Lecture III-a: Many-body methods for nuclear open quantum systems

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In the previous lecture...

What you have learned:

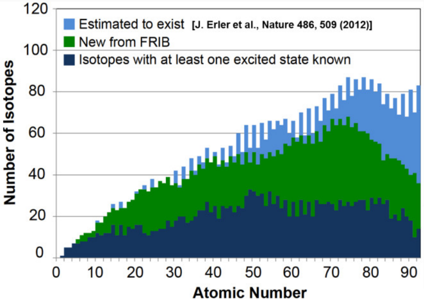
- What is the Berggren basis and how to generate one.

What you will learn (hopefully):

- How several many-body methods were extended using the Berggren basis.

1) The Gamow shell model.
2) The density matrix renormalization group approach for open quantum systems.
3) The coupled clusters theory in the Berggren basis.

Present situation in low-energy nuclear physics



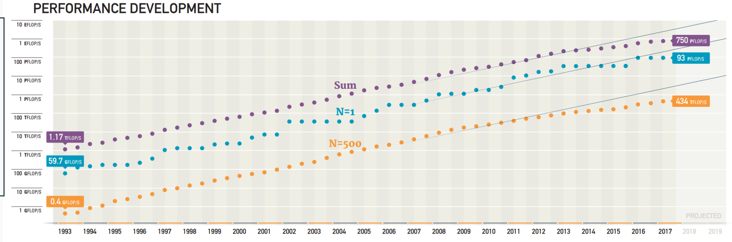
Experimental developments:

- Development of powerful rare isotope beam facilities of new generation.
- Powerful equipment (separators, detectors, etc.) providing better resolution.

Theorists were not idly sitting around either...

Computing:

- Exponential increase in computational power.
- Better parallel algorithms.



The 2015 Long Range Plan for Nuclear Science by the Nuclear Science Advisory Committee, Top500.org.

Trends in low-energy nuclear theory

- **Effective field theory.**
  → Interactions with systematic improvements.
- **Renormalization group techniques.**
  → Similarity RG, improved convergence in many-body methods.
- ***Ab initio* methods.**
  → Coupled clusters, in-medium SRG, truncations in correlations.
- **Uncertainty quantification.**
  → Feedback interaction/many-body observables, Bayes.
- **Couplings to the continuum.**
  → Berggren, density matrix RG, natural orbitals.
- **Microscopic optical potentials.**
  → Dispersion optical model, *ab initio* potentials.

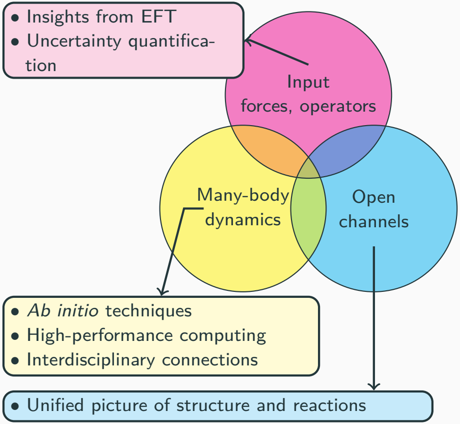


Figure adapted from W. Nazarewicz, J. Phys. G **43** 044002 (2016)

However, limitations are already visible.

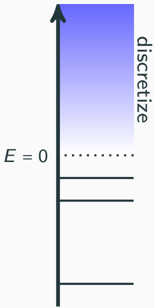
- **Interaction:**
  → In practice, similar reproduction of data by EFT and phenomenological interactions.
  → Proliferation of EFT interactions.

- ***Ab initio*:**
  → Full three-body forces essential, but out of reach for most systems at present.
  → Difficult to go beyond existing approximations.

- **Uncertainty quantification:**
  → Costly to estimate.

- **Continuum couplings:**
  → Computationally very expensive to include (e.g. NCSMC, GSM-CC).

- **Reaction theory:**
  → Optical potentials limited in energy range or by the fitting data.

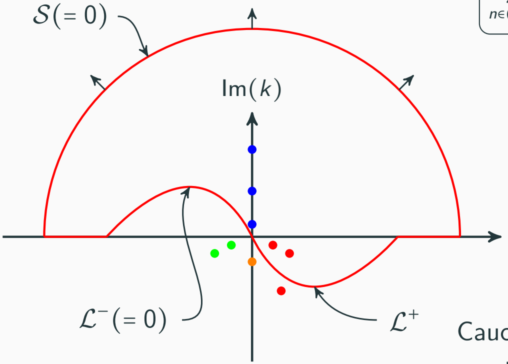


Reminder on the Berggren basis

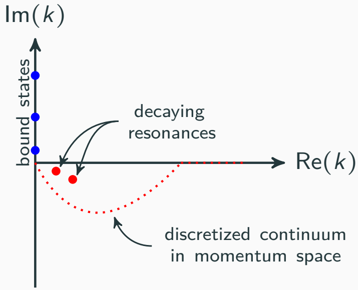
The Berggren basis:

