The single-particle Berggren basis in structure calculations

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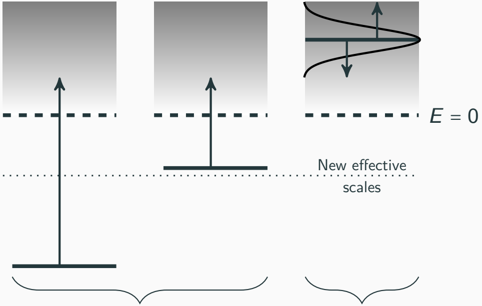
Nuclei as open quantum systems (OQS)

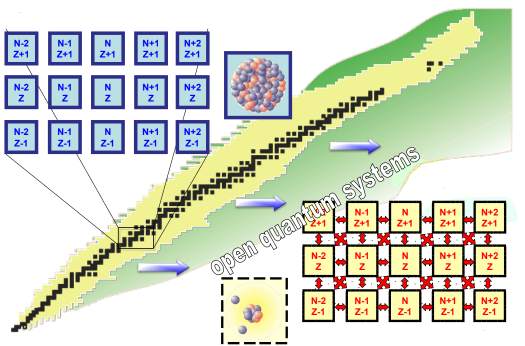
Why do we care about continuum couplings?

→ In short: quantum systems can break apart.



Coupled by excitations $\Rightarrow \Gamma = 0$

Excitations and decay $\Rightarrow \Gamma > 0$

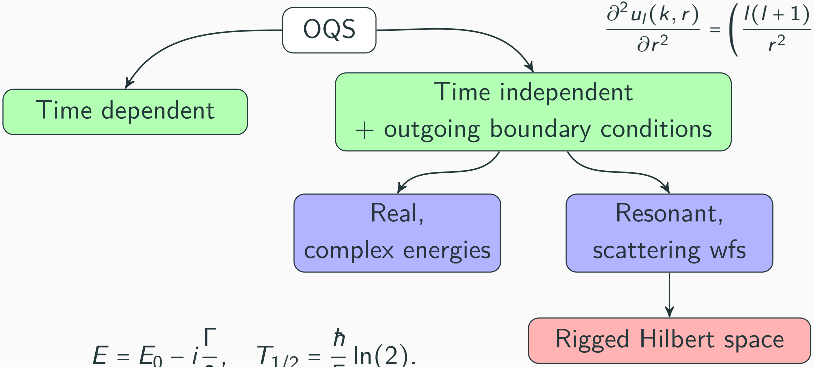


New paradigm: network of OQS!

→ Unification of structure and reactions.

N. Michel *et al.*, J. Phys. G **37**, 064042 (2010)

The two possibilities to deal with OQS:



$$\frac{\partial^2 u_l(k,r)}{\partial r^2} = \left(\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} V(r) - k^2 \right) u_l(k,r).$$

$$u_l(k,r) \underset{r\sim 0}{\sim} C_0(k) r^{l+1}.$$

$$E = E_0 - i\frac{\Gamma}{2}, \quad T_{1/2} = \frac{\hbar}{\Gamma} \ln(2).$$

$$u_l(k,r) \underset{r\to\infty}{\sim} C_+(k) H^+_{l,\eta}(kr) + C_-(k) H^-_{l,\eta}(kr).$$

$C_-(k) = 0$ for bound and decaying states.

J.J. Thomson, Proc. London Math. Society, 197 (1884),
G. Gamow, Z. Physik **51**, 204 (1928), A. F. J. Siegert, Phys. Rev. **56**, 750 (1939)

Resonant and scattering states

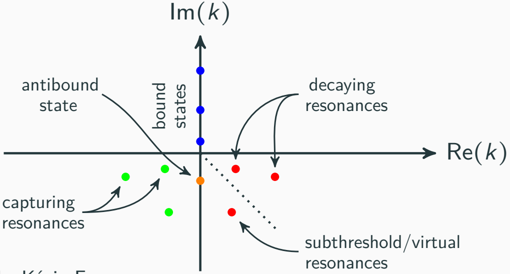
A few definitions:

