Origins and evolution of nuclear energy density functional models

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Goal

- Put EDF into its context

❶ Microscopic approaches of nuclear systems

A) Richness of nuclear systems

B) Strenuous task

C) Strategies

❷ Energy density functional approaches

A) Independent particle picture

B) Historical perspective

C) Miraculous density dependence

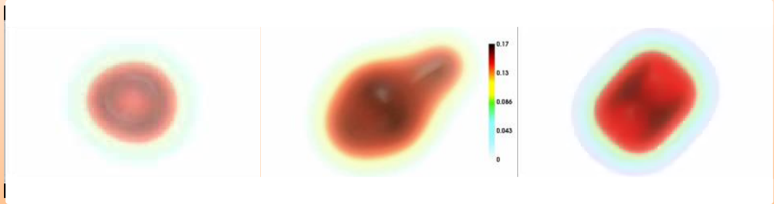
D) Modern interpretation

❶ Microscopic approaches of nuclear systems

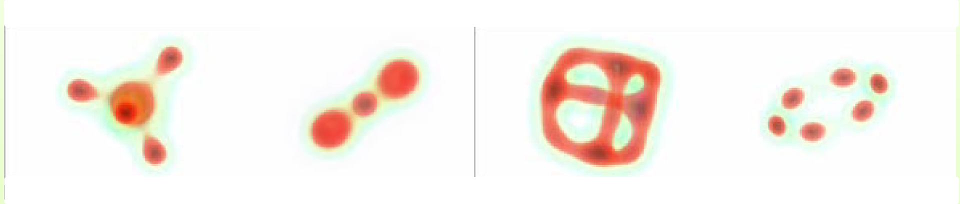
A) Richness of nuclear systems

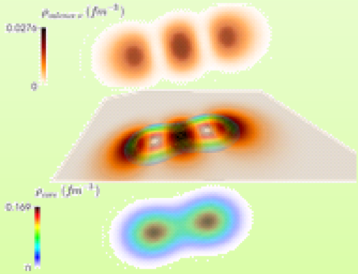
➲ Nuclear systems : huge variety of behaviors

➲ Deformation

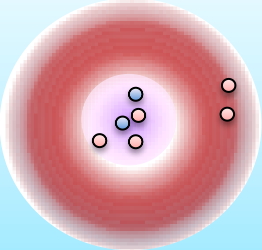


➲ Clustering

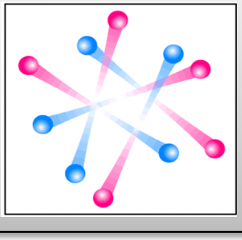




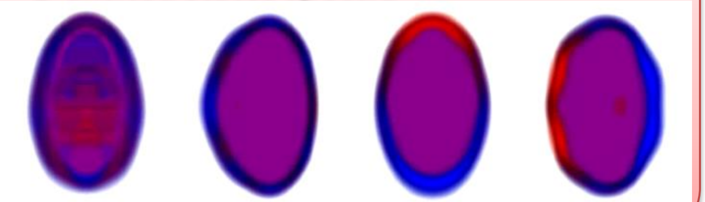
➲ Halo, neutron skin



➲ Superfluidity

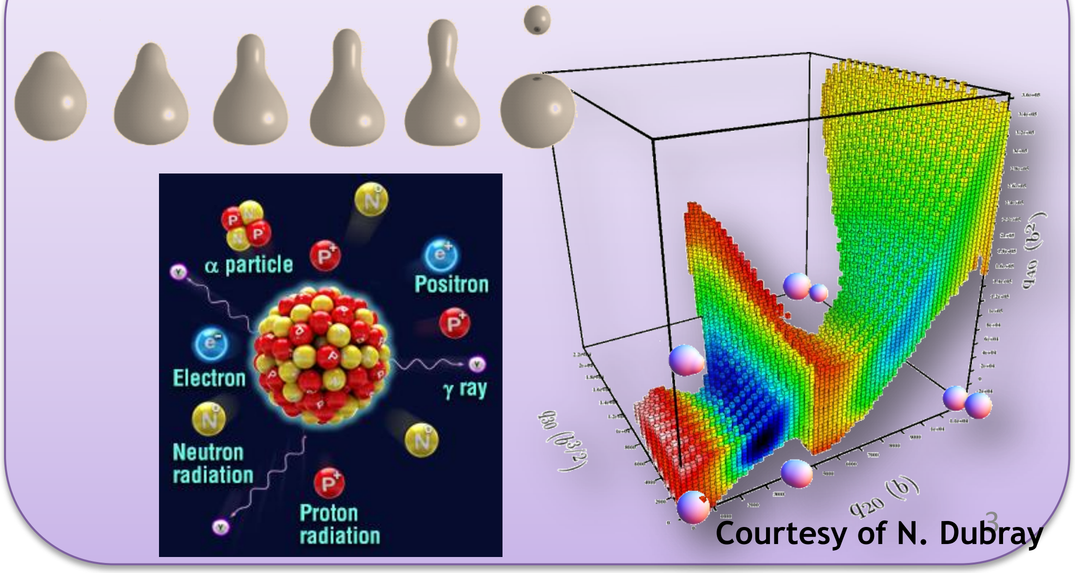


➲ Excited states spectra



Courtesy of D. Peña Arteaga

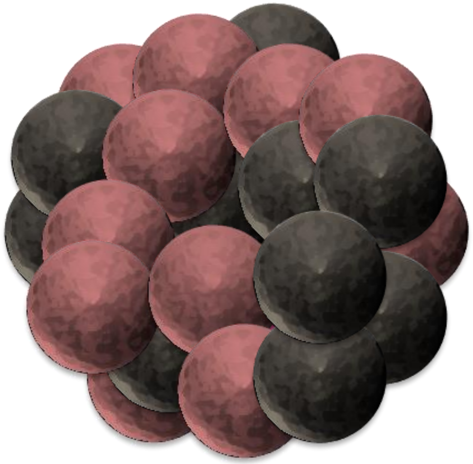
➲ De-excitation modes



Courtesy of N. Dubray

✪ *Cross-fertilization*

➲ Mesoscopic physics



➲ Particle physics

➲ Astrophysics

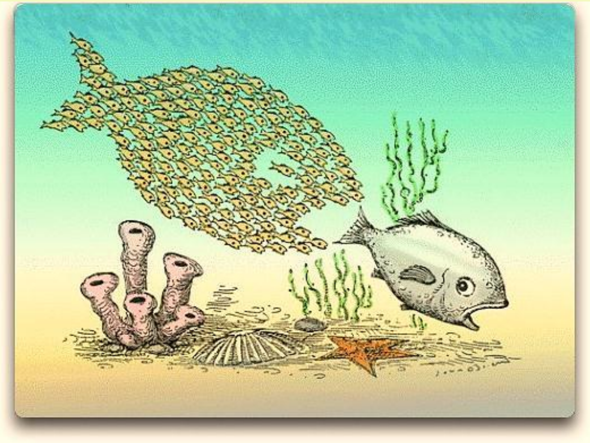
✪ Why such a diversity ?

➲ Emergent phenomena : hallmark of many-body systems

❖ Behavior not reducible to some sort of sum of the behaviors its parts

❖ Behavior not predictable given the full knowledge of the behaviors its parts

❖ Behavior somehow novel by some salient standard

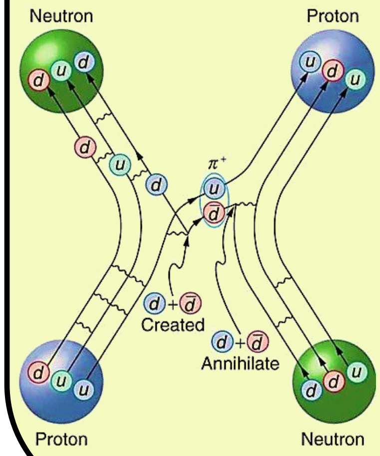


⇒ When many particles interact totally surprising results can emerge

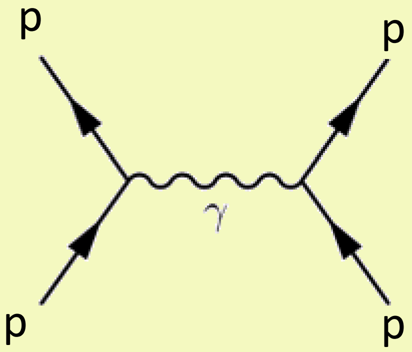
Anderson P.W., Science 177:393-396 (1972)
Batterman R.W., Fond. Phys. 41:1031-1050 (2011)

✪ *Why such a diversity ?*

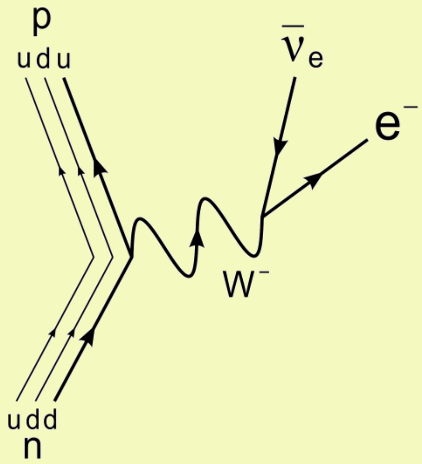
➲ Nuclear systems = mixture of <u>**4**</u> types of <u>**non-elementary**</u> fermions feeling <u>**various**</u> interactions



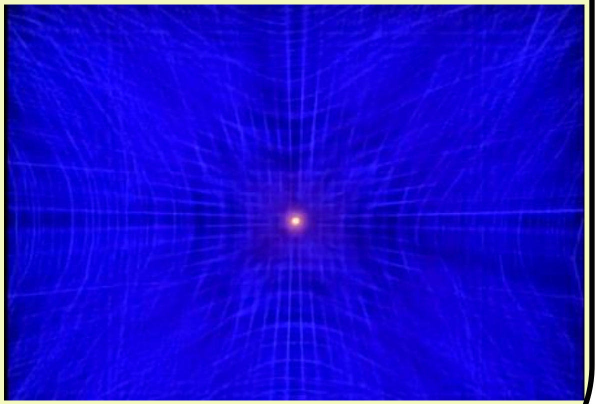
Strong
Binds nucleons in nuclei
⇒ saturation



Electromagnetic
Asymmetry proton/neutron
Limits size nuclei



Weak
Exotic nuclei decay towards stability line

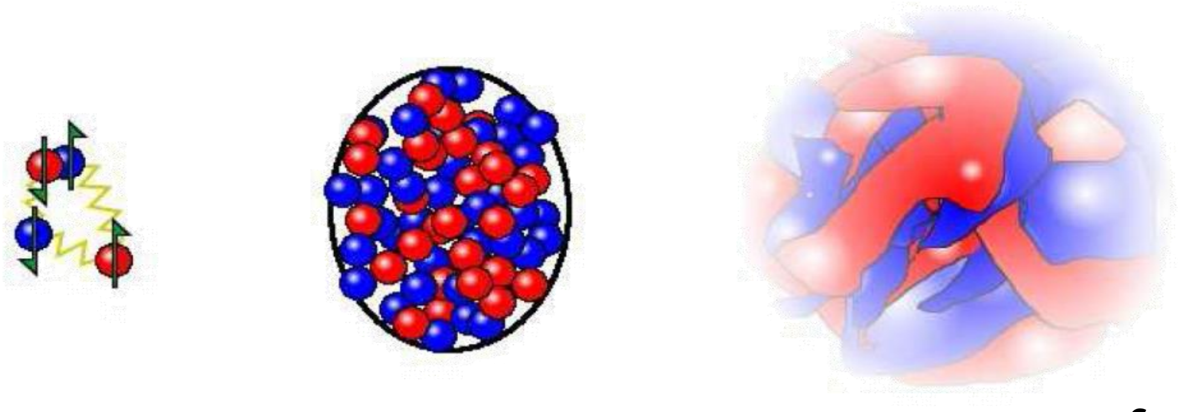


Gravity
Binds neutron in neutron stars

✪ Why such a diversity ?

➲ Finite size effects non negligible

⇒ Adding even one nucleon to a nucleus can lead profound structural changes



Courtesy of T. Duguet

➲ Openness of the nuclear quantum system

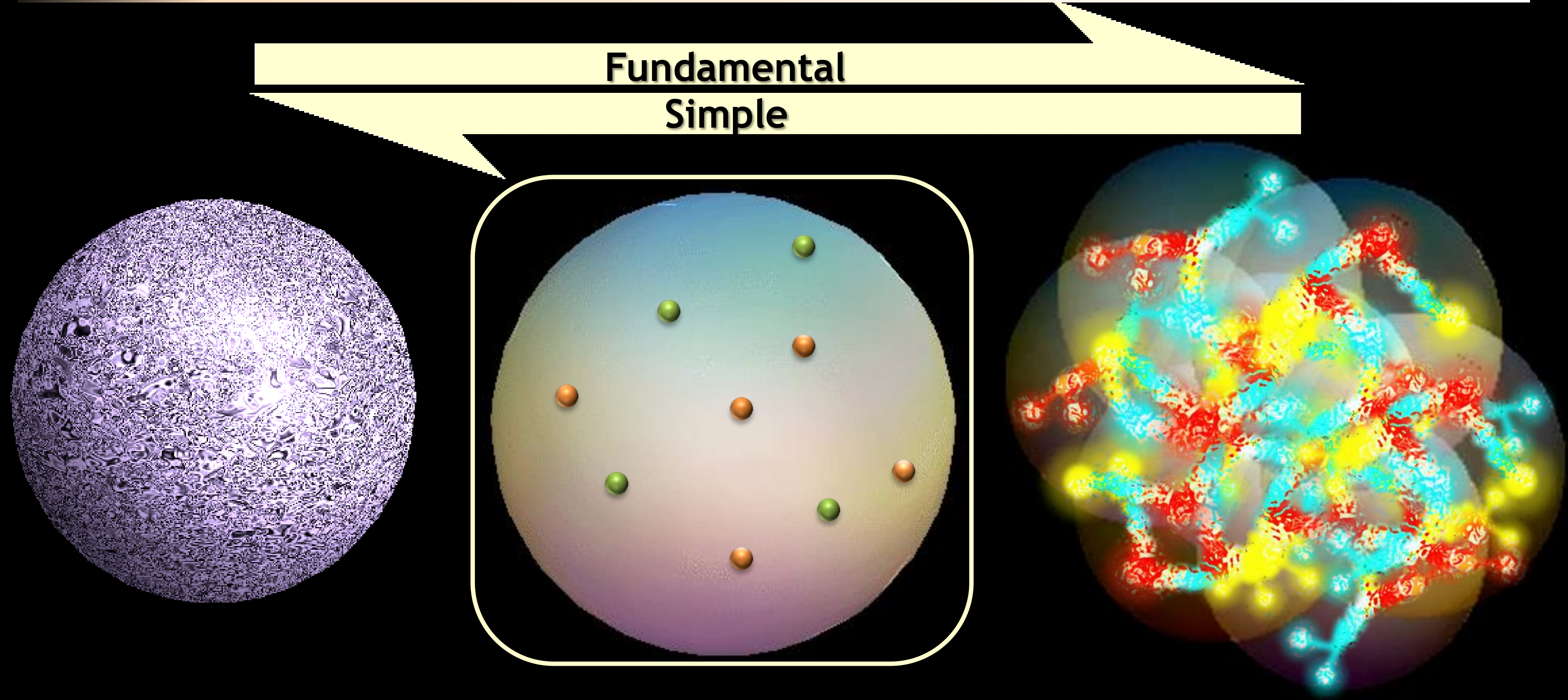
✪ Consequences

➲ Theoretical description of nuclear systems = a hell of a challenge !