→ 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



The Berggren basis in many-body methods

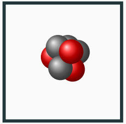
First use of the Berggren basis in structure calculations (CI):

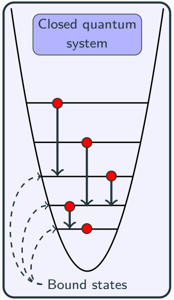
- R. M. Id Betan, R. J. Liotta, N. Sandulescu and T. Vertse (Stockholm-Debrecen group), Phys. Rev. Lett. **89**, 042501 (2002).
  —*Two-particle resonant states in a many-body mean field.*—
- N. Michel, W. Nazarewicz, M. Płoszajczak and K. Bennaceur (Oak Ridge-GANIL group), Phys. Rev. Lett. **89**, 042502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

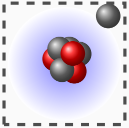
Quasi-stationary formulation of the shell model:

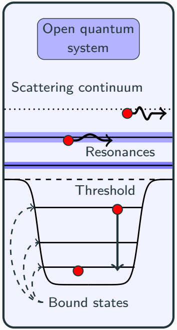




s.p. HO states (bound)
→ MEs, SDs
→ H matrix
→ Many-body bound states

s.p. Berggren states (resonant, scatt.)
→ cont. discretization
→ MEs, SDs
→ H matrix
→ identification
→ Many-body bound states, resonances and scattering states





N. Michel *et al.*, J. Phys. G **36**, 013101 (2009)

The Gamow shell model

Dense, complex-symmetric Hamiltonian matrix:

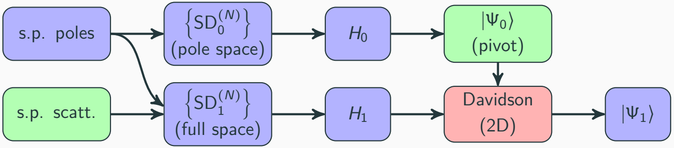
$$\begin{pmatrix} z_{00} & z_{10} & z_{20} \\ z_{10} & z_{11} & z_{21} \\ z_{20} & z_{21} & z_{22} \end{pmatrix}$$

Dense: up to a few percents of nonzero matrix elements.

Complex-symmetrix: There can be a vector $Z \neq 0$ such as $Z^T Z = 0$.

Factorial wall: both in terms of matrix elements density and matrix dimension!

Overlap method:



Many-body resonant solutions are poles of the many-body S-matrix.

Useful to find eigenstates in large-scale problems where full diagonalization is impossible.

Claim: Solutions in the pole space are many-body S-matrix poles.
→ True if s.p. poles ≈ natural orbitals.

The Gamow shell model for reactions

A general problem for many-body methods in the Berggren basis:

When using the Berggren basis, many-body eigenstates are expressed using Slater determinants (or just one):

$$|\Psi^{(A)}\rangle = \sum_i a_i \, |\mathrm{SD}_i^{(A)}\rangle, \qquad \hat{H}\,|\Psi^{(A)}\rangle = E\,|\Psi^{(A)}\rangle, \qquad E = e - i\Gamma/2.$$

However, the width Γ is the total width, it does not tell anything about the decay channels $|\Phi_c\rangle = |\Psi^{(A-1)}\rangle \otimes |\ell, j\rangle$:

$$\langle \Psi^{(A)} | \Phi_{c_0} \rangle \neq 0, \; \langle \Psi^{(A)} | \Phi_{c_1} \rangle \neq 0 \qquad \Rightarrow \qquad \Gamma = \sum_c \Gamma_c .$$

There is no known way to extract reaction channels from a configuration-interaction (CI) method, they must be included by hand using the resonating group method (RGM).

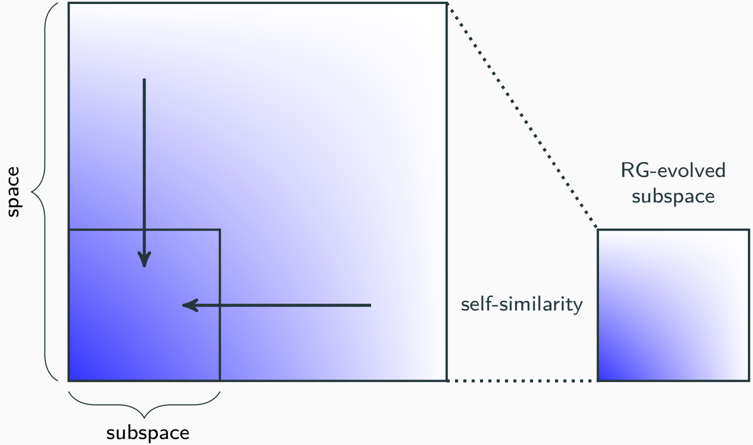
→ This is why the GSM was formulated in the coupled-channels formalism using the RGM.

