherically symmetric Berggren basis, but results were not very accurate for the complex energy of the deformed resonance.

Therefore during my visit at Oak Ridge direct integration method was used for calculating Gamow resonance in a deformed potential.

The coupled channels version of the piecewise perturbation method program, (CCGAMOW) was used for calculating full and partial widths of proton decay from axially symmetric proton emitters at Oak Ridge.
We with Andras Kruppa had the opportunity of working in the group of Witek Nazarewicz and were able to analize experimental results measured in the Oak Ridge National Laboratory.
In a non-adiabatic description of the proton emission from deformed nuclei we (Kruppa, Barmore, Nazarewicz, Vertse) used a modified version of the coupled channels program NONADI in which the degeneracy of the members of the rotational bands has been removed.
We used Berggren's idea in calculating the contribution of the Gamow resonances in shell correction calculations at $T = 0$:
(Vertse, Kruppa, Liotta, Nazarewicz, Sandulescu, Werner)
and at finite temperature:(Sandulescu, Civitarese, Liotta, Vertse).

In 1992 we (Dussel, Liotta, Sofia, Vertse) studied the effect of the finite temperature in giant resonances within the RRPA:

For 2002 it became possible to use of the full Berggren representation in calculating two-particle resonances using a *shell model on the complex energy plane*:
Phys. Rev. Lett.**89**, by the Stockholm group: Id Betan, Liotta, Sandulescu, Vertse (042501)
and by the Oak Ridge-GANIL group: Michel, Nazarewicz, Ploszajczak, Bennaceur, (042502).
In 2003 the Stockholm group (Id Betan, Liotta, Sandulescu, Vertse) calculated two neutron resonances in ^{80}Ni and two proton resonances in ^{102}Te nuclei, the Oak Ridge-GANIL group (Michel, Nazarewicz, Ploszajczak, Okolowicz) made a systematic Gamow shell model calculation for the light neutron-rich nuclei ^{6-10}He and

$^{18-22}O$.

In 2004 Michel, Nazarewicz and Ploszajczak demonstrated rigorously the completeness of the Berggren basis for a charged particle.

Generalized Berggren representation

In 1989 the Berggren representation has been generalized for including a virtual state into the discrete part of the basis (Vertse, Curutchet, Liotta, Bang).
Berggren originally used only true resonant poles with

$$arg(k_n) > -\frac{\pi}{4} \quad \Re(E_n) > 0 \ ,$$

therefore virtual resonances and antibound states were excluded from the Berggren basis.
More recently this generalized Berggren representation was used for the description of halo nuclei ^{11}Li and ^{72}Ca .
We (Id Betan, Liotta, Sandulescu, Vertse, Wyss) observed destructive interference between the virtual state and contour states.
This explains the failure of the early attempt in 1989.

The nice thing was that we could form a bound state in ^{11}Li from only unbound basis states of the ^{10}Li. Which suggests that the generalized Berggren basis is also complete.
In 2006 a similar basis was studied by the Oak Ridge group (Michel, Nazarewicz, Ploszajczak, Rotureau) in order to find the optimal contour and basis. They found that the generalized Berggren basis was the least optimal among the choices they tried.
In our simple model we did not expect that the inclusion of the antibound state could reduce the size of the basis.
The use of the generalized Berggren basis has conceptual advantage compared to the one in which a non existing neutron bound state has been assumed for the unbound ^{10}Li system for the description of the bound ^{11}Li nucleus.

Self consistent calculations

The use of phenomenological potential is a nice playing ground but can be justified only by the results of self-consistent calculations.
It is essential to see how the presence of a resonant state influences the self-consistent mean field.
In 1997 Kruppa, Heenen, Flocard and Liotta used complex scaling in self consistent HF (CSHF) calculations with Skyrme effective interaction to determine binding energies of particle unstable nuclei.
Later (2001) Kruppa, Heenen and Liotta used complex scaling in self consistent HF BCS calculations in which the scattering states of the complex contour was neglected.

