A quantum optimization algorithm for deriving effective shell model hamiltonians

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Università degli Studi della Campania *Luigi Vanvitelli*

INFN Istituto Nazionale di Fisica Nucleare

SM&FT 2022

Outline

- The Nuclear shell model
- The problem of the effective Hamiltonian
- Genetic algorithm (GA)
- Quantum GA
- Use of GA to derive p shell effective interaction
- Conclusions and Outlook

Outline

- The Nuclear shell model

The Nuclear Shell Model

The nuclear many-body problem

Infinite Space, **A** nucleons

$$H\psi_\alpha = E_\alpha\psi_\alpha$$

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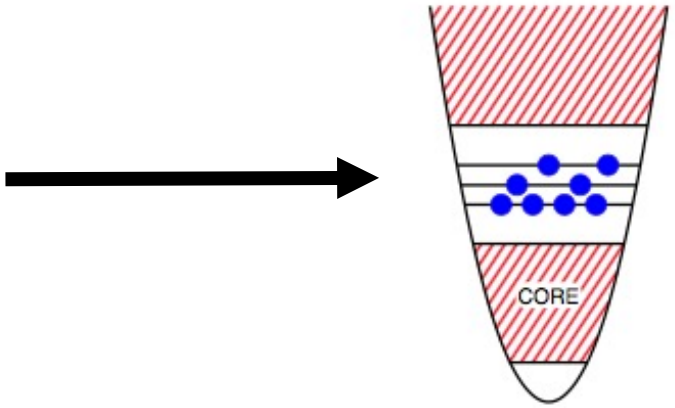

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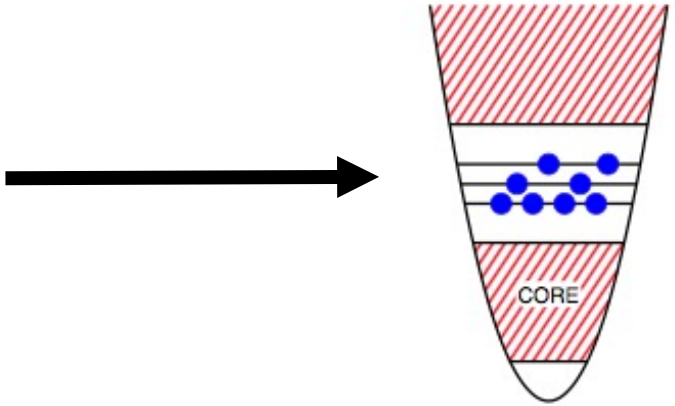

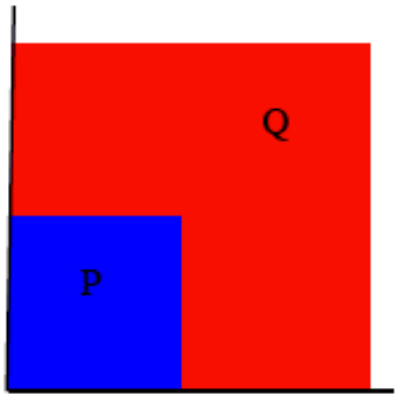

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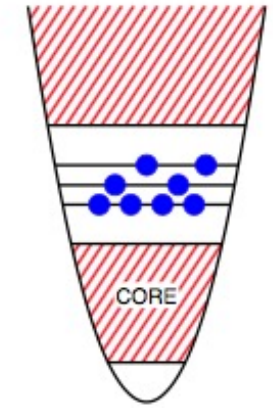

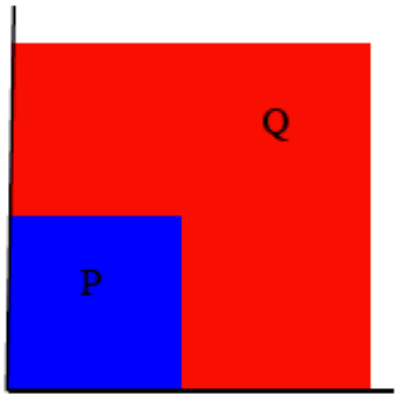

Model Space, v nucleons

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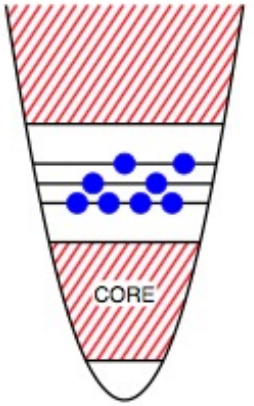
The excitations of the core are absorbed by the effective hamiltonian

$$V_{eff} = V + V\frac{Q}{E - H_0}V_{eff}$$



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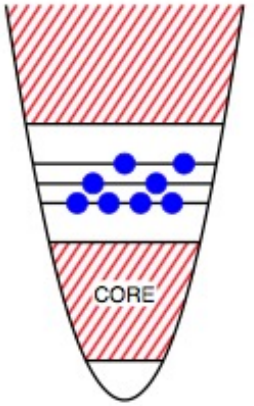