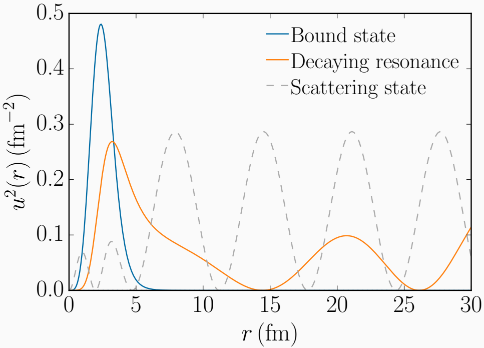
- Resonant states or Gamow states: poles of the *S*-matrix, *i.e.* bound states, virtual or antibound states and resonances (decaying or capturing).

→ Discrete energies.

- Scattering states: nonresonant (continuum) states.

→ Continuous energies.





Connection between Gamow states and the (Green function) resolvent's spectrum in 1954.

R. E. Peierls, Proc. Glasgow Conf. Nucl. Meson Phys., 296 (1954)

T. Berggren: “What can we do with those states? A basis!”

- PhD in 1966 (Lund), groundbreaking work published in 1968:
  T. Berggren, Nucl. Phys. A **109**, 265 (1968)
  —*On the use of resonant states in eigenfunction expansions of scattering and reaction amplitudes.*—
- Connection between the Berggren and Mittag-Leffler expansions:
  T. Berggren and P. Lind, Phys. Rev. C **47**, 768 (1993)
  —*Resonant state expansion of the resolvent.*—
- Interpretation of the imaginary part of observables:
  T. Berggren, Phys. Lett. B **373**, 1 (1996)
  —*Expectation value of an operator in a resonant state.*—

→ Many papers based on the Berggren basis nowadays, still spreading.

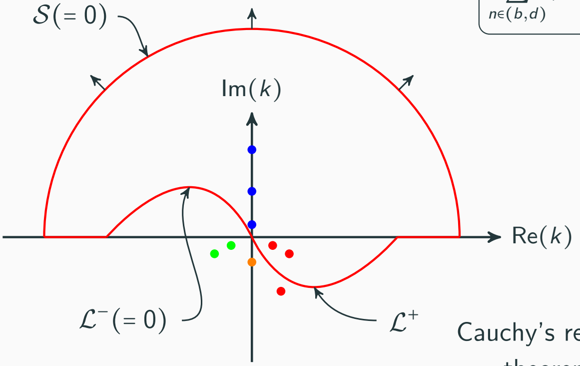
Picture from *Symmetry in the world of atomic nuclei* by I. Ragnarsson and S. Åberg, Lund University.

Definition of the s.p. Berggren basis

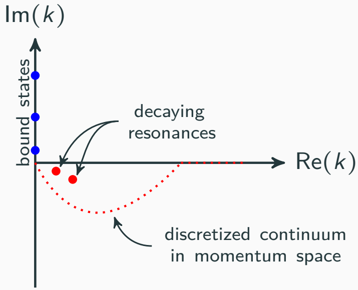
The Berggren basis:

→ Single particle basis including bound states, decaying resonances and scattering states.

$$\sum_{n\in(b,d)} |u_\ell(k_n)\rangle\langle\tilde{u}_\ell(k_n)| + \int_{\mathcal{L}^+} dk\, |u_\ell(k)\rangle\langle\tilde{u}_\ell(k)| = \hat{\mathbb{1}}_{\ell,j}.$$