They got good agreement with the result of HFB calculations in the proton drip line region around the ^{48}Ni nucleus.
This encouraged us to study quasiparticle resonances in phenomenological potentials using full Berggren basis:
Rodolfo Id Betan will give a talk about these results.
Until now I spoke about results in which the Berggren basis used *coordinate representation*.
The advantage of the use of *momentum space* Berggren representation was suggested recently by the Bergen-Oslo group.
I belive that Jan Waagen will speak about these calculations in detail.
Most recently (2006) it was applied in self consistent HF calculations by: Hagen, Hjort-Jensen, and Michel.

Interpretation problems

It is a serious difficulty to accept the fact that in Berggren representation the matrix elements of the operators are complex and the probabilty interpretation of the resonant wave function is lost. This is a price we pay for trying to describe the time dependent process of the decay of a resonance in the stationary picture. (Without solving the time-dependent Shrödinger equation.)
We shall see in the next talk that in this stationary picture the resonant wave function is the product of time dependent and space dependent factors. The t-dependent part decribes an exponential decay of the amplitude, while its radial part oscillates with exponentially growing amplitude reflecting the fact that the farther we are from the nucleus the stronger the source (emitting the particle) has been in time. Since the decay process in this picture is

unlimited both in time and space, the decay process never ends. This is certainly an approximation of the physical process.
In 1984 Romo showed that a narrow Gamow resonance has very large overlap with a properly shaped wave packet
Resonance with small width (large lifetime) is similar to a bound state. For small width the imaginary part of the radial wave function is small inside the nucleus and the wave function is almost real. A narrow resonance shows up as a sharp peak in the reaction cross section and its contribution can more or less certainly be separeted from that of the continuum. Berggren showed in 1978 that the imaginary part of the complex cross section calculated by assuming that the final state is a Gamow resonance describes the interference of that resonance with the non-resonant background. In a later paper (1996) Berggren demonstrated that for an operator wich commutes with the Hamiltonian the expectation value of that operator is the real part of their matrix element and the

square of uncertainty of the expectation value is the negative of the square of the imaginary part of the matrix element. In the case of an operator which does not commute with the Hamiltonian we do not know a definite relation between the imaginary part of the matrix element and the uncertainty of the expectation value. This seems to be an open problem for both of the Berggren representation and of the complex scaling method.

Berggren completeness for complex potential

Complex potential appears in optical potential for scattering and also in the CS Hamiltonian.
How the poles move?
Let us study the pole trajectory of the $1g_{7/2}$ resonant state as the strength of the imaginary part of the potential in a WS potential well changes.

$$h = t + v(r) + v_{so}(r) \quad v(r) = (V_0 + iW)f(r)$$

$$f(r) = -\begin{cases} (1 + exp((r-R)/a)^{-1} & , \text{if } r < r_{max} \\ 0 & , \text{if } r \geq r_{max} \end{cases}$$

The values of the energies are shown in Table 1.

Table 1: Complex energies of the $1g_{7/2}$ neutron resonant states in complex WS potentials.

W	$\Re(E_c)$	$\Im(E_c)$	$\Re(E_d)$	$\Im(E_d)$
0	6.739	0.738	6.739	−0.738
−1.5	6.478	1.464	7.009	−0.043
−6	6.039	3.289	7.858	2.660
1.5	7.009	0.043	6.478	−1.464
6	7.858	−2.660	6.039	−3.289

For real well we have a time reversed pair of poles:

$$E_c = E_d^*$$

of capturing E_c and decaying E_d Gamow resonances with radial wave functions:

$$\tilde{u}_c(r, E_c) = u_d^*(r, E_d) \ .$$

This symmetry is due to the fact that the Hamiltonian is self adjoint:

$$h = h^\dagger$$

for a real potential.
This symmetry is spoiled if $W \neq 0$, since $h \neq h^\dagger$.
For $W < 0$ (emission) the decaying resonance moves into the direction of the real k-axis. At about $W = -1.5 MeV$ it is almost on the real k-axis. If we decrease W further then the decaying pole moves to the upper half of the k-plane i.e to the physical E-sheet:

E_I.
Let us keep the name *decaying resonance* for simplicity although this solution is not a resonance any more.
Here the wave function is a square integrable complex function, since it goes to zero when $r \to \infty$.
For $W < 0$ values the capturing resonance: k_c moves downward, the resonance becomes broader.