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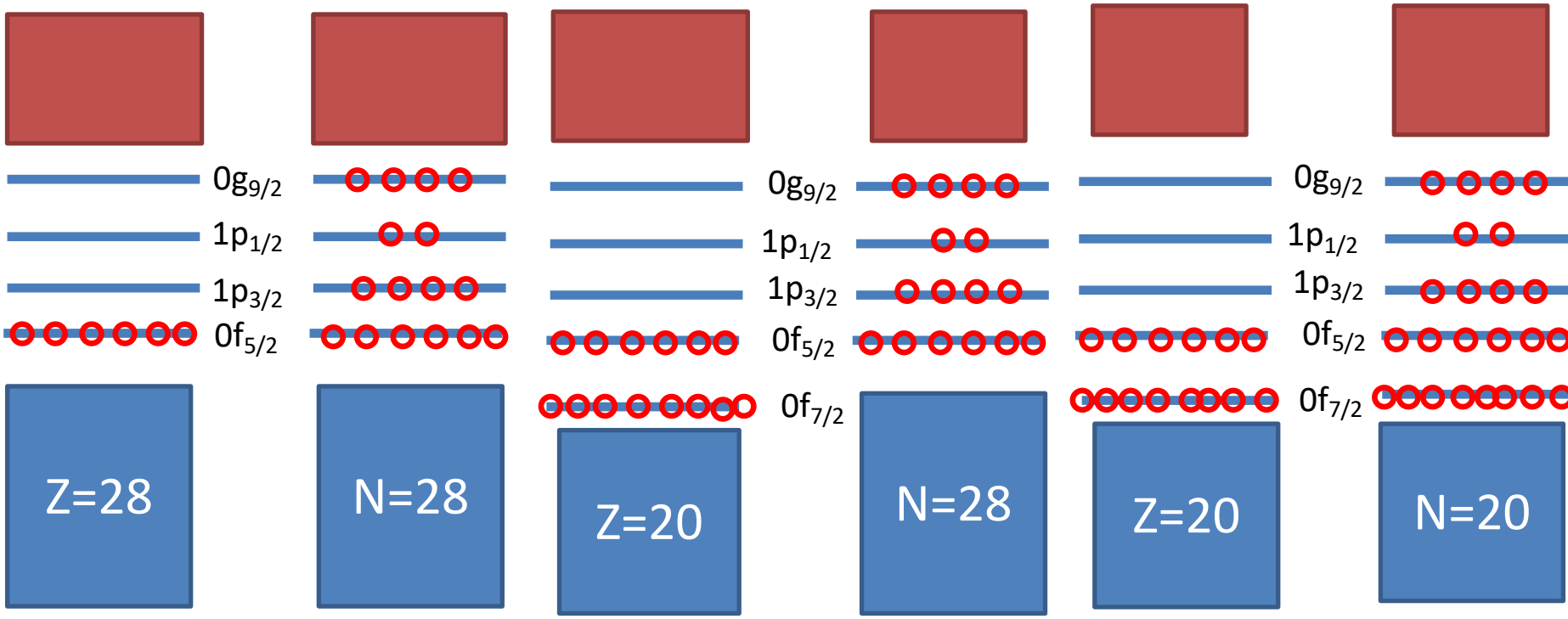
Problems:

1) Size of the Hamiltonian matrix too large as v increases
2) Derivation of the effective Hamiltonian

Definition of the model space

Let's focus for example on ^{76}Se for different cores



Core ^{56}Ni
Z_v=6
N_v=14

Dim= 6.79×10^8

Core ^{48}Ca
Z_v=14
N_v=14

Dim=1.15×10^{12}

Core ^{40}Ca
Z_v=14
N_v=22

Dim= 2.04×10^{13}

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The shell-model hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered

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Two alternative approaches

Microscopical

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V_{NN} ($+V_{NNN}$)

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Microscopical

V_{NN} (+V_{NNN}) ⇒ many-body theory ⇒ H_{eff}

The eigenvalues of H_{eff} belong to the set of eigenvalues of the full nuclear hamiltonian.
This may be provided by a similarity transformation Ω of the full Hilbert-space hamiltonian H.

The shell-model effective hamiltonian

The shell-model hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered

Two alternative approaches

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The ME and the single particle energies are determined using for example best fit procedure fitting experimental data available in the region.

Well known phenomenological potential are for example the Cohen-Kurath in the 0p shell, the USDA and USDB in the 1s0d shell

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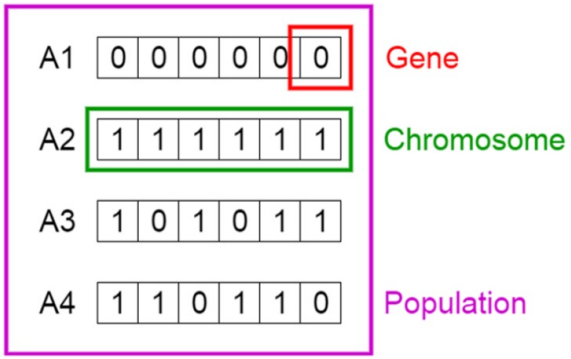
Selection of the individuals most likely to survive in a given environment takes place

They rely on an iterative process that consists in evolving and evaluating a large set of solutions called "population of individuals"

Genetic algorithm (GA)



The idea of selection phase is to select the fittest individuals and let them pass their genes to the next generation.