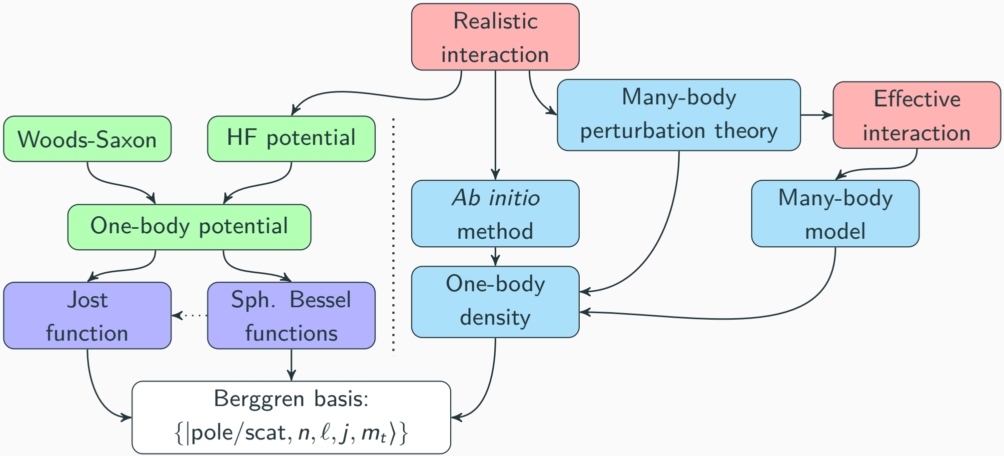


Cauchy's residue theorem



How to generate a s.p. Berggren basis? The truth.

A few options are available to generate a Berggren basis:



Spherical Bessel functions

The easy way to go:

- Analytical solutions, regular at the origin $j_\ell(r)$ (first kind) and ideally ℓ-dependent.
- Extended into the complex plane using a recurrence relation (NIST 10.51(i)) accurate for $\ell < 7$:

$$f_{n+1}(z) + f_{n-1}(z) = \frac{2n+1}{z} f_n(z).$$

- Expand the s.p. Schrödinger eq.:

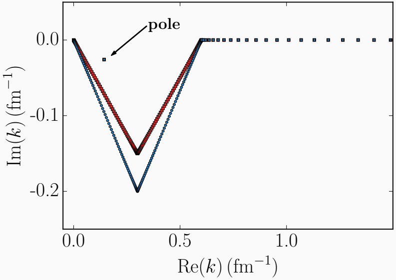
$$\frac{\hbar^2}{2m}\begin{pmatrix} k_0^2 & 0 \\ 0 & k_1^2 \end{pmatrix}\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} + \begin{pmatrix} V(k_0,k_0) & V(k_1,k_0) \\ V(k_0,k_1) & V(k_1,k_1) \end{pmatrix}\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = E\begin{pmatrix} c_0 \\ c_1 \end{pmatrix}$$

- Physical states do not depend on the basis.

$$\frac{\partial^2 \psi_l(k,r)}{\partial r^2} = \left(\frac{l(l+1)}{r^2} - k^2\right)\psi_l(k,r)$$

$$\phi_\ell(kr) = \sqrt{\frac{2}{\pi}} kr j_\ell(kr)$$

$$\int_0^\infty dr\, \phi_\ell(kr)\phi_\ell(k'r) = \delta_{k,k'}$$



The Jost function method(s)

There are in fact two methods:

- Searching the zeros of the outgoing Jost function for poles.
- Directly integrating the "Jost functions" from $r = 0$ to $r \to \infty$.

$$\frac{\partial^2}{\partial r^2} u_{\ell,\eta}(k,r) = \left(\frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2} V(r) - \frac{2\eta k}{r} + k^2 \right) u_{\ell,\eta}(k,r) \text{ with } u_l(k,r) \underset{r\sim 0}{\sim} C_0(k) r^{l+1}.$$

- Solutions at large distances (Hankel functions): $H^{\pm}_{\ell,\eta}(z) = \begin{cases} F_{\ell,\eta}(z) \mp i G_{\ell,\eta}(z) & \text{for } \eta \neq 0 \\ z[j_\ell(z) \mp n_\ell(z)] & \text{for } \eta = 0 \end{cases}$
- General solution (linear combinaison):
  $u_{\ell,\eta}(k,r) = C^+(k) H^+_{\ell,\eta}(kr) + C^-(k) H^-_{\ell,\eta}(kr)$ (at large r) $\Rightarrow u_{\ell,\eta}(k,r) = C^+(k) u^+_{\ell,\eta}(k,r) + C^-(k) u^-_{\ell,\eta}(k,r)$

How can be obtain $u^{\pm}_{\ell,\eta}(k,r)$ and the coefficients?