For absorptive well: $W > 0$ at about $W = +1.5MeV$ k_c moves to the negative part of the real k-axis. If we increase $W > 0$ further, k_c moves on the upper half of the k-plane.

We can see from the energies in Table I and also in the figure 3. that the same sort of symmetry of the poles we had for $W = 0$ remains, if we use consider the poles belonging to h and $h^\dagger$ i,e, with

the same imaginary strenghts $|W| > 0$ but with different sign for the capturing and deacying poles, respectively. Therefore we can consider the time reversed solution again as the same resonance as we did it in the real potential case. The time reverse of the emission is the absorption therefore the above identification can be justified.

In this case the $\Im(k)$ values are the same and $\Re(k_c) = -\Re(k_d)$. For the energies the real parts are the same and $\Im(E_c) = -\Im(E_d)$. So by using complex potential we can shift either the decaying or the capturing resonance to the upper half of the k-plane i.e. to the physical energy sheet : with $W = 6$ MeV $k_c = (-0.62, +0.10)$ and with $W = -6$ MeV $k_d = (0.62, +0.10)$.

1 Diagonalization in a Berggren basis of a real potential

Now we can take a Hamiltonian h_0 with real potential and calculate the Berggren basis of this h_0 with different complex contours. In these Berggren representations we can calculate the matrix of the perturbed Hamiltonian h_1 with complex potential. If we diagonalize this matrix we can get eigenenergies of h_1 and compare it to the numerically exact result.

With $W = -6MeV$ the imaginary part of $E_d = 7.958 + i2.660MeV$ is positive. This change of sign appeared because the pole moved to the physical energy sheet from the unphysical one.

With the real contour A we use the traditional space in which we are able to expand all outgoing solutions with k from the upper

half k-plane.

With complex contour B the diagonalization reproduces the first $3-4$ decimal digits of the numerically exact results in Table I. Let us try to expand now the decaying resonance in h_1 with $W=-6$ at $7.958+i2.660$ MeV with different E-contours in table II.

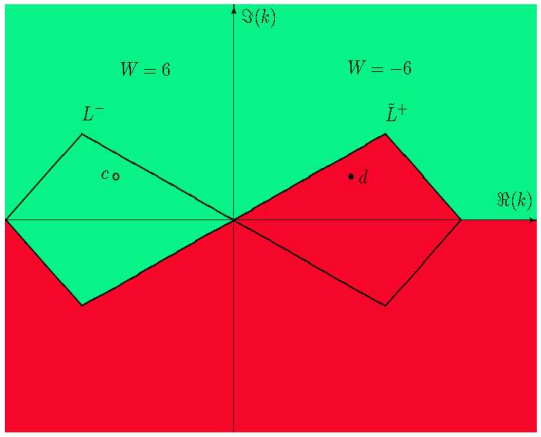
- A vertices: $(0,0)40(3.4,0.0)50(7.9,0.0)30(190,0)$.
- B vertices: $(0,0)40(3.4,-3.4)50(7.9,-7.9)30(190,0)$.
- C vertices: $(0,0)40(3.4,0.34)50(7.9,0.0)30(190,0)$.
- D vertices: $(0,0)40(3.4,3.4)50(7.9,0.9)30(190,0)$.
- E vertices: $(0,0)40(3.4,3.4)50(7.9,3.0)30(190,0)$.

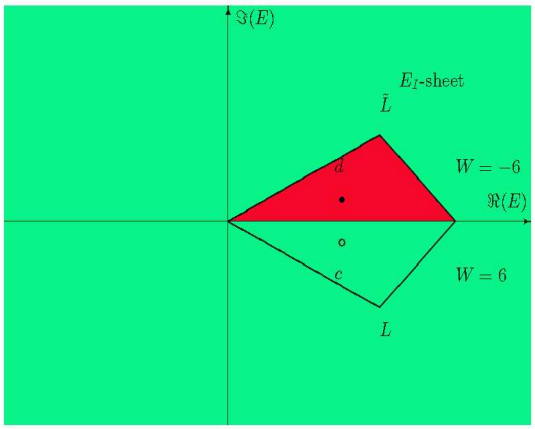
With contour B we included the decaying, with D and E the capturing resonance at $E_d = 6.73863, -i0.73787$ and at $E_c = 6.73863, i0.73787$into the basis.