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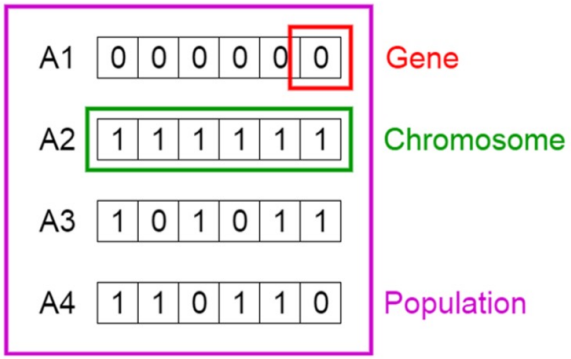

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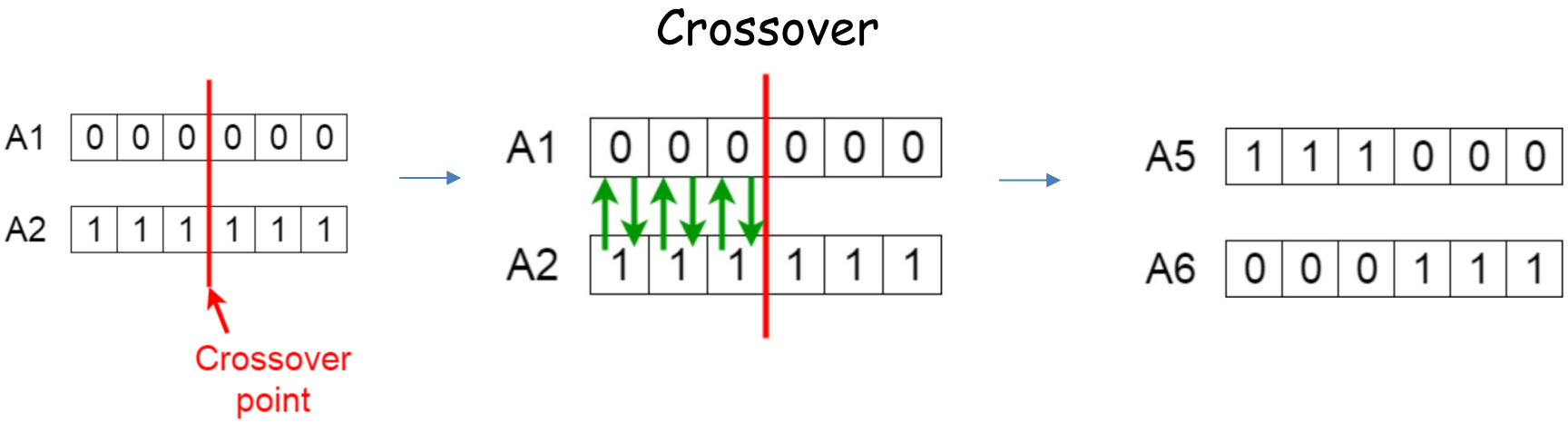

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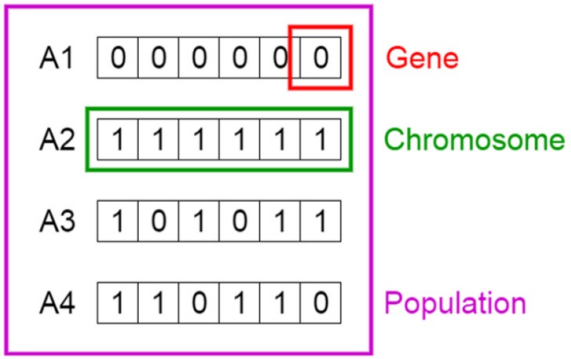