- ❖ Perturbative methods can hardly be used as is
- ❖ Statistical treatment does not apply

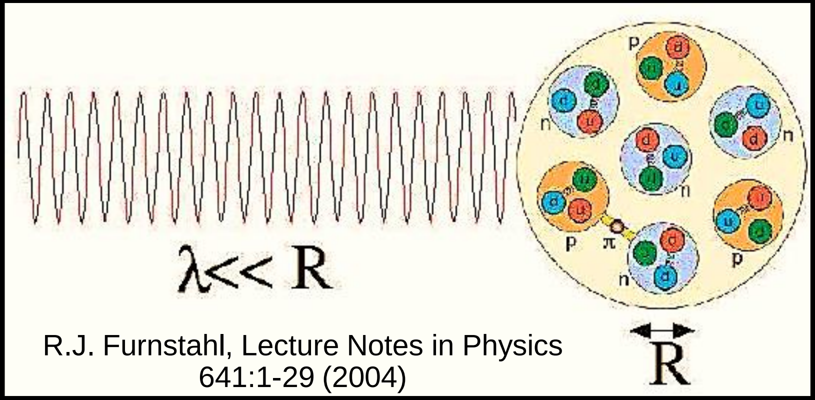
➲ Proliferation of nuclear models

✪ Relevant degrees of freedom

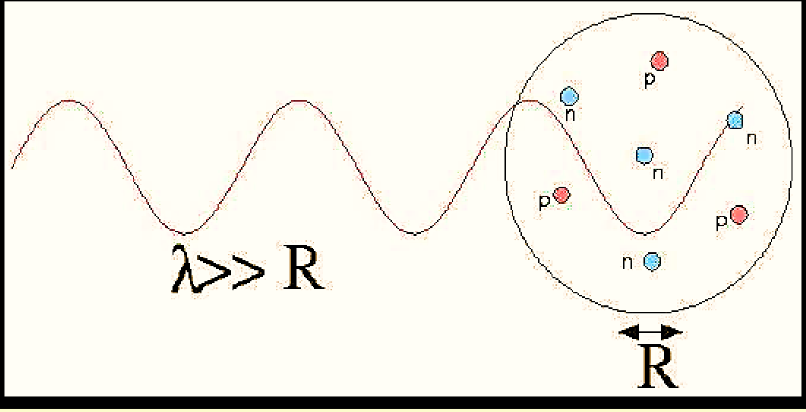


Fundamental

Simple



R.J. Furnstahl, Lecture Notes in Physics 641:1-29 (2004)



➊ Microscopic approaches of nuclear systems

B) Strenuous task

✪ What is a microscopic approach of the nucleus ?

➲ Nucleus = A point-like nucleons in interaction

$$H = \sum_{i=1}^{A} T_i + \sum_{i<j=1}^{A} V_{ij} + \sum_{i<j<k=1}^{A} V_{ijk} + \ldots$$

➲ Difficulties

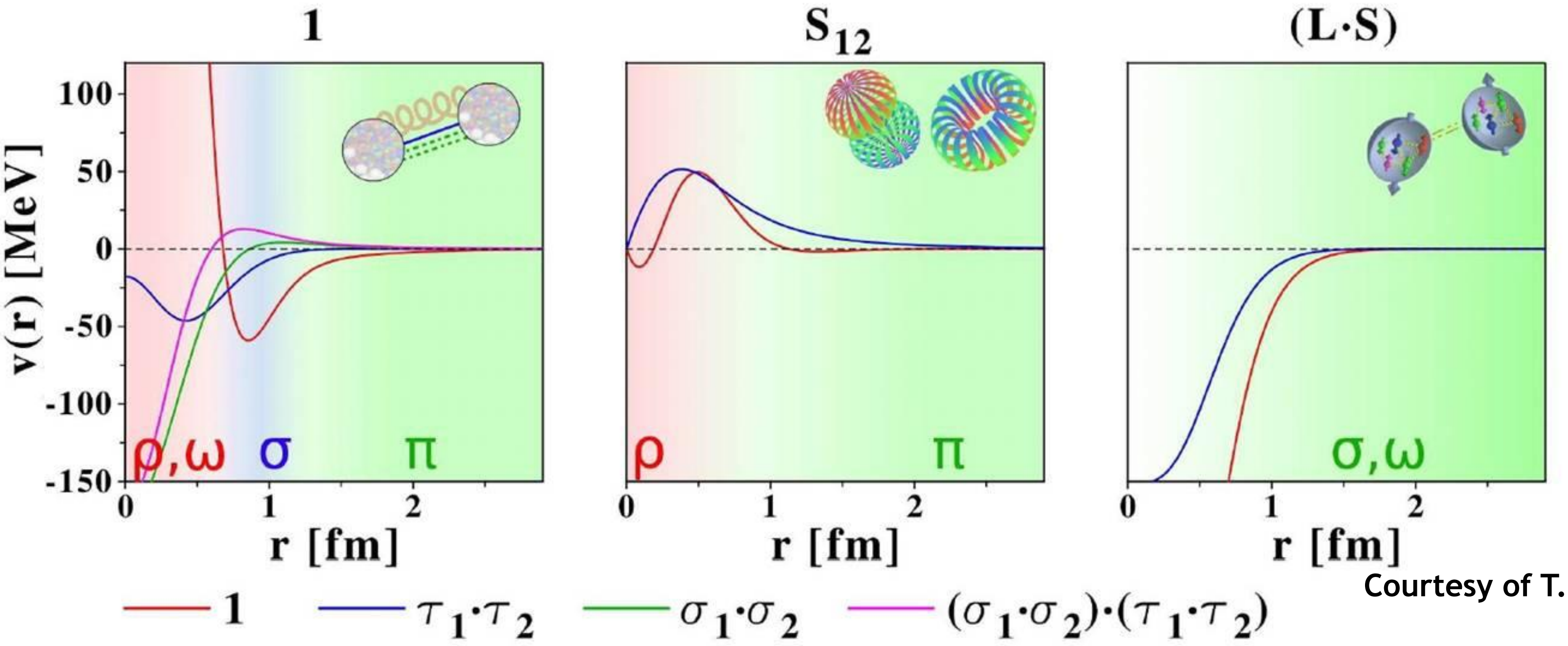
- ❖ Treatment of the inter nucleonic interactions
- ❖ Many-body problem

✪ Inter nucleonic interaction

➲ In Real life, nucleons = **composite** particles involving quarkic and gluonic degrees of freedom

❖ Strong interaction between nucleons reminiscent of strong interaction between their quarks and gluons

⇒ Complicated form for the corresponding NN potential (non-local, spin orientation dependent, …)



Courtesy of T. Duguet

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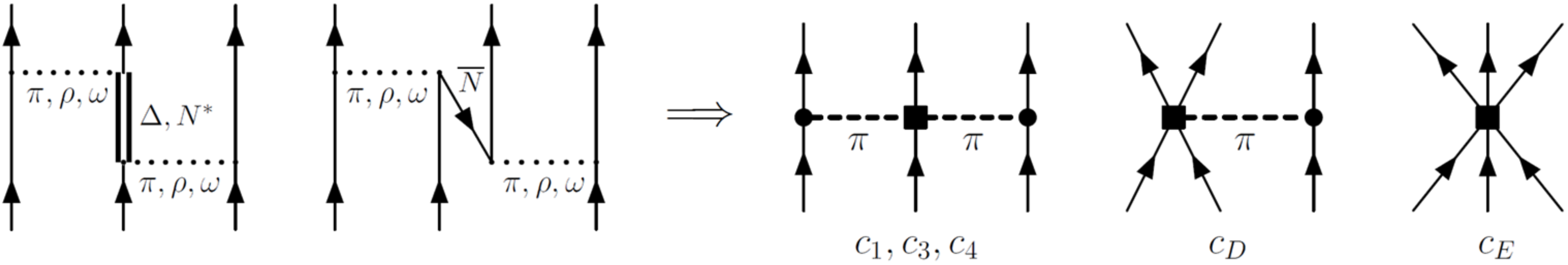
❖ Internal structure ⇒ existence of more than pairwise interactions in the point-like picture



Bogner et. al, Prog.Part.Nucl.Phys.65:94-147 (2010)

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➲ In principle, inter-nucleonic interactions should be derived from QCD

✪ QCD in a nutshell – building of the gauge theory

➲ QCD = non-abelian gauge theory of the strong interactions based on SU(3)$_c$

❖ Idealized lagrangian density of free quarks :

$$\mathcal{L} = \sum_{j=1}^{N_f} \bar{\psi}_j \left(i \not\partial \right) \psi_j$$

- *flavor*
- *Quark field*

❖ Quark field in the fundamental representation of SU(3)$_c$:

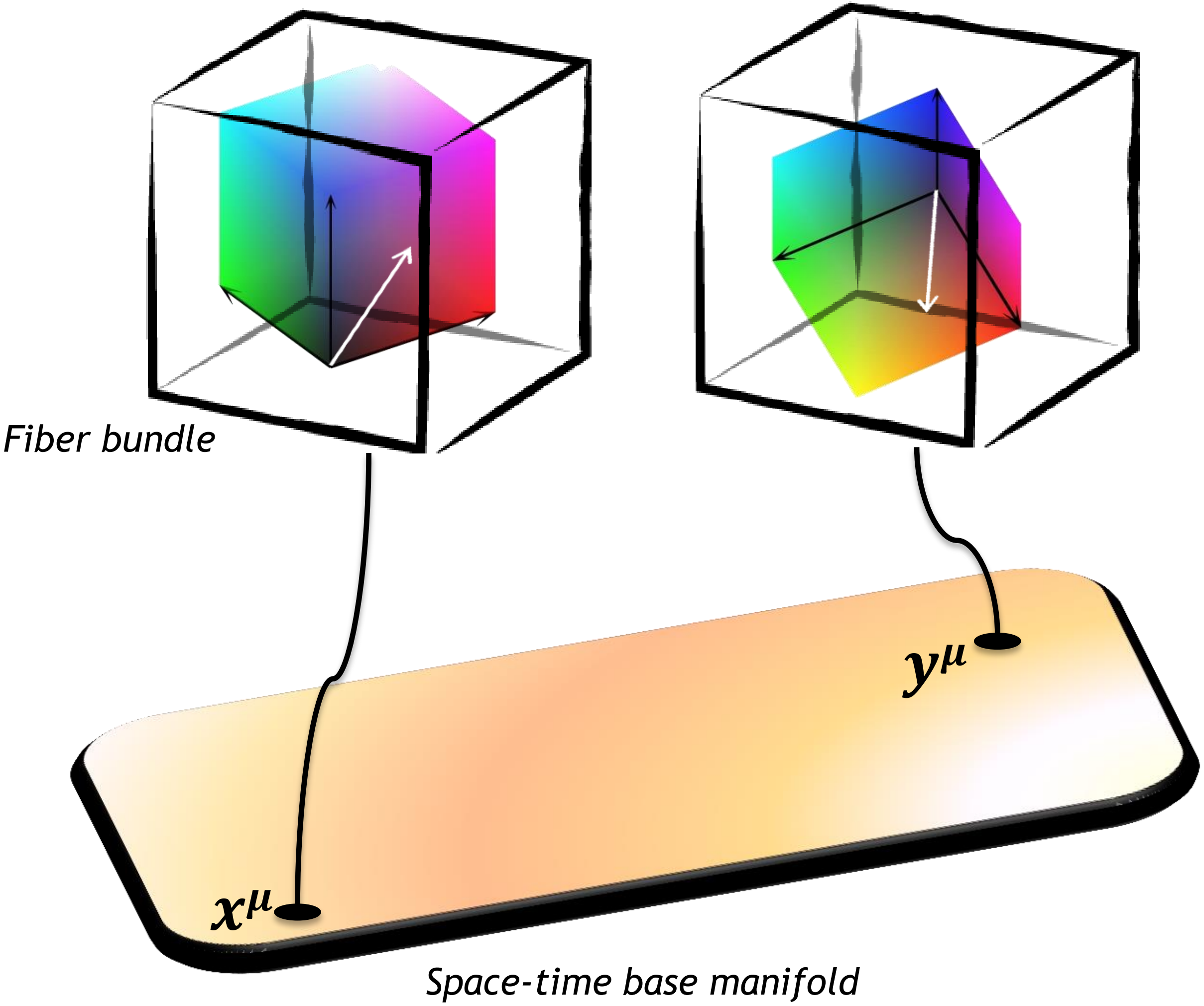
$$\psi_j(x^\mu) \equiv \begin{pmatrix} q_j^{red}(x^\mu) \\ q_j^{green}(x^\mu) \\ q_j^{blue}(x^\mu) \end{pmatrix}$$

❖ Invariance under **global** rotation in gauge space : $\psi_j(x^\mu) \rightarrow e^{i\theta_a T_a} \psi_j(x^\mu)$

➲ Now ask the Lagrangian to be invariant under **local** gauge transformation

$$\psi_j(x^\mu) \rightarrow e^{i\theta_a(x^\mu) T_a} \psi_j(x^\mu)$$

✪ QCD in a nutshell – building of the gauge theory



➲ Gauge field (connection) : gives a mean to compare internal frames at different space-time points (parallel transport)