Table 2: Energies of the *decaying resonance* calculated by diagonalizing h_1 with $W = -6$ MeV using the Berggren basis of a real Hamiltonian.

contour	$\Re(E)$	$\Im(E)$
A	7.85834	2.6606
B	7.85818	2.6606
C	7.85834	2.6606
D	7.85710	2.6603
E	7.89681	3.0077
exact	7.85882	2.6606

One can see in Table II. that the *decaying resonance* lying on the physical E-sheet can be reproduced precisely using contours A,B,C and less accurately with contour D. The pole disappears if we use contour E, since the pole is below the contour E in the physical sheet, i.e. in the red region in fig.3.





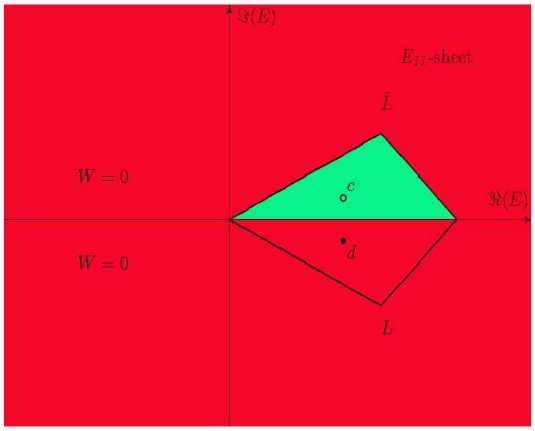


Figure 3: Poles of S-matrix on the complex k and E-sheets. Berggren basis with $\tilde{L}$ expands functions with asymptotics e^{ikr} taken from the green region. On the E_I-sheet the poles in complex potential are shown.

2 Diagonalization in a Berggren basis of a complex potential

Let us exchange the unperturbed and the perturbed Hamiltonians and try to calculate the Berggren basis of a Hamiltonian h_0 with complex potential:

$$W = -6MeV \ .$$

In this complex potential we have a *decaying resonance* (a square integrable outgoing state) at

$$E_d = 7.858181 + i2.660594 \quad k_d = 0.61988489 + i0.102092715$$

Since now h_1 has real potential we have a pair of resonances at energies listed in the first raw of Table 1. If we want to calculate the decaying one we have to use an L contour shown in Fig. 2.

The vertices of the energy contours are the following:

- A with vertices:$(0,0)40(3.4,-3.5)50(7.9,-3.8)30(190.0,0.0)$
- B is complex straight line contour with $arg(E_{cont}) = -0.46365$ with last vertex: $(190,-95)$

With both contours we included the *decaying resonance* of h_0 into the Berggren basis since this pole is on the physical energy sheet and the contours are on the unphysical sheet as one can see in Fig. 3. The results of the diagonalization are shown in Table 3. The diagonalization using contour A reproduces the decaying resonance in the real Hamiltonian h_1 up to 5 decimal digits accuracy. If we use the contour B (the straight line contour with $arg(Econt) = -0.463647609$ we get a somewhat less accurate agreement but this value shows that the return to the real axis

is not really necessary. Note that this contour looks like a rotated E-axis in CS method. In both cases the resonance is built mainly on the *decaying resonance*.

Table 3: Energy of the decaying resonance calculated by diagonalizing the matrix of the real Hamiltonian using the Berggren basis of a complex Hamiltonian with $W = -6MeV$ with different L contours and the numrically exact eigenvalue of the resonance.

contour	$\Re(E)$	$\Im(E)$
A	6.73863	-0.73787
B	6.73936	-0.73790
exact	6.73863	-0.73787

We can repeat the diagonalization by using the Berggren basis of the complex potential with absorption strength $W = 6$ in h_0 . The results are basically the same, i.e. we can reproduce the numerically exact energy of the capturing resonance with the same accuracy as we did when we used Berggren basis of a real Hamiltonian.

Results of numerical calculations suggest that the Berggren completeness might be valid for non self-adjoint Hamiltonians with complex optical potential.