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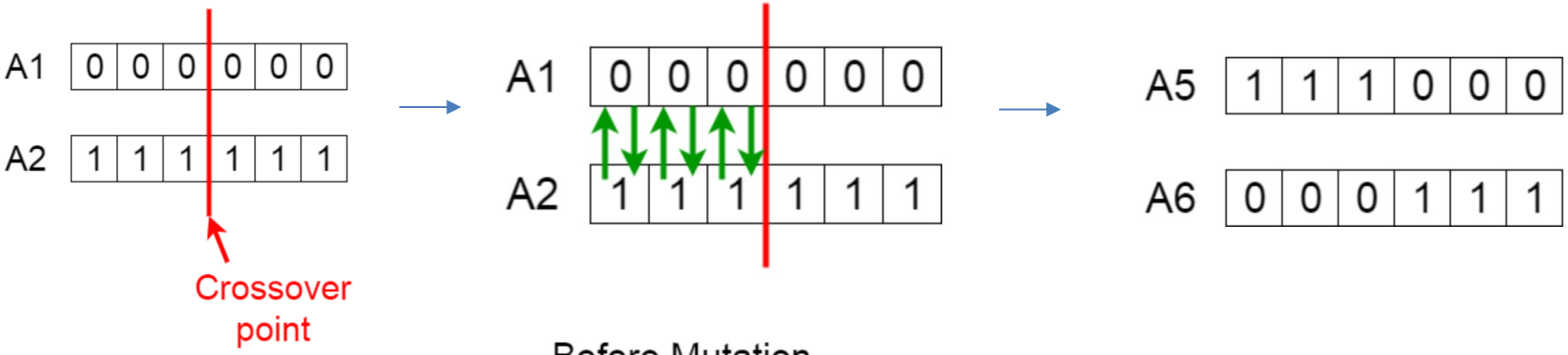
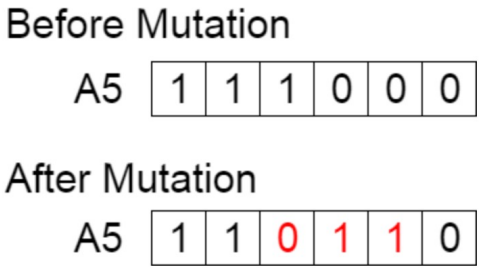
Crossover



Mutation



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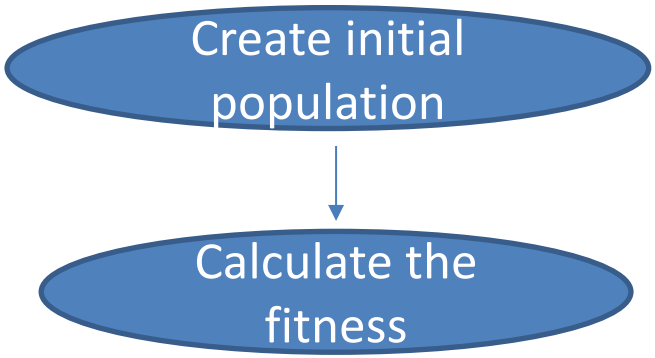

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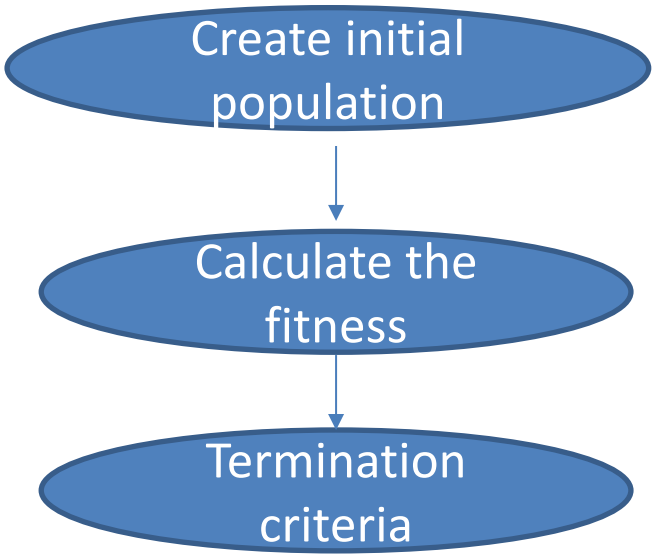

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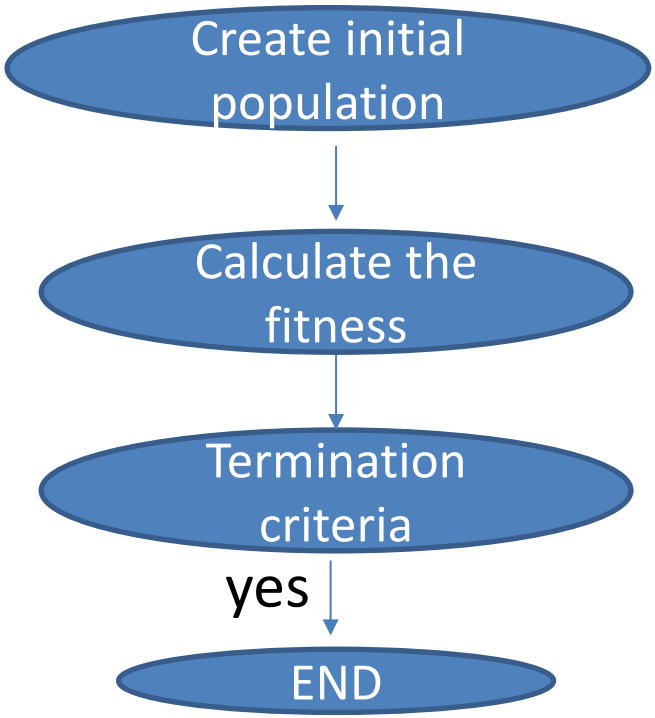