(I am not going to explain how, this is not a reaction theory lecture...)

Y. Jaganathen *et al.*, Phys. Rev. C **89**, 034624 (2014); K. Fossez *et al.*, Phys. Rev. C **91**, 034609 (2015)
F. de Grancey, A. Mercenne *et al.*, Phys. Lett. B **758**, 26 (2016)

The density matrix renormalization group method

Two powerful ideas: renormalization group + density matrix based truncation scheme.

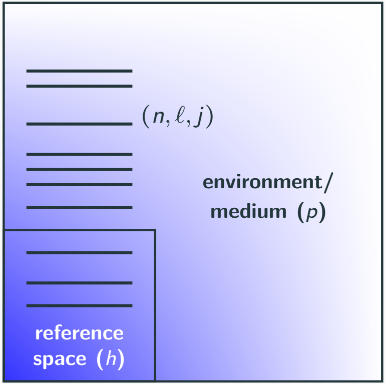


- The RG-evolved subspace is a compressed version of the whole space. It looks the same.
- Keeping all the information is computationally expensive. A truncation scheme is helpful.
- One can write the many-body wave function in a factorized form.

S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); S. R. White, Phys. Rev. B **48**, 10345 (1993)

The density matrix renormalization group method

Density matrix based truncation scheme:



- Many-body wave function: $|\Psi\rangle = \sum_{h,p} \Psi_{h,p} |h\rangle \otimes |p\rangle$.
- Density matrix reduced in the reference space:
$$\rho^{(r)}_{p,p'} = \sum_h \Psi_{h,p} \Psi_{h,p'}.$$
- The eigenvectors of $\rho^{(r)}_{p,p'}$ are linear combinations of the original (n, ℓ, j) shells.
- The eigenvalues $\{\varepsilon_n\}$ of $\rho^{(r)}_{p,p'}$ measure the importance of the new shells in the many-body wave function.

→ The DMRG criterion: $\varepsilon_n > \varepsilon$ (gently breaks the many-body completeness).

J. Dukelsky and G. G. Dussel, Phys. Rev. C **59**, R3005(R) (1999), J. Dukelsky and S. Pittel, Rep. Prog. Phys. **67**, 513 (2004)
T. Papenbrock and D. J. Dean, J. Phys. G **31**, S1377 (2005)

The density matrix renormalization group method

DMRG for the nuclear many-body problem:

- Works well in condensed matter (sites, neighboors only) or cold atom physics (contact interaction).
- In the shell model, HO shells are significantly different than natural orbitals (for a given state).
- The nuclear interaction acts on nucleons even if they are on different (distant) shells.

M-scheme DMRG:

- Seemed to work using simple $\hat{H}$, but slow convergence to wrong energies with realistic interactions.
- Little by little, the DMRG truncation breaks the rotational invariance in the M-scheme.

J-scheme DMRG:

- Correct energies in the J-scheme, but still slow convergence (HO, HF shells).
- Important increase of the complexity of the algorithm.

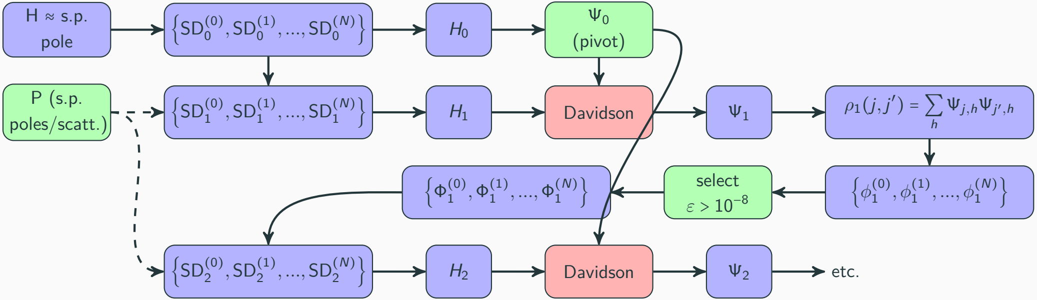
In principle, one must do a warm-up, sweep-down, sweep-up, etc.

S. Pittel and J. Dukelsky, Rev. Mex. Fis. **49 Supl. 4**, 82 (2003),
J. Dukelsky and S. Pittel, Rep. Prog. Phys. **67**, 513 (2004)

Gamow-DMRG or DMRG in the Berggren basis:

- In the Berggren basis there are: 1) resonant/pole states, and 2) scattering/continuum states.