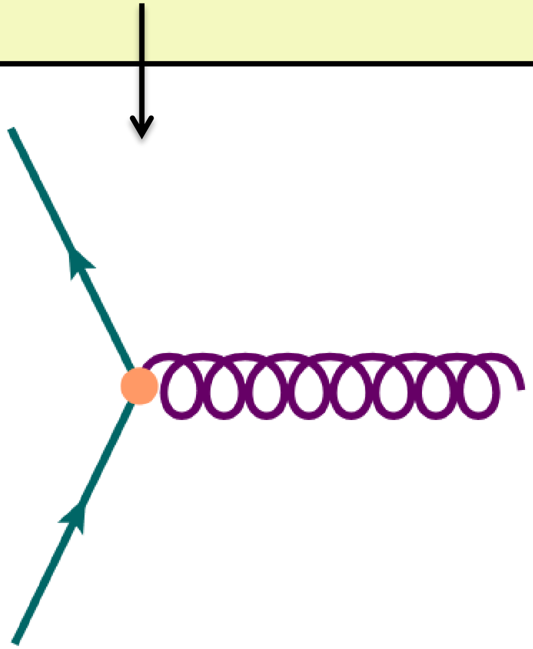
➲ Covariant derivative : measures deviation from parallel transport

$$\partial_\mu \to D_\mu = \partial_\mu - iA_\mu$$

✪ QCD in a nutshell – building of the gauge theory

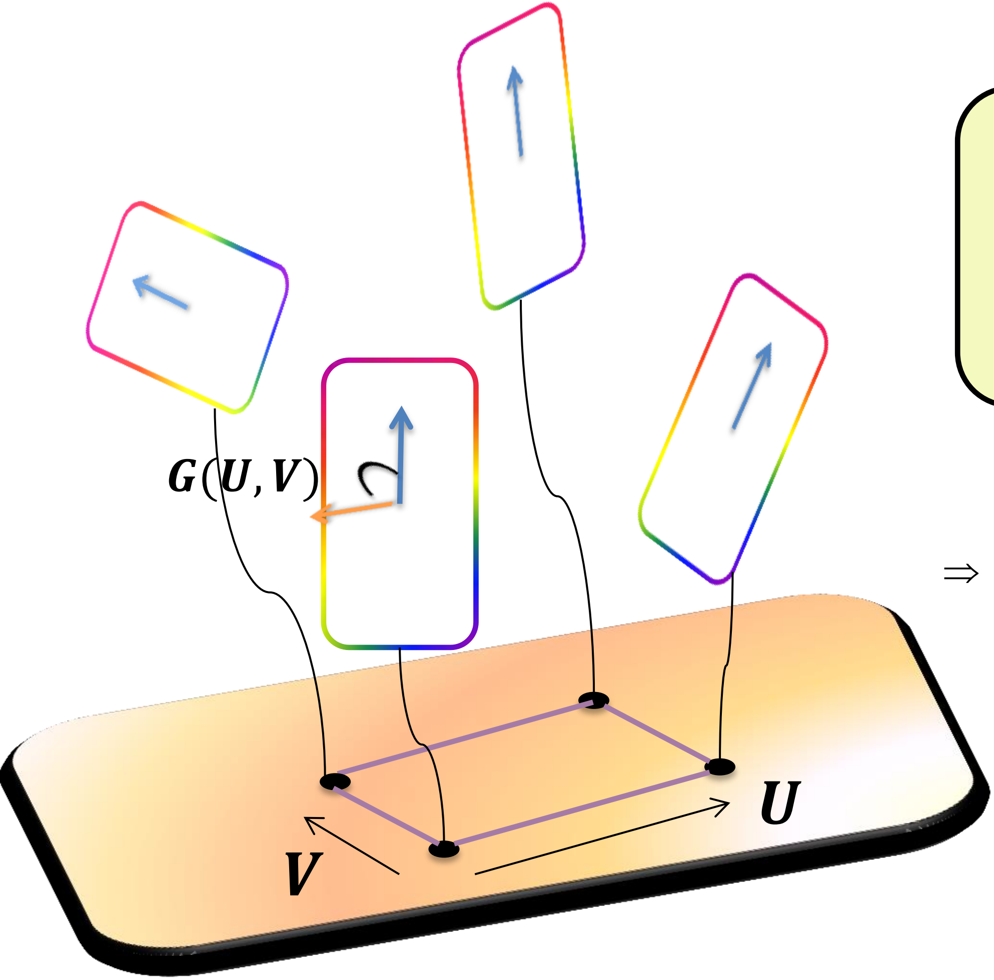
➲ Local symmetry requirement ⇒ interaction :

$$\mathcal{L} = \sum_{j=1}^{N_f} \bar{\psi}_j \left(i \not{D}\right) \psi_j = \sum_{j=1}^{N_f} \bar{\psi}_j \left(i\not{\partial} + \gamma_\mu A^\mu\right) \psi_j$$



$$A_\mu^{here} = g A_\mu^{usual}$$

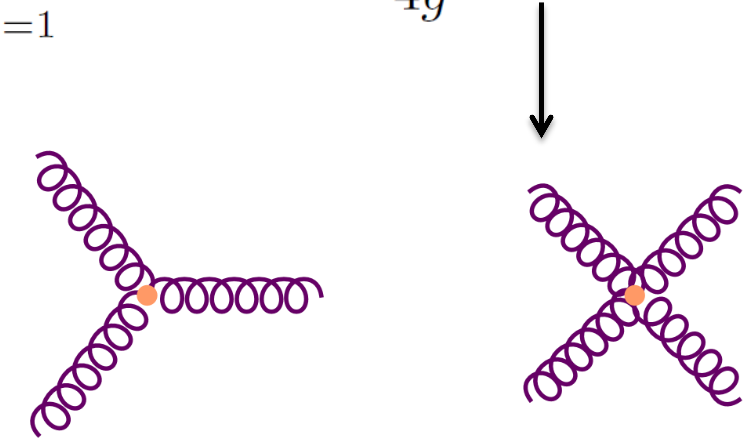
✪ QCD in a nutshell – building of the gauge theory



➲ Connection curvature : obstruction to the closure in the fiber bundle ⇒ chromo - electric and magnetic fields

$$G_{\mu\nu} \equiv i\left[D^{\mu}, D^{\nu}\right] = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} + i\left[A_{\mu}, A_{\nu}\right]$$

$$\Rightarrow \mathcal{L} = \sum_{j=1}^{N_f} \bar{\psi}_j \left(i \not{D}\right) \psi_j - \frac{1}{4g^2} Tr G^{\mu\nu} G_{\mu\nu}$$



Cubic and quartic gluon self-interaction : makes life interesting

✪ *QCD in a nutshell – symmetries*

➲ Theory exhibits host of symmetries variously hidden

$$\mathcal{G}_{apparent} = SU(3)_c \times SU(N_f)_L \times SU(N_f)_R \times U(1)_B \times U(1)_A \times \mathcal{R}^{+}_{scale}$$

$$\downarrow$$

$$x^\mu \to \lambda x^\mu; A^\mu \to \lambda^{-1} A^\mu; \psi \to \lambda^{-1}\psi$$

$$\mathcal{G}_{actual} \;=\; SU(3)_c \times SU(N_f)_L \times SU(N_f)_R \times U(1)_B \times Z_A^{N_f}$$

Subgroup that survives quantization

Asymptotic freedom, chiral anomaly

$$\to \; SU(3)_c \times SU(N_f)_{L+R} \times U(1)_B$$

Symmetry subgroup of the G.S.

Chiral condensation

$$\to \; SU(N_f)_{L+R} \times U(1)_B$$

Color confinement

✪ QCD in a nutshell – asymptotic freedom

➲ Renormalization of QCD spoils classical scale invariance

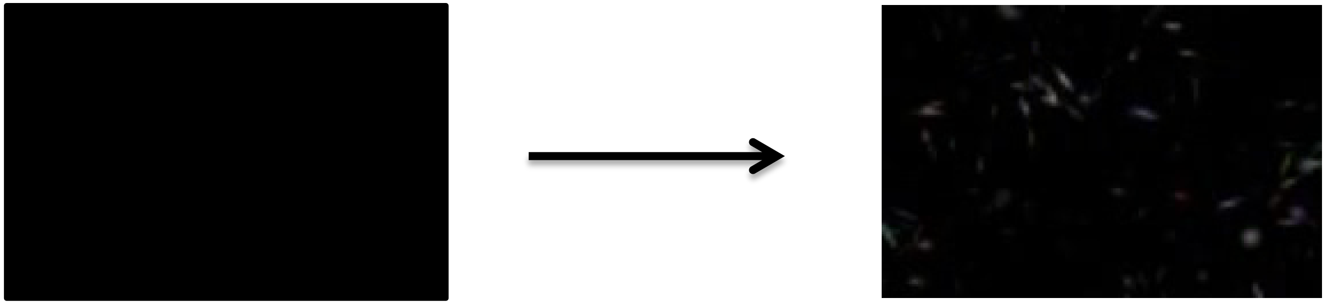
➲ Nominally empty space full of virtual particle-antiparticle pairs of all types

⇓

➲ Vacuum = dynamical medium exhibiting dielectric and paramagnetic behaviors

⇓

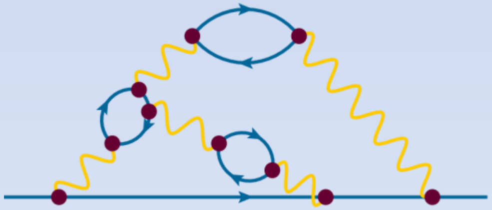
➲ Coupling constant depends of the scale of observation

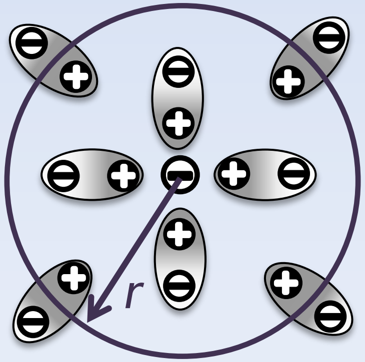


Classical vacuum → *Quantum vacuum*

✪ QCD in a nutshell – asymptotic freedom

QED



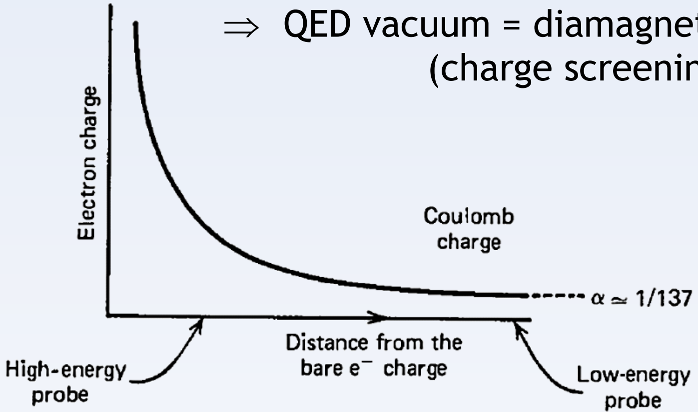


$$V\left(r\right)=\frac{\mathcal{V}\left(r\right)}{\varepsilon\left(r\right)}$$

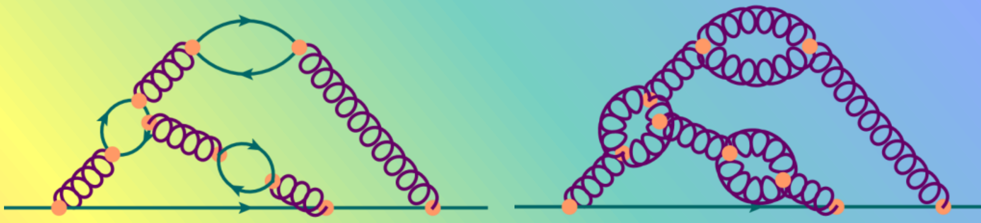
$$\varepsilon\left(r\right)\mu\left(r\right)=1$$

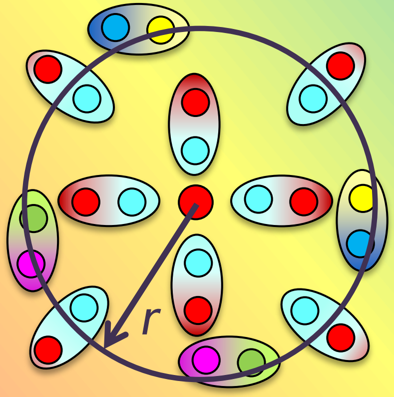
$\varepsilon > 1 \quad \mu < 1$

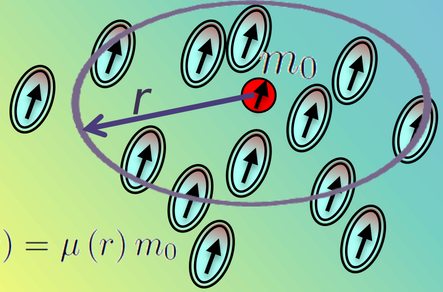
⇒ QED vacuum = diamagnet
(charge screening)