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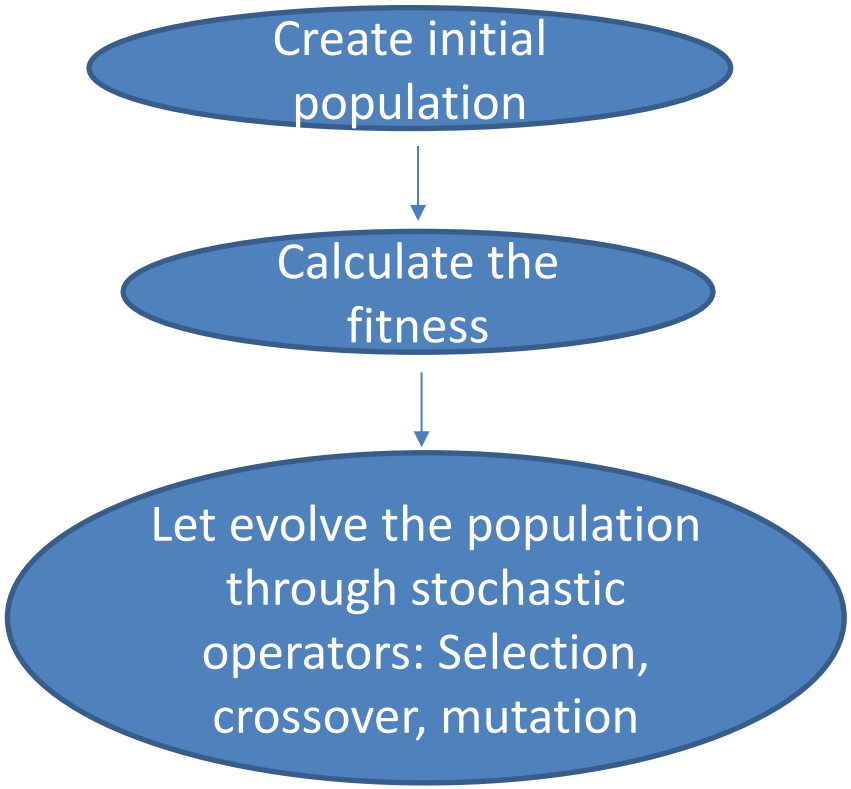

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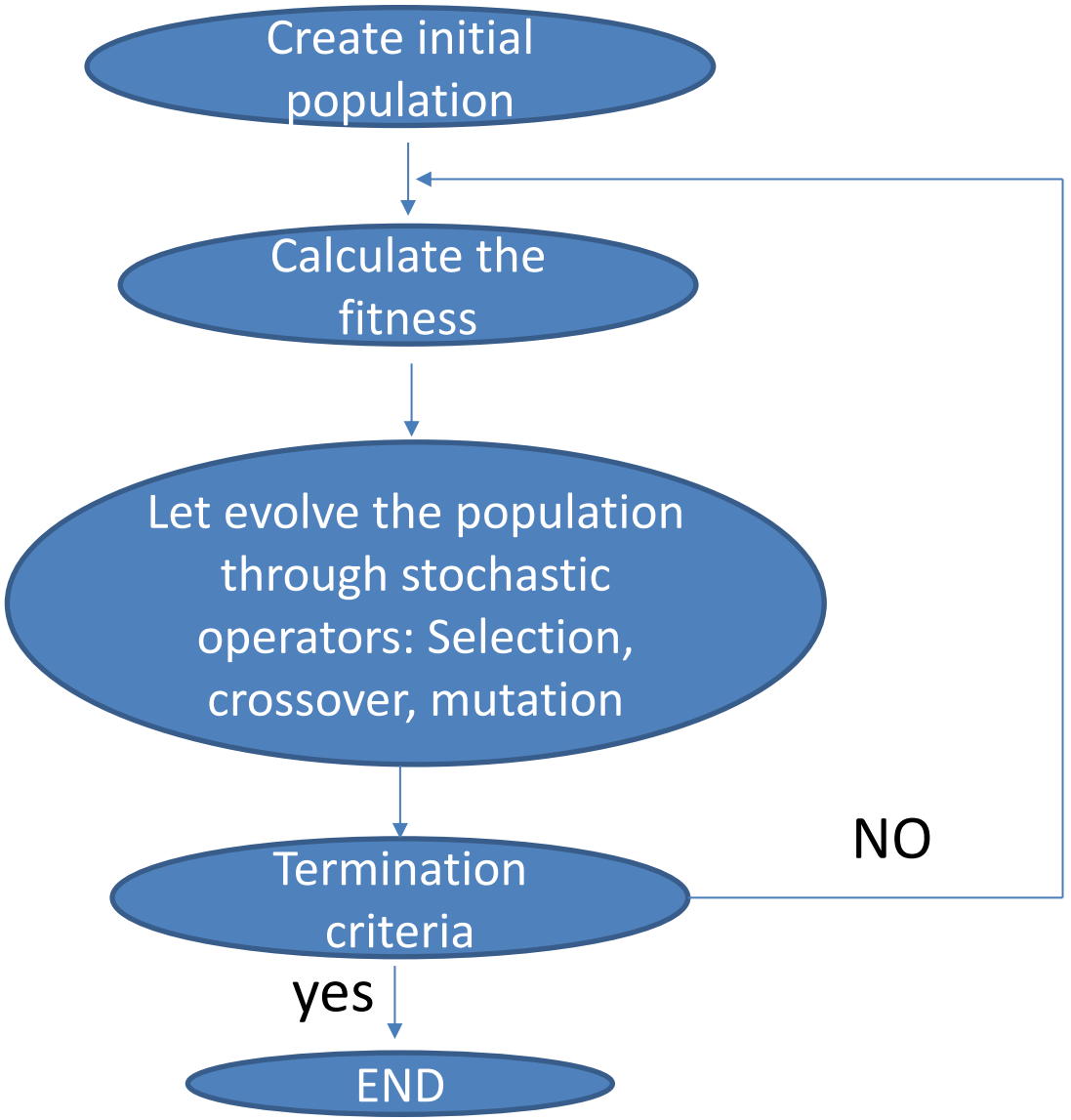

