Lecture II: Quasi-stationary formalism and Berggren basis

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What you have learned:

- At low energy, nuclei must be treated as open quantum systems, and this requires a unification of nuclear structure and reactions.
- Several options are available to extend many-body methods into the continuum.
- Among those options, the Berggren basis offers a practical way to extend bound state methods beyond one- and two-body resonances.

What you will learn (hopefully):

- What is the Berggren basis.
- How to generate a s.p. Berggren basis.

Why do we care about continuum couplings?

 \rightarrow In short: quantum systems can break apart.



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

The quasi-stationary formalism

The two possibilities to deal with OQS:



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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).
- \rightarrow Discrete energies.
- Scattering states: nonresonant (continuum) states.
- → Continuous energies.





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

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



How to generate a s.p. Berggren basis?

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 $r \rightarrow \infty$.

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

- Solutions at large distances (Hankel functions): $H_{\ell,\eta}^{\pm}(z) = \begin{cases} F_{\ell,\eta}(z) \mp iG_{\ell,\eta}(z) & \text{for } \eta \neq 0 \\ z[j_{\ell}(z) \mp n_{\ell}(z)] & \text{for } \eta = 0 \end{cases}$
- General solution (linear combinaison):

 $u_{\ell,\eta}(k,r) = C^+(k)H^+_{\ell,\eta}(kr) + C^-(k)H^-_{\ell,\eta}(kr) \text{ (at large } r) \Rightarrow u_{\ell,\eta}(k,r) = C^+(k)u^+_{\ell,\eta}(k,r) + C^-(k)u^-_{\ell,\eta}(k,r)$

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

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:

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

 \rightarrow 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)!

The Jost function method(s)

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



- 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.

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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) 12

Normalization: exterior complex-scaling method

Rigged Hilbert space norm, regularization methods:



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

Exterior complex-scaling:

$$\mathcal{N}^{2} = \int_{0}^{R} dr \, u_{\ell,\eta}^{2}(r) + \left(C^{+}(k)\right)^{2} \int_{R}^{\infty} dr \left(H_{\ell,\eta}^{+}(kr)\right)^{2} = \mathcal{I}_{R} + \left(C^{+}(k)\right)^{2} \int_{0}^{\infty} dx \left(H_{\ell,\eta}^{+}(k[R + xe^{i\theta}])\right)^{2} e^{i\theta} dx$$

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).

The Berggren basis:

- 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).

Thank you for your attention!