QCD



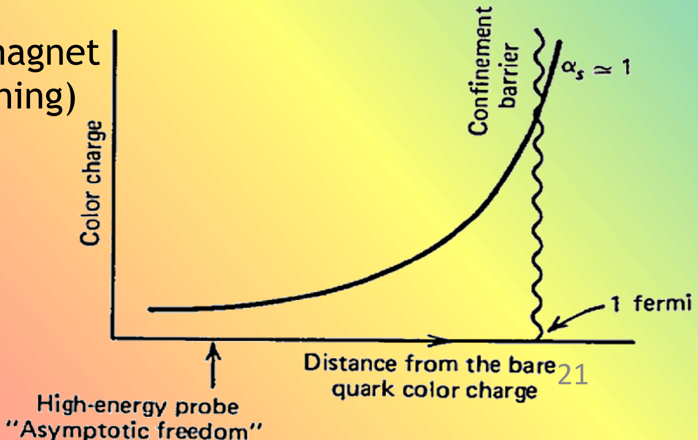




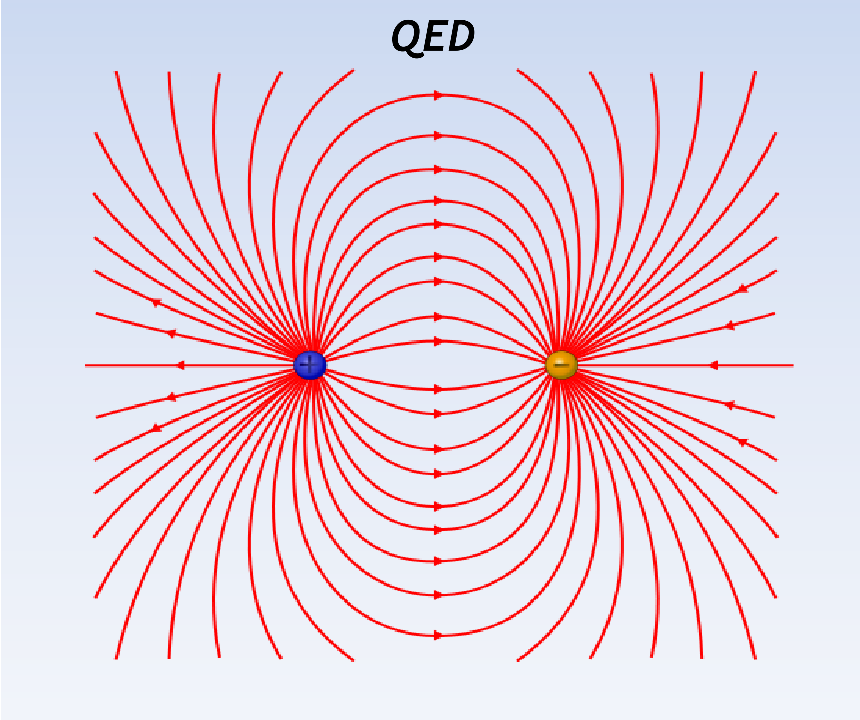
$m\left(r\right)=\mu\left(r\right)m_0$

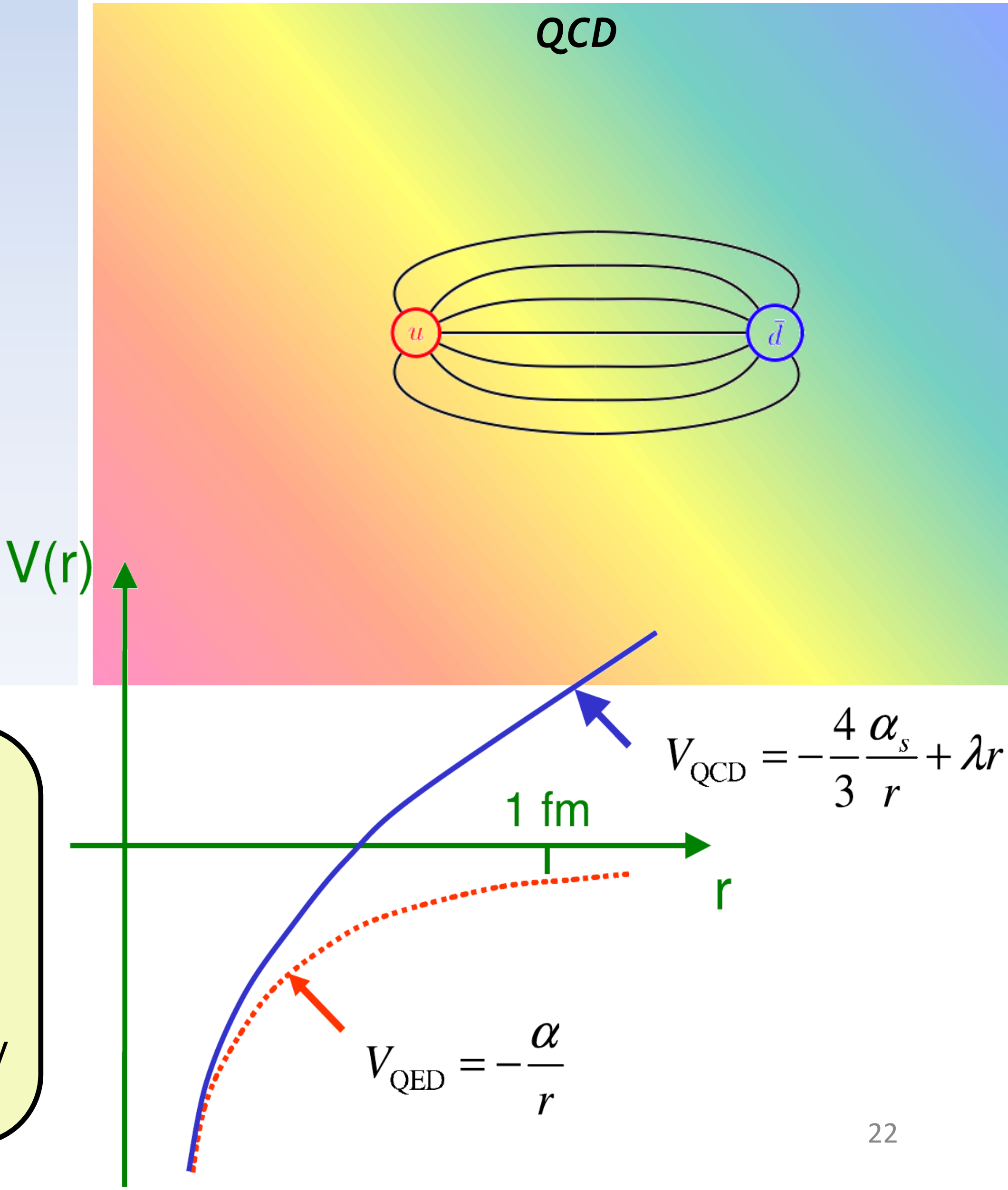
$\mu > 1 \quad \varepsilon < 1$

⇒ QCD vacuum = paramagnet
(charge antiscreening)



✪ QCD in a nutshell – color confinement





$$V_{\text{QCD}} = -\frac{4}{3}\frac{\alpha_s}{r} + \lambda r$$

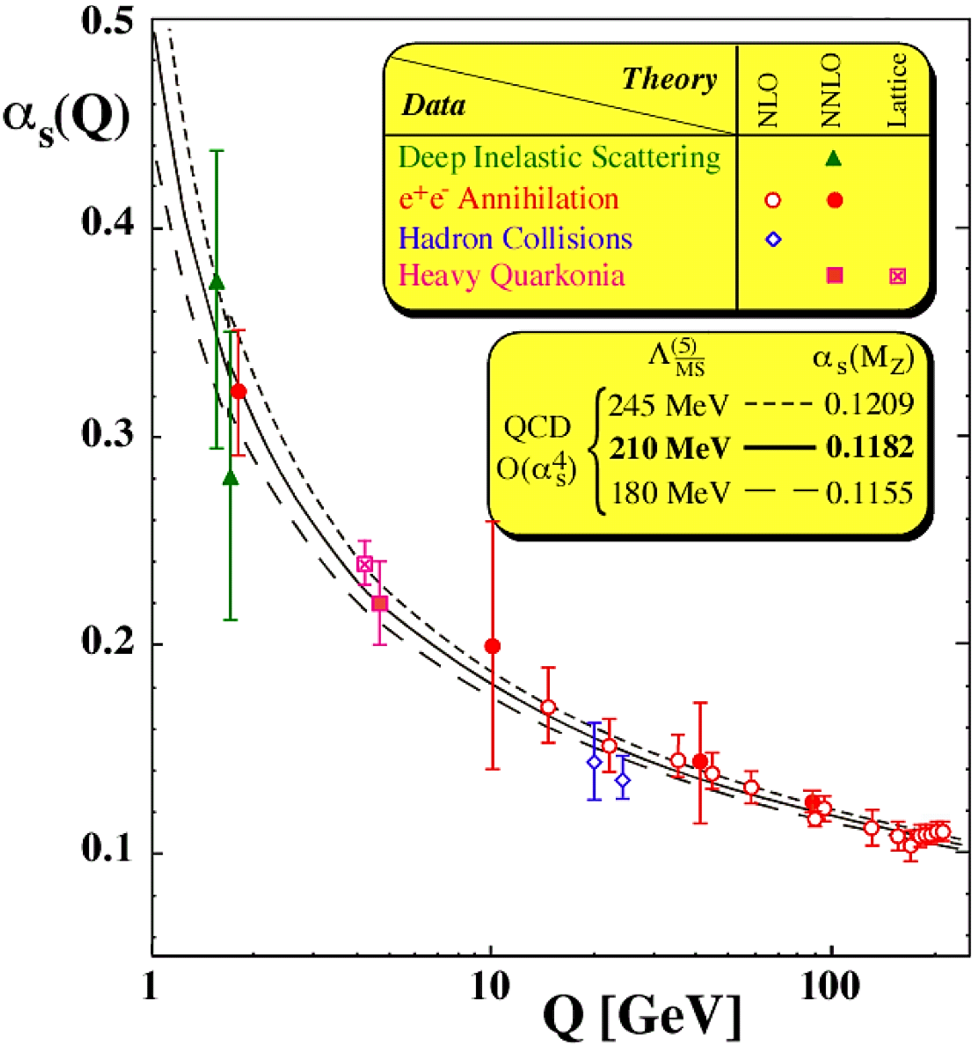
$$V_{\text{QED}} = -\frac{\alpha}{r}$$

➲ QCD vacuum = dual superconductor (Cooper pairs of chromo-magnetic charges condense)

❖ Dual Meissner effect ⇒ chromo electric flux tube ⇒ linear potential

Quarks are born free, but everywhere they are in chains

✪ Inter nucleonic interaction



➲ Features of low energy QCD :

- ❖ Asymptotic freedom
- ❖ Color confinement

➲ Implications for nuclear structure:

- ❖ No simple relation between NN potential and quarks potential
- ❖ Degrees of freedom different from QCD

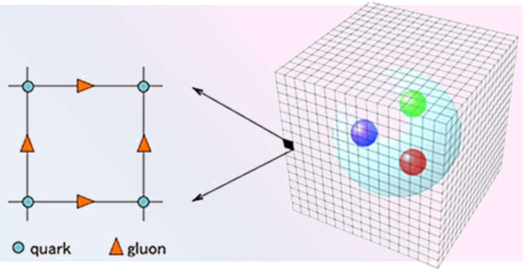
✪ *Inter nucleonic interaction*

➲ Lattice QCD

❖ Wick rotation ⇒ QFT→ SFT

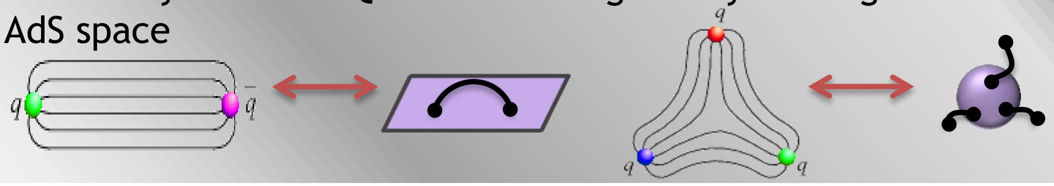
❖ Discretized Euclidian space-time

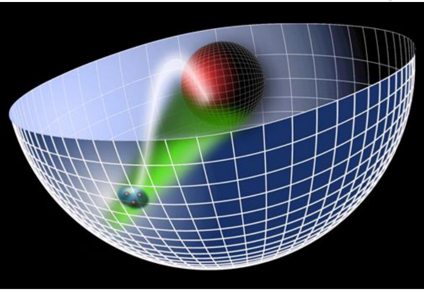
❖ QCD fields expanded on the lattice, correlation functions evaluated with Monte Carlo techniques



➲ Holographic QCD

❖ Duality between QCD and a string theory in a higher dimensional AdS space



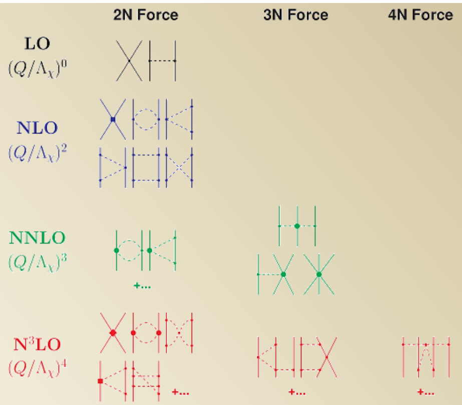


➲ Chiral effective field theory

❖ Based on effective low-energy d.o.f. + constrained by symmetries and symmetry breaking pattern of underlying theory

❖ High energy dynamics generically parameterized by contact terms

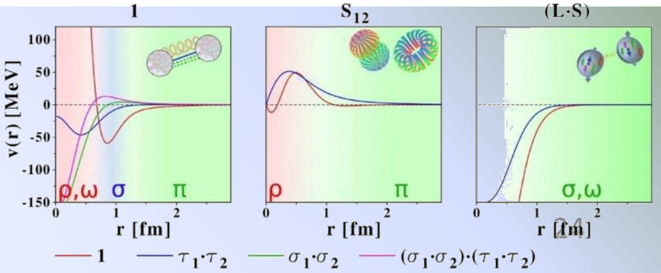
❖ Hierarchy of contributions to inter-nucleonic interactions



➲ Phenomenological interactions (in free space)

❖ Ansatz compatible with symmetry of the 2 (3) nucleons system

❖ Parameters fitted to accurately reproduce phase shifts



✪ Many-body problem

$$\widehat{H} = \sum_{i=1}^{A} \frac{\widehat{p}_i^2}{2M} + \sum_{i<j=1}^{A} \widehat{v}_{ij} + \sum_{i<j<k=1}^{A} \widehat{v}_{ijk} + \ldots$$

➲ Solve the eigenvalue equation (or time dependent version) of the Hamiltonian :

$$\sum_{i=1}^{A} \frac{-\hbar^2}{2M} \overrightarrow{\nabla}_i^2 \ \psi_\alpha(1,2,\ldots,A) + \ \frac{1}{2} \sum_{i=1}^{A} \sum_{j\neq i=1}^{A} \int d^3r'_i \int d^3r'_j \ \langle ij|\widehat{v}_{ij}|i'j'\rangle$$

$$\psi_\alpha(1,2,\ldots,i',\ldots,j',\ldots,A) = E_\alpha \ \psi_\alpha(1,2,\ldots,A)$$

➲ Encodes how nucleons behavior is modified by the presence of other nucleons

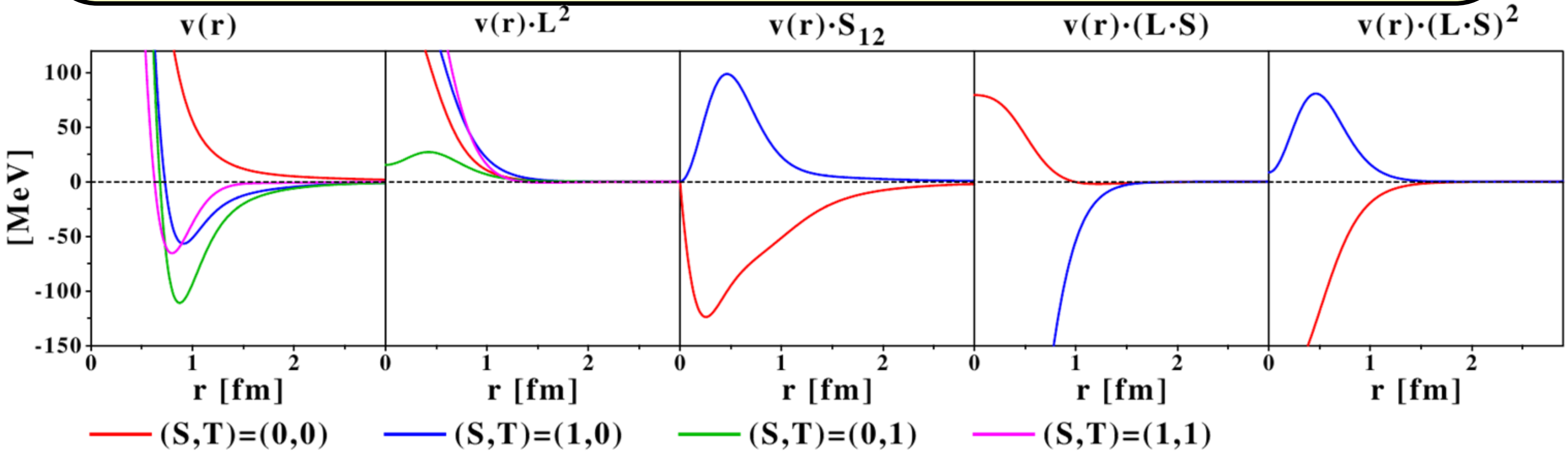
- ❖ EMC effect neglected
- ❖ Modification of the nucleonic interactions (Pauli principle principally)