Genetic algorithm (GA)

What is the advantage of using evolutionary algorthms like GA with respect to algorithm based on Gradient for example?

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What is the advantage of using evolutionary algorthms like GA with respect to algorithm based on Gradient for example?

- Starting from a population EA algorithms are more robust
- The possibility to end up with in local minima is minimized, complete exploration of the space
- Computational advantage: No computation of the gradient

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Quantum GA

First implementation for the binary case

Quantum GA is a hybrid quantum/classical algorithm able to perform genetic optimization by using quantum and classical computers

In detail, quantum computers are used to implement the entire evolutionary optimization process, while classical computers perform the fitness function evaluations

Extension to the real case is ongoing

G. Acampora and A. Vitiello, Information Sciences 575 (2021) 542–562

Quantum GA

The quantum chromosome

The quantum chromosome allows to efficiently embed a large portion of a classical genetic population on a single quantum register

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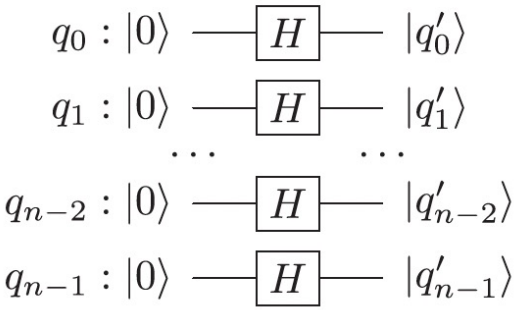

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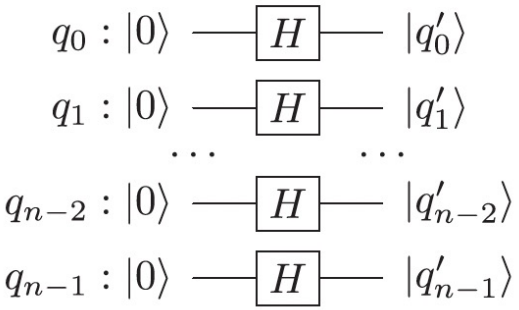

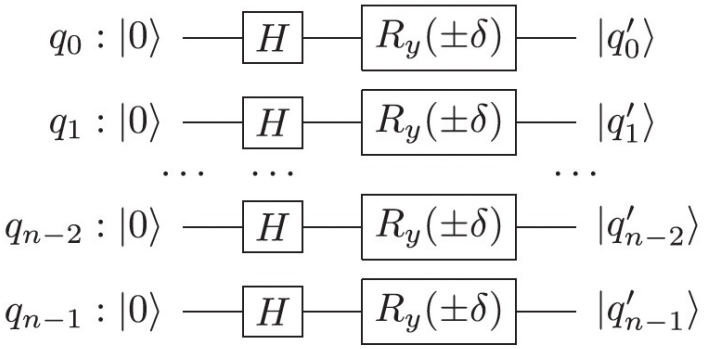

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A single n-qubit quantum register can embody all 2^n-bits configurations simultaneously

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Thanks to the application of the quantum measurement, a single fitness function evaluation is required to evaluate its quality.

Potential exponential advantage!!!