→ Natural division that fits well the reference space *vs.* medium DMRG division.



Formulated in J-scheme, makes use of natural orbitals.

First proposed in Rev. Mex. Fis. **5 Suplemento 2**, 74 (2004),
J. Rotureau *et al.*, Phys. Rev. Lett. **97**, 110603 (2006), J. Rotureau *et al.*, Phys. Rev. C **79**, 014304 (2009)

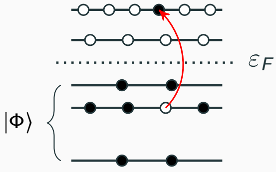
The coupled clusters theory

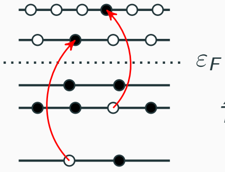
A powerful method: similarity transformation on a normal-ordered Hamiltonian:

- Reference state $|\Phi\rangle$ treated as an effective vaccum using normal-ordering.
- Similarity transformation (non-unitary) to avoid building the $\hat{H}$ matrix.

$$\hat{H} = \sum_{p,q} \varepsilon_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{p,q,r,s} \langle pq||rs\rangle \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r$$
$$= E_0 + \sum_{p,q} f_{pq} \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{p,q,r,s} \Gamma_{pqrs} \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} = E_0 + H_N.$$

$$\boxed{\begin{aligned} &\langle\Phi|\hat{H}_N|\Phi\rangle = 0, \\ &\bar{H} = e^{\hat{T}} \hat{H}_N e^{-\hat{T}}, \\ &\hat{T} = \sum_{n=1}^{A} \hat{T}_n. \end{aligned}}$$





$$\hat{T}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1, i_2, \ldots, i_n \\ a_1, a_2, \ldots, a_n}} t_{i_1, i_2, \ldots, i_n}^{a_1, a_2, \ldots, a_n} \hat{a}_{a_1}^\dagger \hat{a}_{a_2}^\dagger \cdots \hat{a}_{a_n}^\dagger \hat{a}_{i_1} \hat{a}_{i_2} \cdots \hat{a}_{i_n}.$$

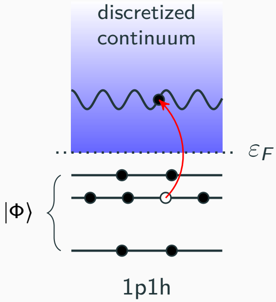
→ Set of non-linear equations for the amplitudes.

G. Hagen *et al.*, Rep. Prog. Phys. **77**, 096302 (2014)

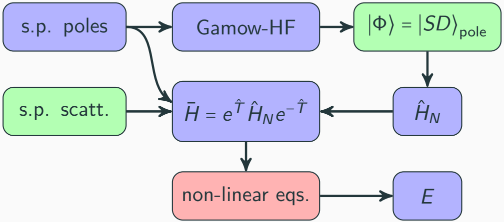
The coupled clusters theory

In the Berggren basis:

- Non-symmetric $\hat{H}$ matrix → complex non-symmetric.
- Does not care much about the size of the s.p. basis!
- Most exotic nuclei can be described with one and two particles in the continuum.



Identification of many-body resonances:



→ Size-extensive approach for nuclear open quantum systems.

G. Hagen *et al.*, Phys. Lett. B **656**, 169 (2007)

Known issues

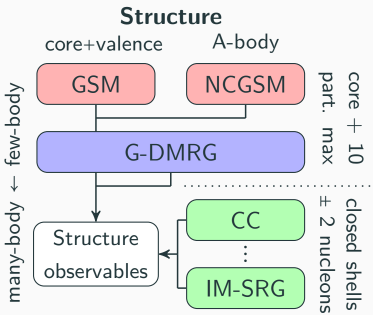
Several issues are still bothering practitioners:

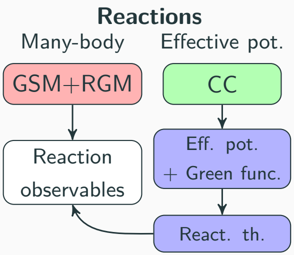
- Identification of many-body resonances in the complex energy spectrum (especially for broad resonances).
- Factorization of the intrisic and center-of-mass eigenstates in *ab initio* calculations.
- Reduction of the basis size (s.p. or many-body).
- Diagonalization of complex-symmetric matrices.
-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

Summary

Many-body methods in the Berggren basis:

- Several techniques have been extended successfully into the continuum.





- Still a lot of work must be done to unified nuclear structure and reactions.

Thank you for your attention!