✪ *Many-body problem*

➲ Nucleonic interactions are complicated

- ❖ Complex structure (including tensor term)
- ❖ Hard core
- ❖ bound state (deuteron) and resonant state (di-neutron)

⇒ Nuclear many-body problem highly nonperturbative



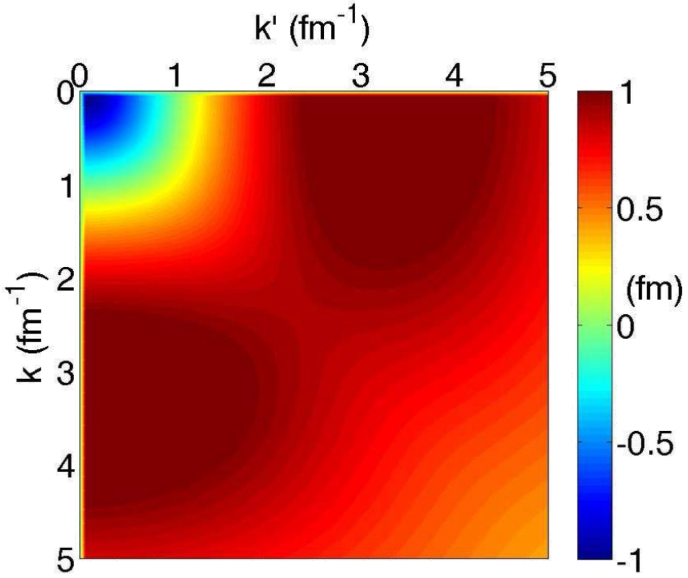
V. Rotival

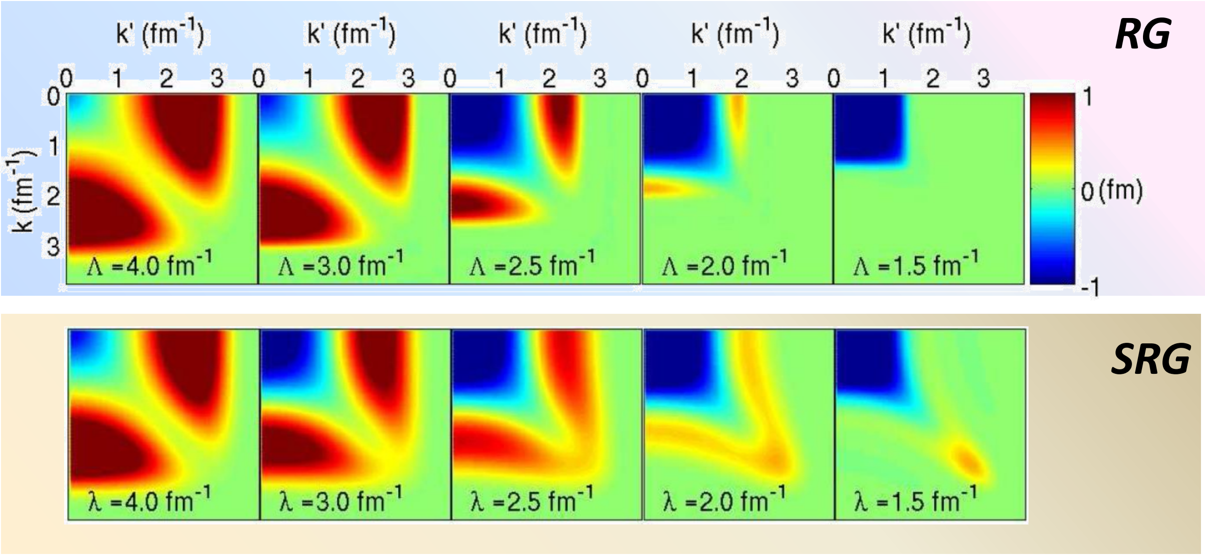
➲ NNN interaction treatment unavoidable

✪ *Many-body problem*

➲ Low momentum NN interaction : make the many body problem more perturbative

❖ Downfold high energy modes and work in a subspace in which only low energy modes and low-energy effects of the virtual modes are taken into account





UCOM

Bogner et. al, Prog.Part.Nucl.Phys.65:94-147 (2010)
Roth et al, Phys. Rev. C 72, 034002 (2005)

➊ Microscopic approaches of nuclear systems

C) Strategies

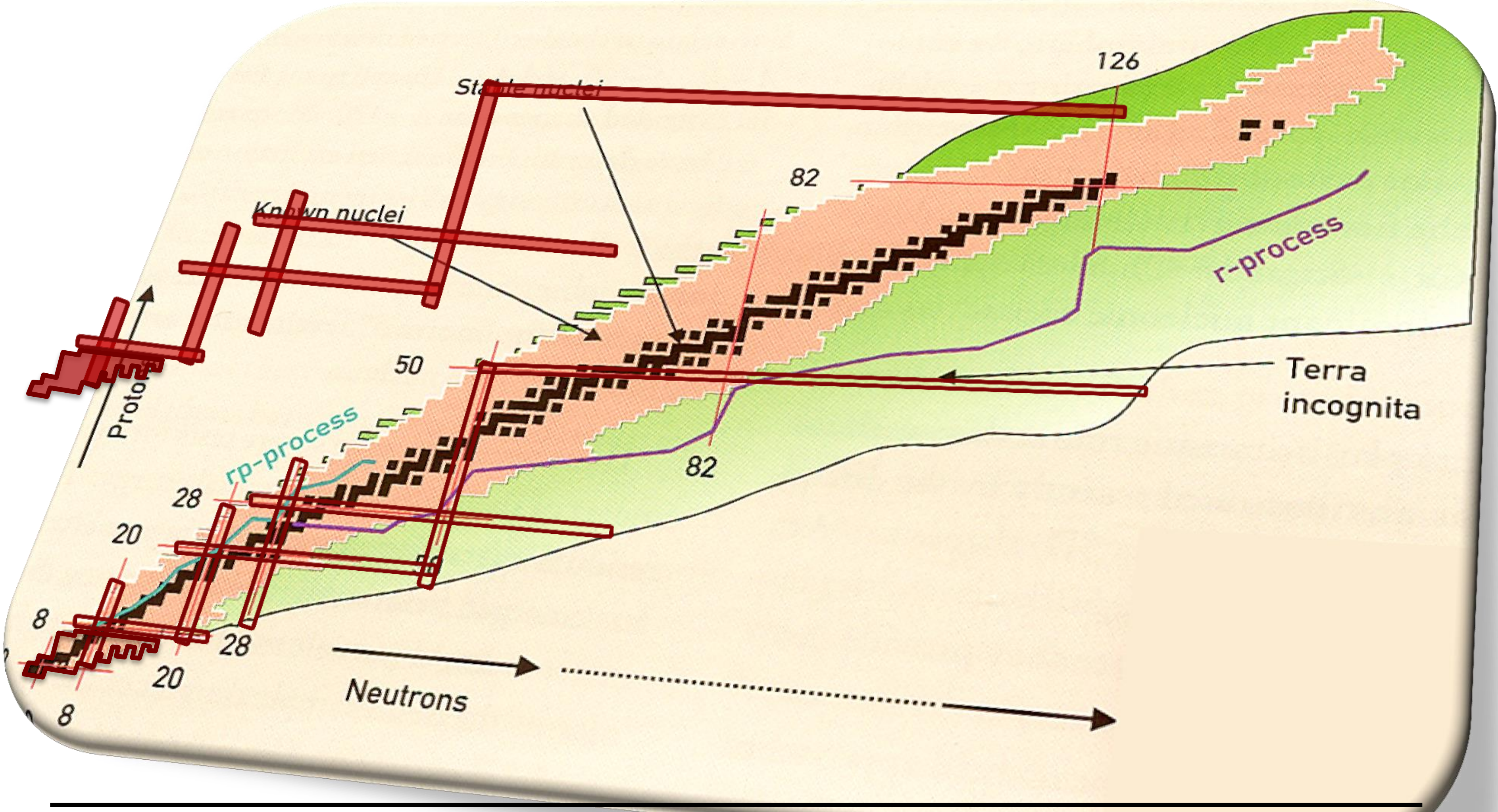
✪ *Three categories*

➲ Ab-initio approaches

- ❖ Treat as exactly as possible the many-body problem starting from NN (+NNN) interactions in free space
- ❖ Form of the many-body wavefunction sought general enough to embed nucleonic correlations
- ❖ Outrageous size of the Hilbert space impose limitations

✪ Three categories

Ab-initio



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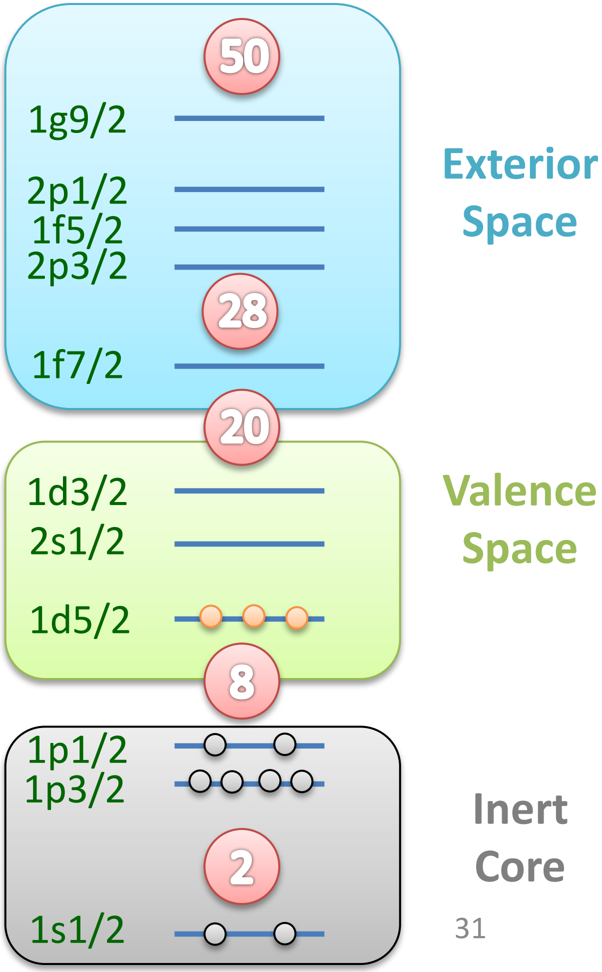
➲ Configuration interaction

- ❖ Drastic truncation of Hilbert space
- ❖ In practice, effective interaction in the valence space fitted to data => calculation impossible for valence space with no known data



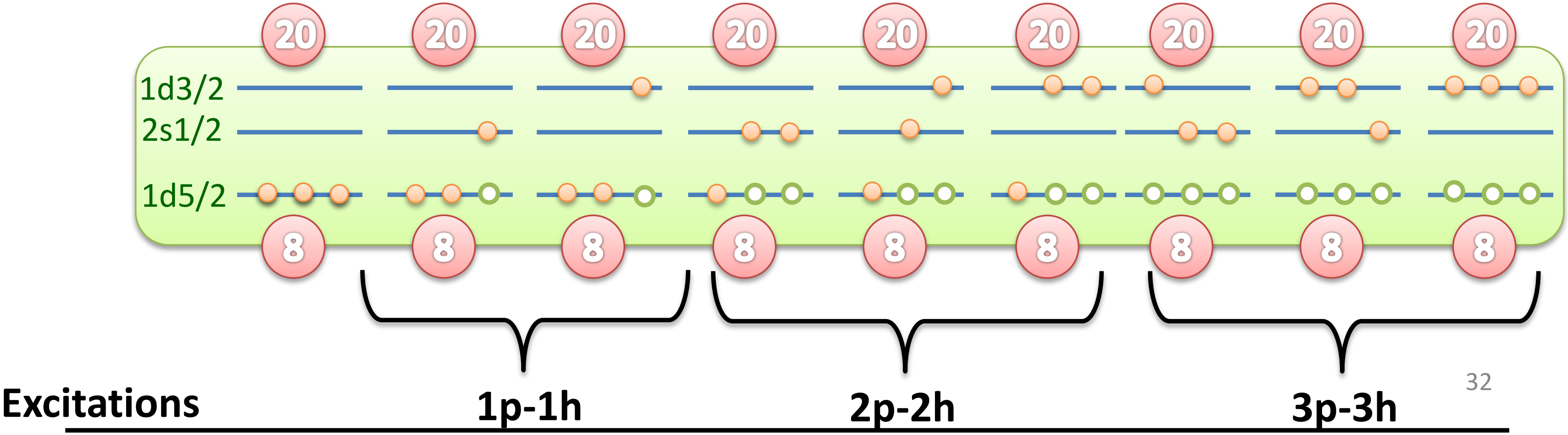
➲ Ab-initio approaches

- ❖ Treat as exactly as possible the many-body problem starting from NN (+NNN) interactions in free space
- ❖ Form of the many-body wavefunction sought general enough to embed nucleonic correlations
- ❖ Outrageous size of the Hilbert space impose limitations

➲ Configuration interaction

- ❖ Drastic truncation of Hilbert space
- ❖ In practice, effective interaction in the valence space fitted to data => calculation impossible for valence space with no known data
- ❖ Nucleonic correlations accounted for by configuration mixing