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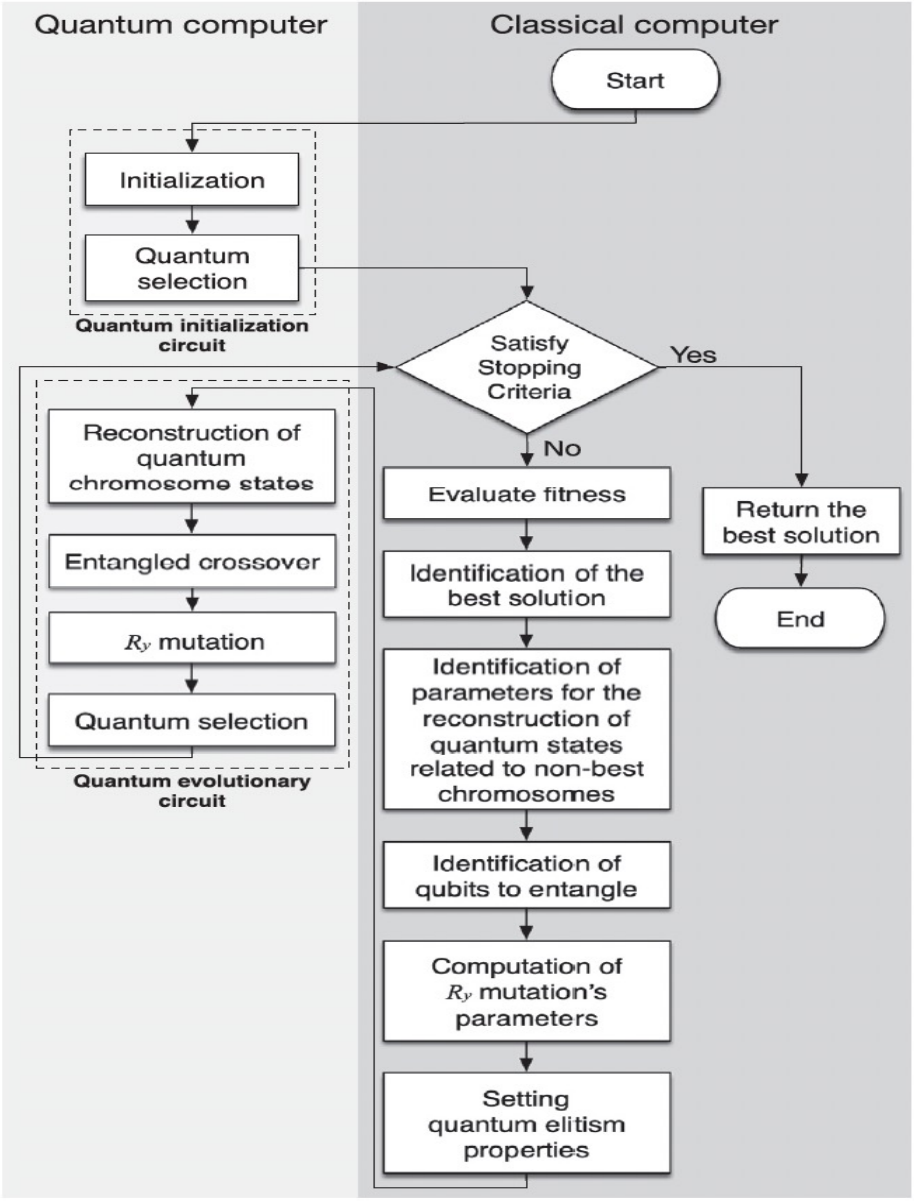
Quantum GA



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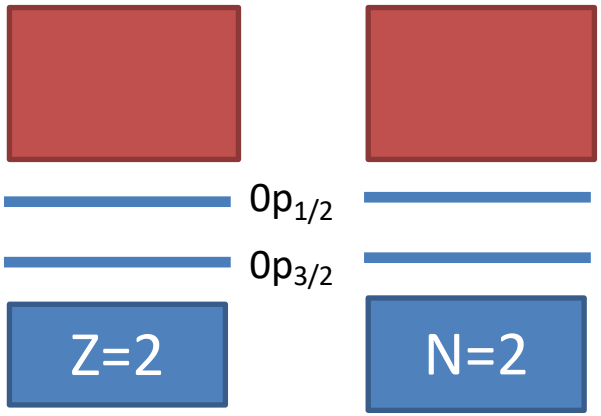
Use of GA to derive shell model effective interactions

We are testing the extension to the real case on the calculation of an effective interaction for p-shell nuclei



In the J coupled scheme there are 34 TBME and 4 sp ME

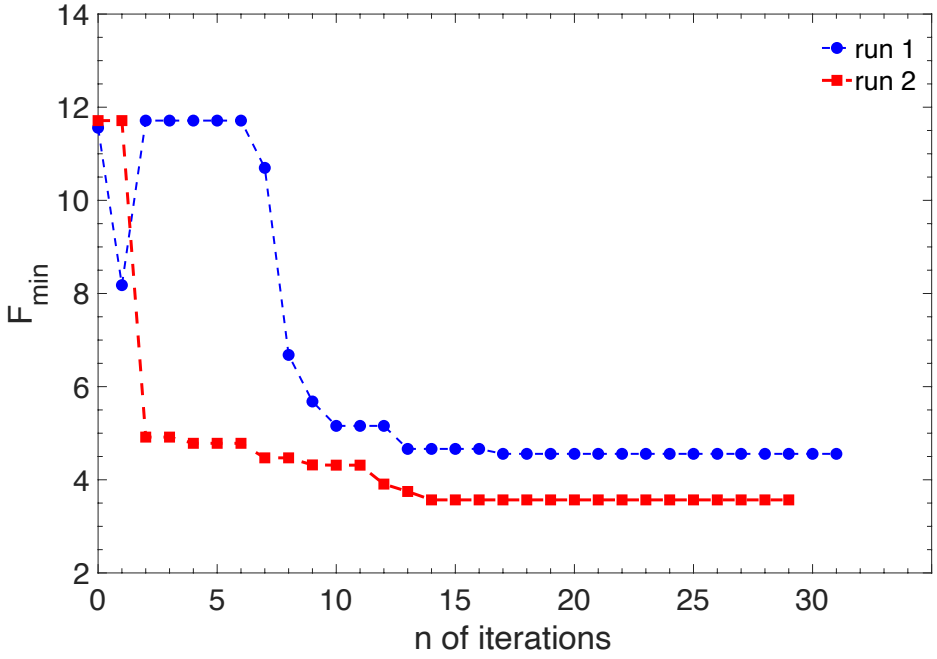
One of the most famous p shell interaction is the Cohen-kurath interaction