R. G. Newton, *Scattering Theory of Waves and Particles*, Springer-Verlag, New-York (1982, 2nd ed.) [p.341],

The Jost function method(s)

The first method: searching the zeros of the outgoing Jost function for poles.

- Integrate from zero to $r = R$, then matching conditions:

$$\begin{cases} \frac{d}{dr}\left(C^+(k)H^+_{\ell,\eta}(kR) + C^-(k)H^-_{\ell,\eta}(kR)\right) = \frac{du_\ell(k,R)}{dr} \\ C^+(k)H^+_{\ell,\eta}(kR) + C^-(k)H^-_{\ell,\eta}(kR) = u_\ell(k,R) \end{cases}$$

→ The differentiability of $u_\ell(k,r)$ is not ensured for outgoing states $(C^-(k) = 0)$!

- Definition of the outgoing and incoming Jost functions:

$$\mathcal{J}^\pm_\ell(k) = W(u^\pm_\ell(k,r), u_\ell(k,r)) = u^\pm_\ell(k,r)\frac{du_\ell(k,r)}{dr} - u_\ell(k,r)\frac{du^\pm_\ell(k,r)}{dr}.$$

→ No r-dependance by def., we only need to vary k to get: $\mathcal{J}^+_\ell(k) = 0$ and hence the differentiability.

Basically a search of zeroes for outgoing states (poles)!

R. G. Newton, *Scattering Theory of Waves and Particles*, Springer-Verlag, New-York (1982, 2nd ed.) [p.341],

The Jost function method(s)

The second method: directly integrating the "Jost functions" from $r = 0$ to $r \to \infty$.

Initial condition:
$$\mathcal{F}^{\pm}_{\ell,\eta}(0,k) = 1$$

"Jost function":
$$\frac{\partial}{\partial r}\mathcal{F}^{\pm}_{\ell,\eta}(r,k) = \mp\frac{i}{k}H^{\mp}_{\ell,\eta}(kr)\frac{2\mu}{\hbar^2}V(r)u_\ell(r,k)$$

Wave function:
$$u_\ell(r,k) = \frac{1}{2}\left(\mathcal{F}^{+}_{\ell,\eta}(r,k)H^{+}_{\ell,\eta}(kr) + \mathcal{F}^{-}_{\ell,\eta}(r,k)H^{-}_{\ell,\eta}(kr)\right)$$

- Start the integration of $\mathcal{F}^{+}_{\ell,\eta}(r,k)$ at $r = 0$, compute the wave function, iterate, etc.
- The connection with the Jost function: $\lim_{r\to\infty}\mathcal{F}^{+}_{\ell,\eta}(r,k) = \mathcal{J}^{+}_{\ell,\eta}(k)$, and obviously: $C^{\pm}(k) = \frac{1}{2}\mathcal{J}^{\pm}_{\ell,\eta}(k)$.

Very simple method that gives the wave function and ANCs simultaneously, **but you need to know where are the poles beforehand.**

R. G. Newton, *Scattering Theory of Waves and Particles*, Springer-Verlag, New-York (1982, 2nd ed.) [p.341],
H. Masui *et al.*, Prog. Theor. Exp. Phys. **2013**, 123A02 (2013)

Normalization: exterior complex-scaling method

Rigged Hilbert space norm, regularization methods:

Rigged Hilbert space norm

Resonant states:

$$\mathcal{N}^2 = \langle \tilde{u}_{\ell,\eta} | u_{\ell,\eta} \rangle = \int_0^{\infty} dr \, u_{\ell,\eta}^2(r) = 1$$

Scattering states:

$$C^+(k) C^-(k) = \frac{1}{2\pi}$$

- Several possibilities to regularize the integral: Ya. B. Zel'dovich, uniform and exterior complex-scaling (UCS,ECS).