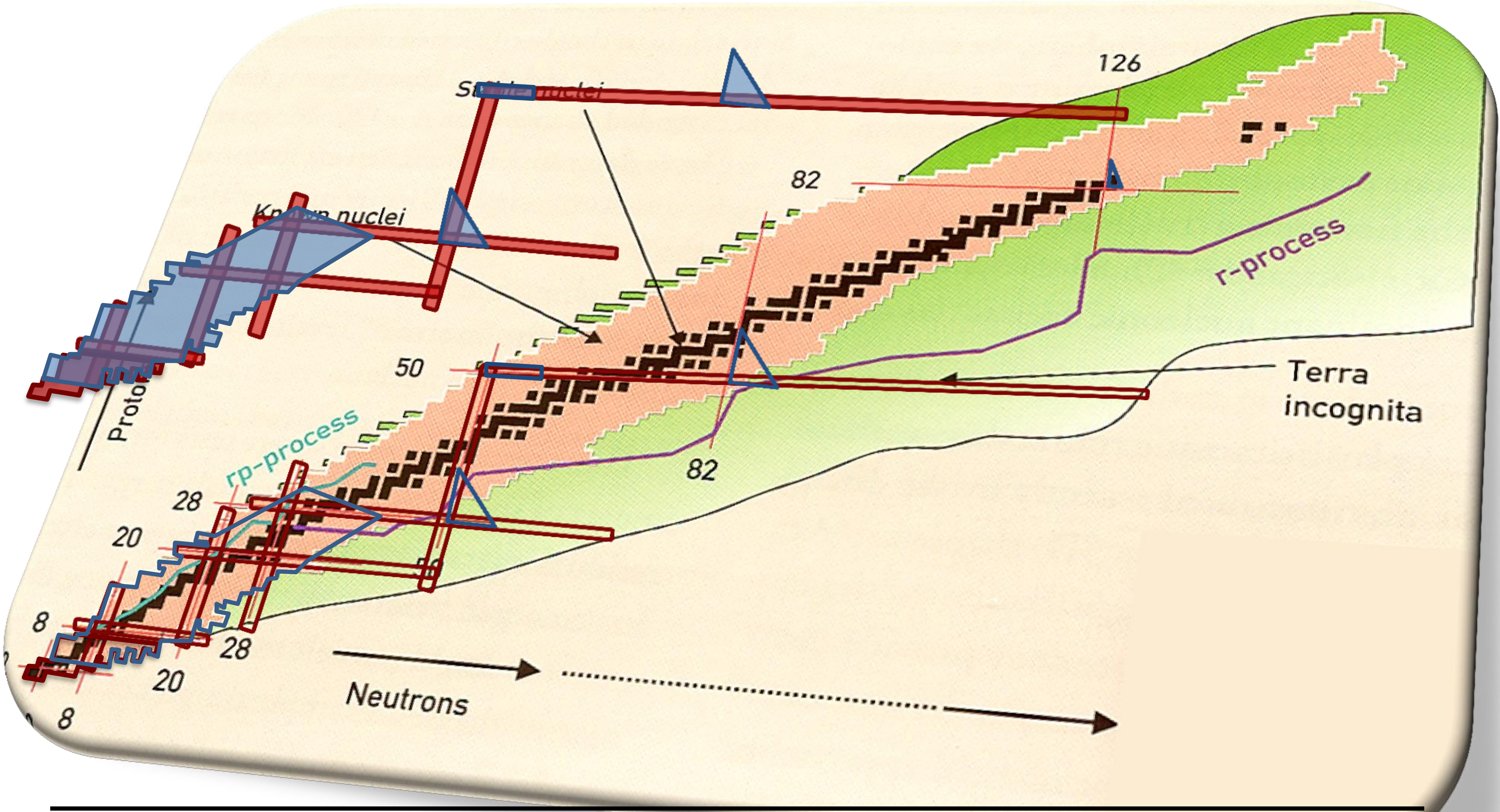
$$|\psi\rangle = \alpha_1|\varphi\rangle_1 + \alpha_2|\varphi\rangle_2 + \alpha_3|\varphi\rangle_3 + \alpha_4|\varphi\rangle_4 + \alpha_5|\varphi\rangle_5 + \alpha_6|\varphi\rangle_6 + \alpha_7|\varphi\rangle_7 + \alpha_8|\varphi\rangle_8 + \alpha_9|\varphi\rangle_9$$



✪ Three categories

Ab-initio

Configuration interaction



✪ Three categories

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➲ Energy Density Functional

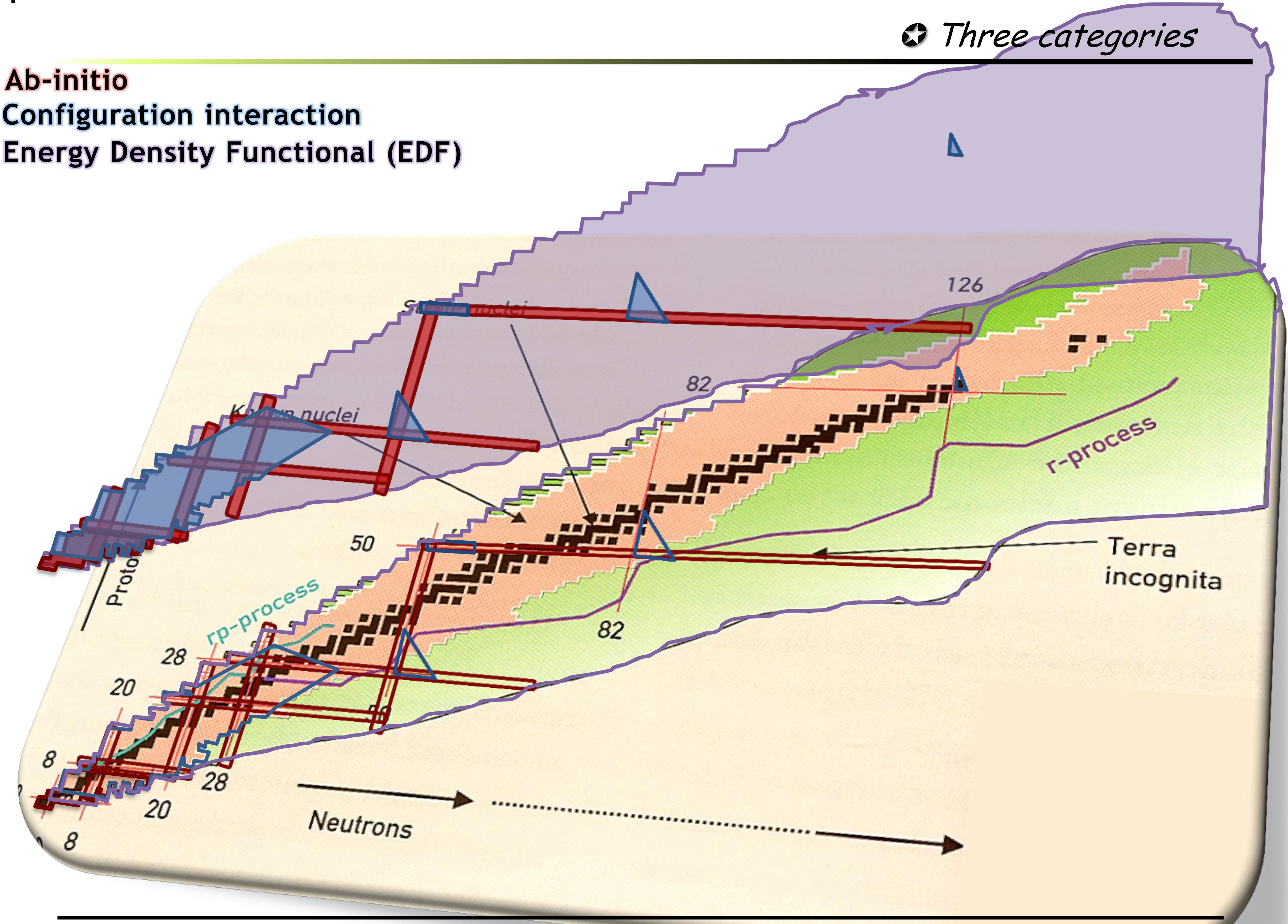
- ❖ Independent particle picture
- ❖ 2-step approach with symmetry breaking and restoration at its very core
- ❖ Universal framework, reasonable computing time
- ❖ Lack of error estimation, not controlled extrapolation

✪ *Three categories*

Ab-initio

Configuration interaction

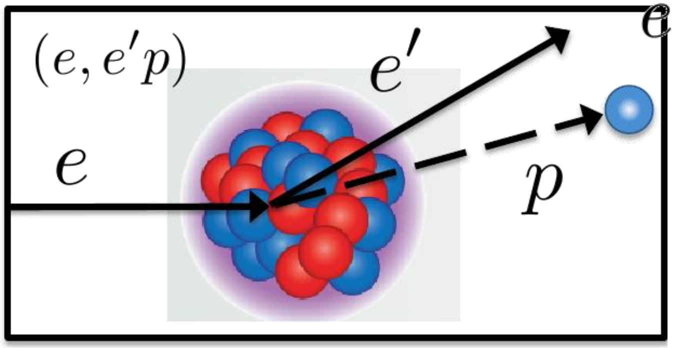
Energy Density Functional (EDF)

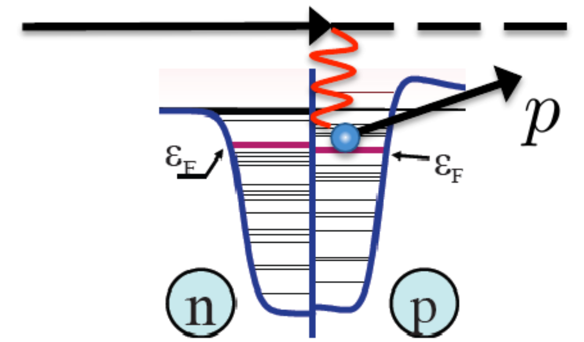


❷ Energy Density Functional approaches

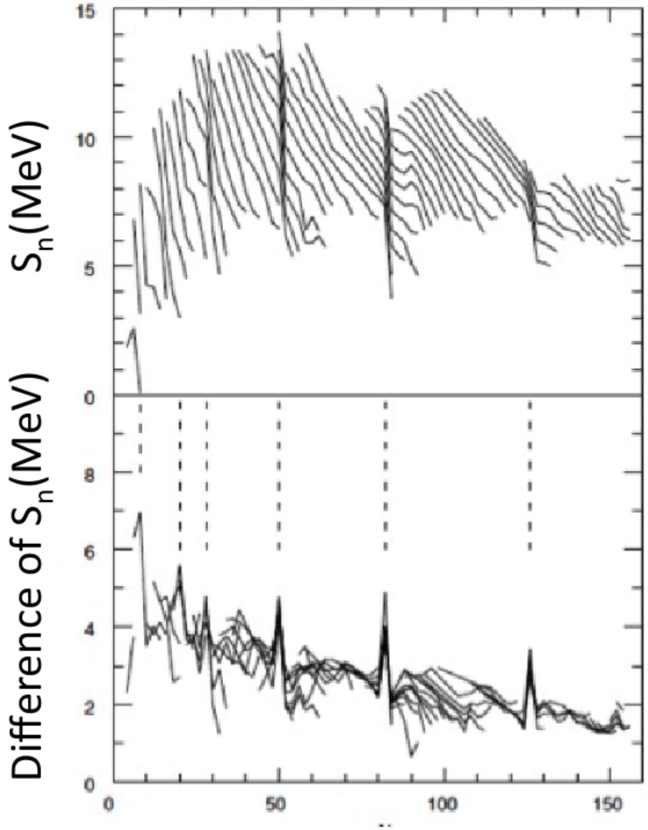
A) Independent particle picture

✪ Evidence for an independent particle picture

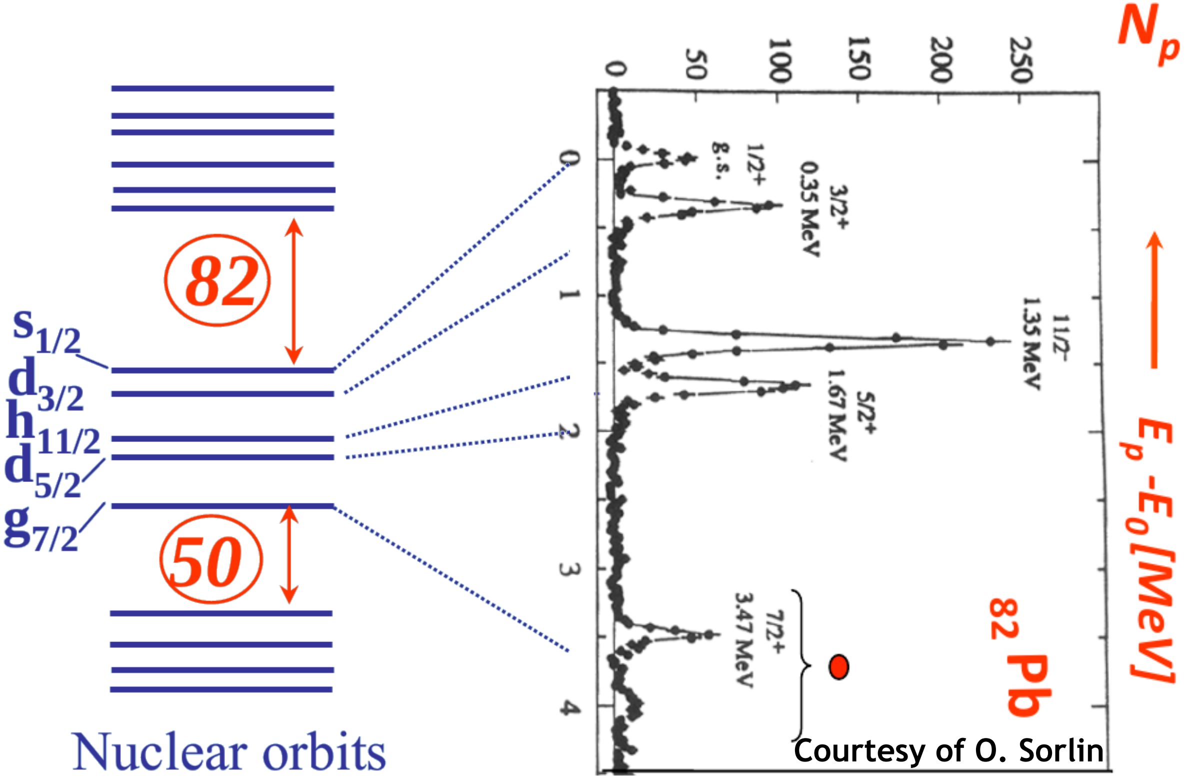




D. Lacroix (EJC 2011)



Discontinuities associated with magic numbers



Courtesy of O. Sorlin

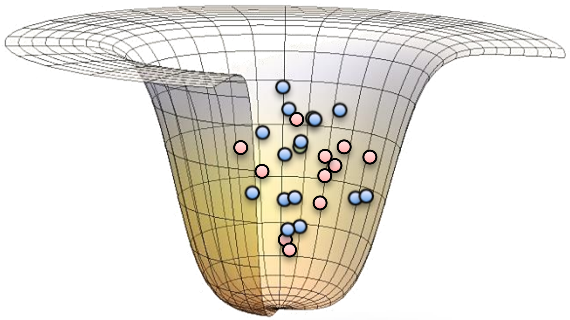
✪ *Rationale for an independent particle picture*

➲ Pauli exclusion principle restricts the phase space for NN collisions

➲ But not a necessary condition : independent particle like behavior would be as prominent if nucleons were bosons interacting with the same forces

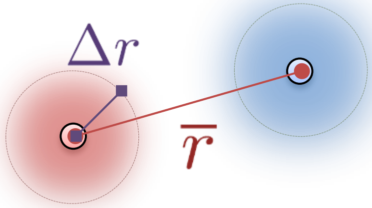
⇒ **More nuanced understanding is needed**