At that time they made the fit (1965) there were 50 experimental levels, and not all of them were put in the fit nowadays we have more than 150 data

They performed a least square fit analysis, neglecting the coulomb interaction -> only a subset of the 34 TBME is linearly independent

S. Cohen and D. Kurath, Nuclear Physics 73 (1965) 1--24

Use of GA to derive shell model effective interactions

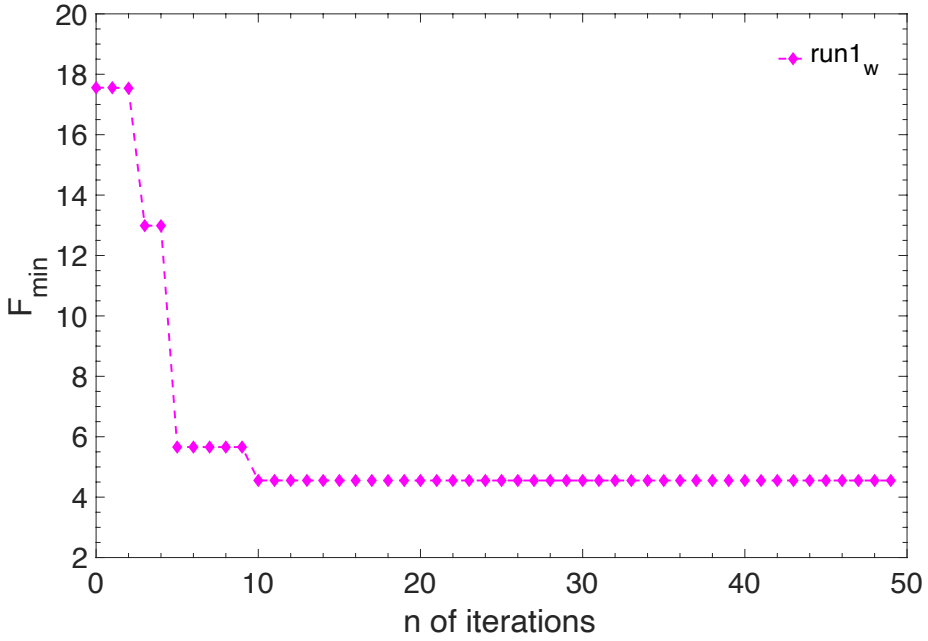


The first thing to show is that GA converges

Preliminary

$$f(\theta_i) = \sum w_j \left(E_j^{th}(\theta_i) - E_j^{exp} \right)^2$$

120 states of different p-shell nuclei



GA Real

The second thing to analyze are the results

We are trying to fit, at same time, gs and excited states energies

Ground state with respect to ^{4}He

Nucleus	J^π	E^{exp}	Eth (CK)	Eth (GA)
^{6}He	0^+	-0.975	-3.909	-4.930
^{8}He	0^+	-3.100	-3.123	-6.213
^{8}Be	0^+	-28.203	-31.119	-29.782
^{12}C	0^+	-63.866	-71.044	-66.613
^{13}N	$½^-$	-65.809	-75.229	-67.816
^{15}N	$½^-$	-87.193	-97.527	-90.838

Preliminary

Excitation energy of excited states

Nucleus	J^π	E_x^{exp}	E_{th} (CK)	E_{th} (GA)
^{6}He	2^+_1	1.797	4.542	1.797
^{8}He	2^+_1	3.100	4.715	2.731
^{8}Be	2^+_1	3.030	3.819	2.553
^{12}C	2^+_1	4.440	4.647	4.549
^{13}N	$3/2^-$	3.502	3.587	5.144
^{15}N	$3/2^-$	6.324	6.362	7.128

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Conclusions

- From very preliminary results GA seems to be able to determine an effective interaction for the 0p shell wich can be potentially better than the CK interaction

Outlook

- Try different populations and improve the Fitness definition

- Once we are ready, we can move to the Quantum GA, for N=34 parameters we will need n=6 qubits

- We will continue with other regions.

- This procedure con be used also to modify already existing effective interactions

Other applications???

Thank you