Exterior complex-scaling:

$$\mathcal{N}^2 = \int_0^R dr \, u_{\ell,\eta}^2(r) + \left(C^+(k)\right)^2 \int_R^{\infty} dr \left(H_{\ell,\eta}^+(kr)\right)^2 = \mathcal{I}_R + \left(C^+(k)\right)^2 \int_0^{\infty} dx \left(H_{\ell,\eta}^+(k[R + xe^{i\theta}])\right)^2 e^{i\theta}$$

The Coulomb and centrifugal barriers

Just a note about long-range terms in the Hamiltonian:

- The effect of the centrifugal barrier ($1/r^2$) can be included exactly when using ℓ-dependent spherical Bessel basis states.
- Including the effect of the Coulomb barrier ($1/r$) requires Hankel functions in the complex plane (Only two codes published so far?).

It is, of course, always possible to go around the problem and directly integrate the centrifugal and Coulomb barrier in the Schrödinger eq., but for an inevitable loss of accuracy in sensitive calculations (*i.e.*, reactions, some atomic physics problems).

I. J. Thompson *et al.*, J. Comp. Phys. **64**, 490509 (1986) [see FRESCO],
N. Michel, Comp. Phys. Comm. **176**, 232 (2007).

The Berggren basis in many-body methods

First use of the Berggren basis in structure calculations (CI):

- R. M. Id Betan, R. J. Liotta, N. Sandulescu and T. Vertse (Stockholm-Debrecen group), Phys. Rev. Lett. **89**, 042501 (2002).
  —*Two-particle resonant states in a many-body mean field.*—
- N. Michel, W. Nazarewicz, M. Płoszajczak and K. Bennaceur (Oak Ridge-GANIL group), Phys. Rev. Lett. **89**, 042502 (2002).
  —*Gamow shell model description of neutron-rich nuclei.*—

Beyond the Gamow shell model:

- Realistic (effective) GSM interactions:
  G. Hagen *et al.*, Phys. Rev. C **71**, 044314 (2005), Phys. Rev. C **73**, 064307 (2006).
- DMRG: J. Rotureau *et al.*, Phys. Rev. Lett. **97**, 110603 (2006).
- Coupled clusters + Berggren: G. Hagen *et al.*, Phys. Lett. B **656**, 169 (2007).

Current trend in Gamow many-body approaches

Configuration interaction based
(can be *ab initio*)

Gamow
shell model

↓

Factorial wall.

Density matrix
renormalization group

Correlation truncated based
(*ab initio*)

Coupled clusters
in the Berggren basis

↓

Limited to closed-shell
nuclei ± 2 particles.

In-medium
similarity renormalization group
in the Berggren basis.

Renormalization group based

→ Berggren basis approaches: yes, but combined with renormalization group methods to reach FRIB physics. *Ab initio* for guidance only at present.

Known issues

Several issues are still bothering practitioners:

- Identification of many-body resonances in the complex energy spectrum (especially for broad resonances).
- Factorization of the intrisic and center-of-mass eigenstates in *ab initio* calculations.
- Reduction of the basis size (s.p. or many-body).
- Diagonalization of complex-symmetric matrices.
- Interpretation of complex observables.
- No access to individual decay channels (requires a RGM extension).

Outside of the Berggren basis island

Feshbach projection formalism

CSM, SMEC

Uniform complex-scaling

Fadeev-Yakubowski,
many others*

Berggren basis
+ truncations in correlations

CCT/Berggren

Opportunity:
IM-SRG/Berggren

Resonating group method
+ outgoing boundary conditions

NCSM/RGM,
NCSM/SS-HORSE,
NCSMC, GSM/CC

Berggren basis
+ configuration interaction

GSM, NCGSM,
DMRG, GSM/CC

Many ongoing developments: algorithm,
uncertainties, natural orbitals...

Concluding remarks

The Berggren basis (just my opinion):

- The Berggren basis proved to be a versatile tool (essentially a basis expansion).
- Energies and widths come out simultaneously (no extraction method).
- The many-body asymptotic comes for “free” (critical to scale to many-body resonances).
- Many developments are still possible (that we see, certainly not a dead-end, newcomers).
- Connections/comparisons with others approaches reveal strengths/weaknesses (4n).

→ People willing to **learn** (Kristina, Calvin,...)
are meeting people willing to **share** (ask me, Jimmy,...).

Thank you for your attention!

(NC)GSM vs DMRG