✪ Rationale for an independent particle picture

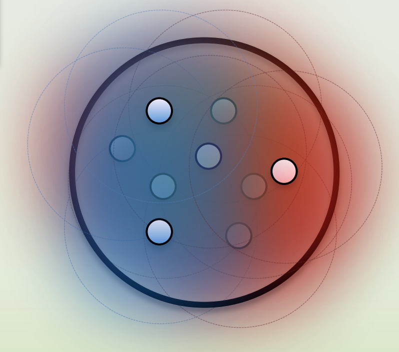


$$\alpha = \frac{\Delta r}{\overline{r}} = f(\Lambda)$$

$$\Lambda = \frac{E_{kin}^{ZP}}{E_{pot}} = \frac{\hbar^2}{M a^2 V_0}$$

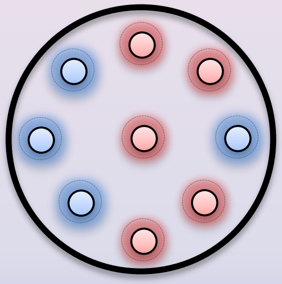


$\alpha > 1$



➲Quantum liquid

$\alpha < 1$



➲Crystalline phase

- ➲ Nuclear forces too weak to localize nucleons in a crystalline structure

  $\Rightarrow$ Ground state of quantum liquid type with delocalized structure and elementary excitations with long mean free path

Mottelson, Les Houches LXVI, 25 (1998)
Ebran et al, Nature 487, 341-344 (2012)

✪ *Fermi liquid theory*

➲ G.S. and low-lying excitations of the interacting system in one-to-one correspondence with the quantum states of the non interacting

➲ Stability of the Fermi surface (topological concept) (except with respect to Cooper pairing)

➲ Landau quasiparticles : nucleon + cloud of excitations created by the propagation of the nucleon in the nuclear medium (Bogoliubov qp = superposition of Landau quasiparticle and quasihole)

Horava, PRL 95, 016405 (2005)

❷ Energy Density Functional approaches

B) Historical perspective

✪ Many-body perturbation theory

➲ Goal : find that nuclei can be fairly well described in terms of an appropriate set of s.p. states + effective interaction between particles in these states

$$H = \sum_{i=1}^{A} t_i + \sum_{i<j=1}^{A} v_{ij}$$

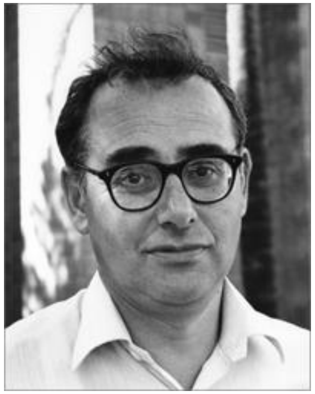
$$= \underbrace{\left\{ \sum_{i=1}^{A} (t_i + Ui) \right\}}_{H_0} + \underbrace{\left\{ \sum_{i<j=1}^{A} v_{ij} - \sum_{i=1}^{A} U_i \right\}}_{H_1}$$

➲ Unperturbed Hamiltonian gives the single particle picture

➲ Residual interaction generates correlations

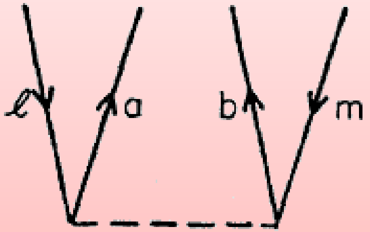
✪ Many-body perturbation theory

➲ Perturbative expansion of the exact energy

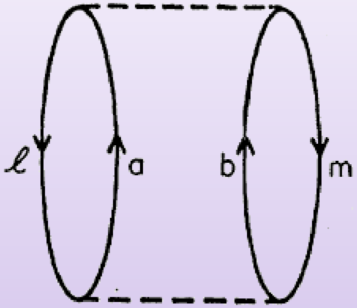


$$E = E_0 + \langle \Phi_0 | H_1 | \Phi_0 \rangle + \left\langle \Phi_0 \middle| H_1 \frac{1}{E_0 - H_0} P H_1 \middle| \Phi_0 \right\rangle + \cdots$$

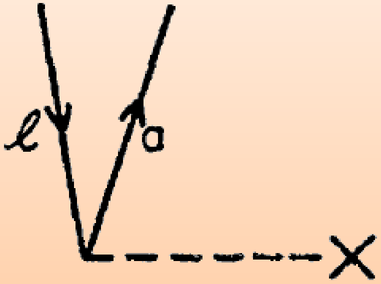
$$H_1 = \sum_{pqrs} \langle pq | v | rs \rangle a_p^\dagger a_q^\dagger a_s a_r - \sum_{pq} \langle p | U | q \rangle a_p^\dagger a_q$$



$$\langle ab | v | lm \rangle a_a^\dagger a_b^\dagger a_l a_m | \Phi_0 >$$



$$\left\langle \Phi_0 \middle| H_1 \frac{1}{E_0 - H_0} P H_1 \middle| \Phi_0 \right\rangle$$

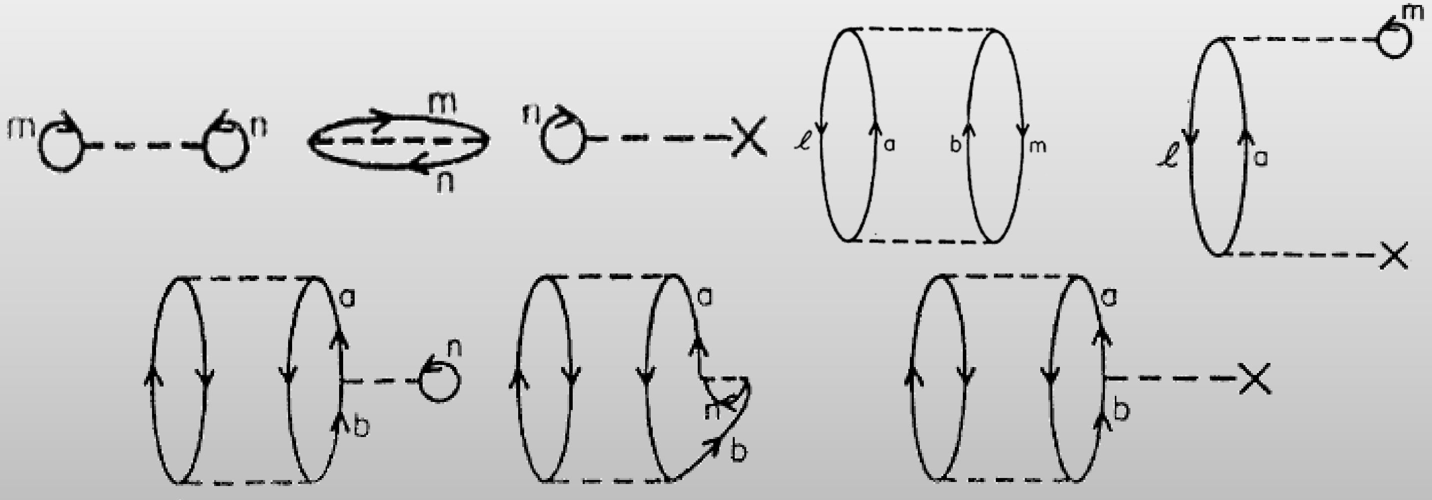


$$\langle a | U | l \rangle a_a^\dagger a_l | \Phi_0 >$$

Day, Rev Mod Phys 39, 719 (1967)

✪ Many-body perturbation theory

$E = E_0 +$



➲ All is about an inspired choice for the mean field U

$$\langle p \mid U_{\mathrm{HF}} \mid q\rangle = \sum_{n\leq A} \left(\langle pn \mid v \mid qn\rangle - \langle pn \mid v \mid nq\rangle\right)$$

$$E_{\mathrm{HF}}[\rho] = \sum_{ij} t_{ij}\rho_{ji} + \frac{1}{2}\sum_{ij,kl} \overset{(a)}{v_{ij,kl}}\,\rho_{ki}\rho_{lj}$$

$$\rho_{ij} = \langle a_i^{\dagger} a_j \rangle$$

Bare NN interaction

✪ *Hard core potentials*

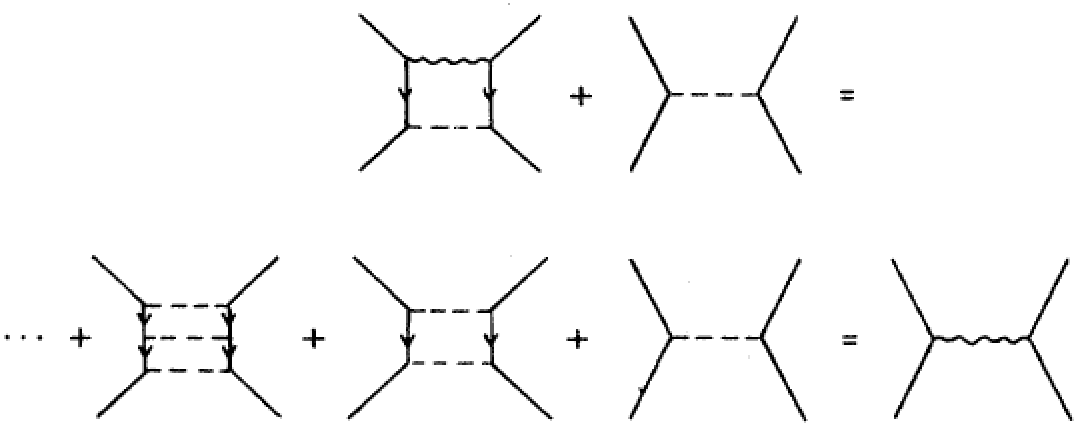
➲ Hard core potentials

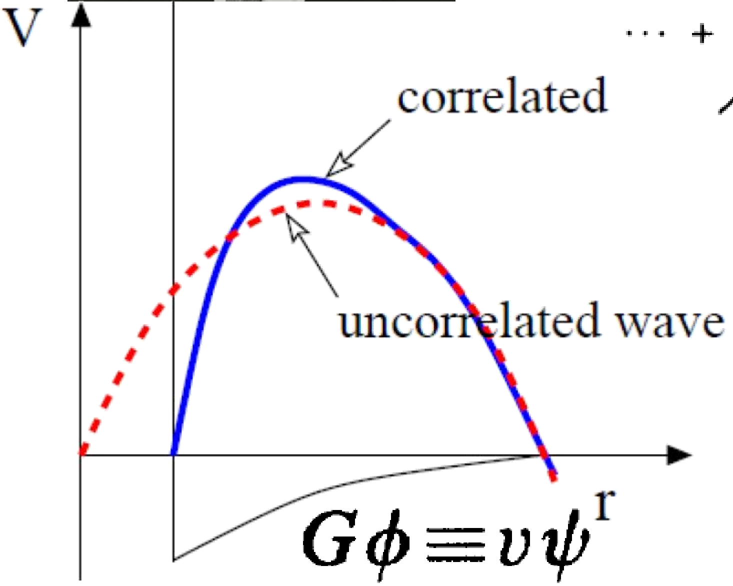
- ❖ Divergence of the Hartree-Fock matrix elements of the bare interaction
- ❖ Rearrangement of the perturbation expansion

✪ Hard core potentials

➲ Brueckner reaction matrix : rearrangement of the perturbative expansion with summation of ladder diagrams to all orders

$$G(W) = v - v(Q/e)G(W)$$

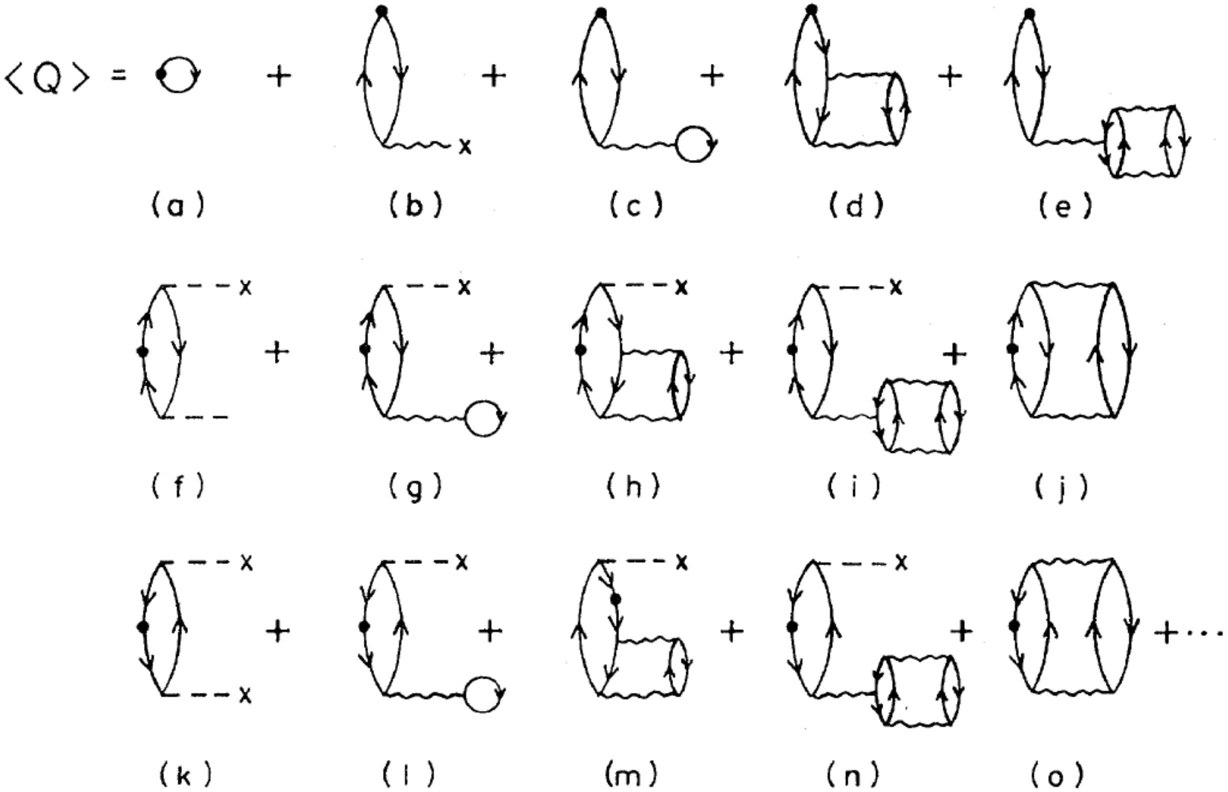


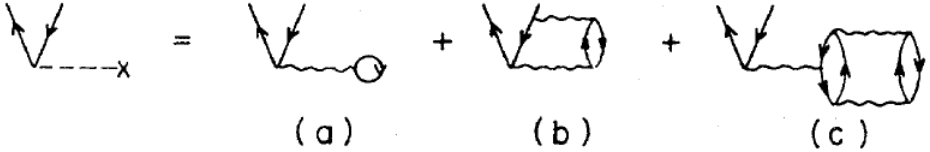


$$G\phi \equiv v\psi$$

✪ Hard core potentials

➲ Mean field U chosen to cancel the maximum of dominant diagrams arising in the expectation value of a 1-body operator





Negele, Rev Mod Phys 54, 913 (1982)

✪ *Hard core potentials*

➲ Diagrammatic definition of U is precisely obtained by formal variation of the approximate expression for the energy :

$$E=\sum_{\nu}\langle\nu|T|\nu\rangle+\frac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|G(\varepsilon_{\nu}+\varepsilon_{\nu'})|\nu\nu'-\nu'\nu\rangle$$

Reaction matrix

$$G(W)=v-vQ\frac{1}{QTQ-W}QG(W)\ ,$$

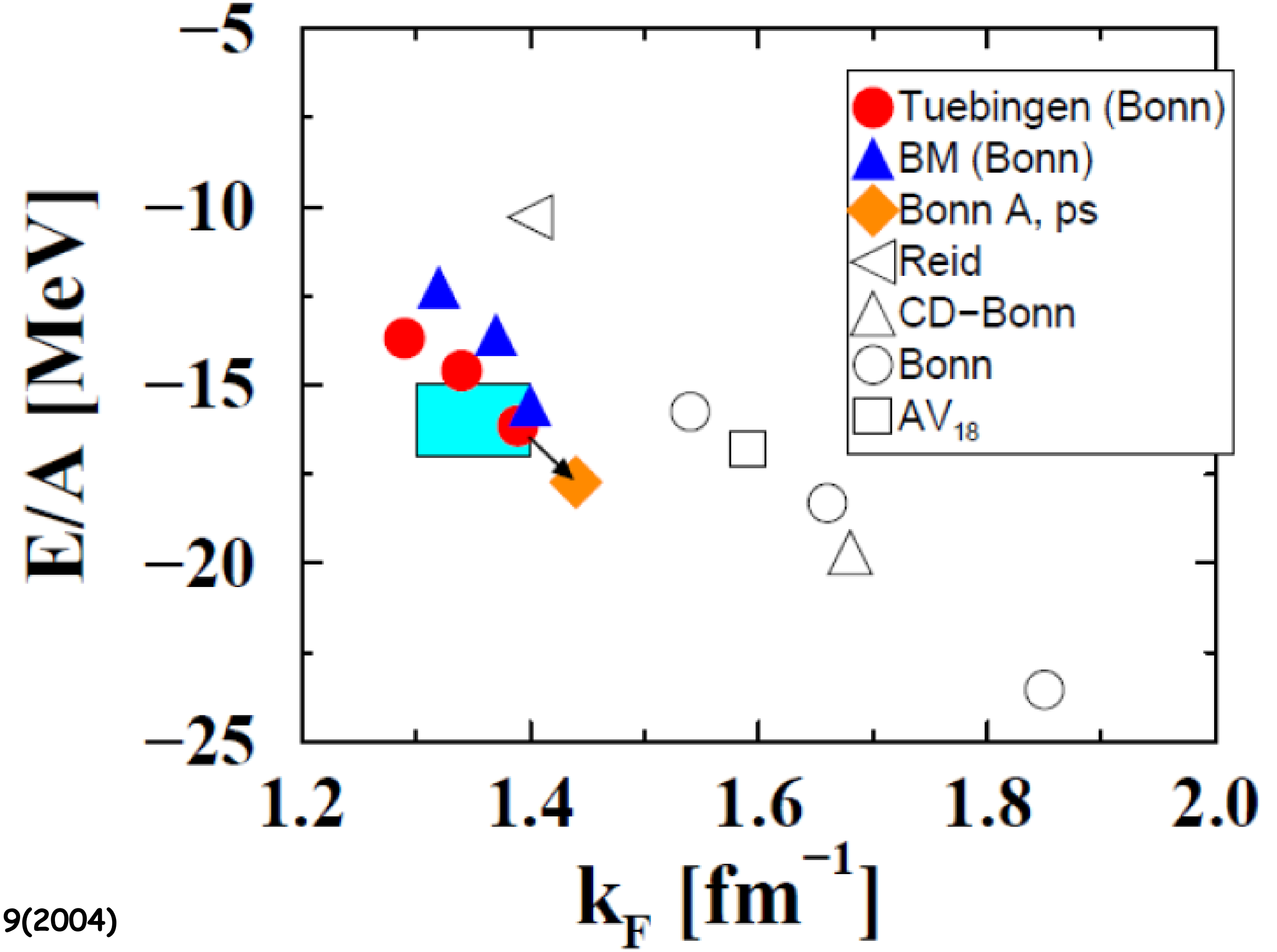
$$\varepsilon_{\nu}=\langle\nu|T|\nu\rangle+\sum_{\nu'}\langle\nu\nu'|G(\varepsilon_{\nu}+\varepsilon_{\nu'})|\nu\nu'-\nu'\nu\rangle$$

$$Q=\sum_{\rho\rho'}|\rho\rho'\rangle\langle\rho\rho'|$$

Davies et al, PRC 10, 2607 (1974)

✪ *Hard core potentials*

➲ Without 3 body force, bad reproduction of nuclear matter saturation (Coester line)



Fuchs, LNP 641:119(2004)

✪ Non singular potential

➲ Hard core potentials

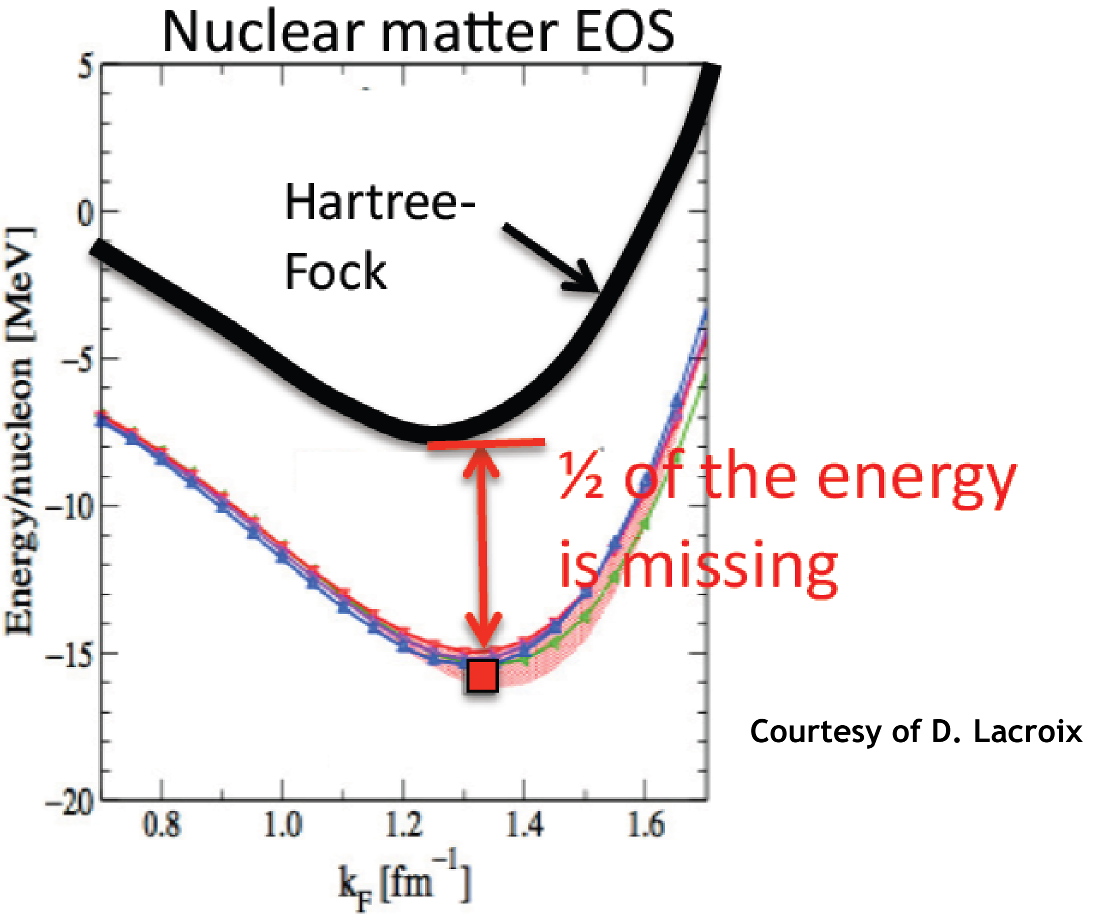
- ❖ Divergence of the Hartree-Fock matrix elements of the bare interaction
- ❖ Rearrangement of the perturbation expansion

➲ Potentials with non singular repulsion

- ❖ “Ordinary” Hartree-Fock can be used (convergence of the perturbation expansion not assured)

✪ Non singular potential

➲ Bad reproduction of nuclear matter saturation properties at the Hartree-Fock level



Courtesy of D. Lacroix

Bogner, et al, NPA 763 (2005)

✪ *Effective interactions*

➲ Hard core potentials

- ❖ Divergence of the Hartree-Fock matrix elements of the bare interaction
- ❖ Rearrangement of the perturbation expansion

➲ Potentials with non singular repulsion

- ❖ "Ordinary" Hartree-Fock can be used (convergence of the perturbation expansion not assured)
- ❖ Rearrangement of the perturbation expansion

➲ Effective interactions

- ❖ deduced from the bare interaction (LDA, DME) + phenomenological corrections for higher order contributions

or

- ❖ purely phenomenological

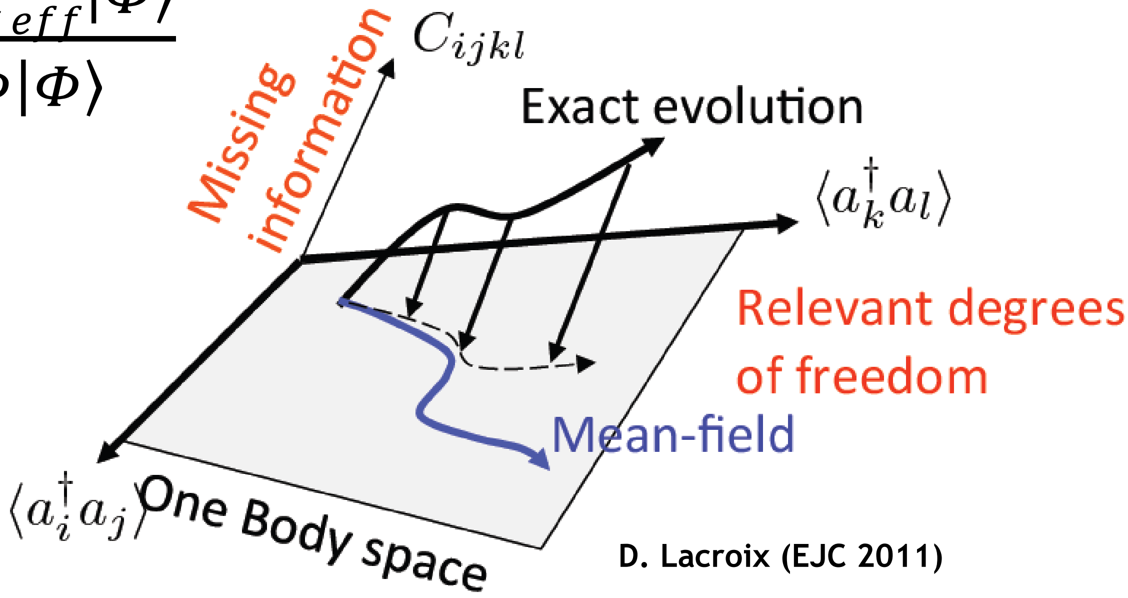
✪ Effective interactions

➲ Start from Hamiltonian with an effective interaction (still independent of the density at this stage) consistent with a single particle picture

$$H_{eff} = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{v}|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

Effective interaction

$$E = \frac{\langle \Psi | H_{exact} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \frac{\langle \Phi | H_{eff} | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$



D. Lacroix (EJC 2011)

✪ Hartree-Fock Theory

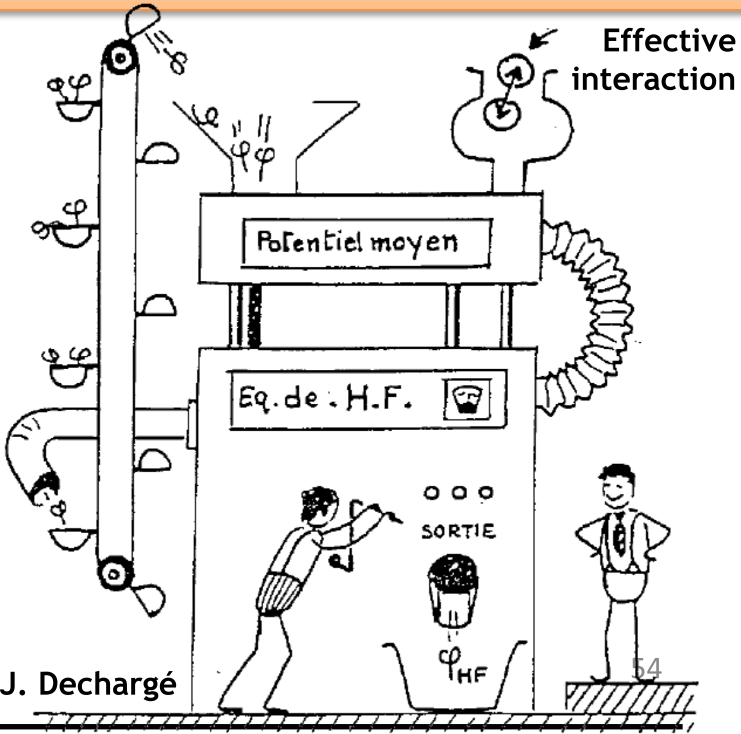
➲ Deduce the energy and Hartree-Fock equation with Rayleigh-Ritz variational principle

$$E_{\mathrm{HF}}[\rho] = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \sum_{ij} t_{ij}\rho_{ji} + \frac{1}{2}\sum_{ij,kl}\tilde{v}_{ij,kl}\rho_{ki}\rho_{lj} = \mathrm{Tr}(t_1\rho_1) + \frac{1}{2}\mathrm{Tr}(\tilde{v}_{12}\rho_1\rho_2)$$

$$\delta\left[E_{\mathrm{HF}}[\rho] - \Lambda\mathrm{Tr}(\rho^2-\rho)\right] = 0 \Rightarrow [h[\rho],\rho] = 0$$

$$h[\rho] = t + \underbrace{Tr_2(\tilde{v}_{12}\rho_2)}_{U[\rho]}$$

$$h[\rho]|\varphi_\alpha\rangle = \varepsilon_\alpha|\varphi_\alpha\rangle$$



J. Dechargé

✪ Hartree-Fock Theory

➲ Relation between total energy and single particle energies

$$E_{HF} = \sum_t \langle t|\ \frac{\widehat{p}^2}{2M} + \frac{1}{2}\widehat{U}[\rho]\ |t\rangle$$

$$E_{HF} = \sum_t \langle t|\ \widehat{h}[\rho] - \frac{1}{2}\widehat{U}[\rho]\ |t\rangle = \frac{1}{2}\sum_t \langle t|\ \widehat{h}[\rho] + \frac{\widehat{p}^2}{2M}\ |t\rangle$$

$$E_{HF} = \sum_t \varepsilon_t - \frac{1}{2}\sum_t \langle t|\ \widehat{U}[\rho]\ |t\rangle = \frac{1}{2}\sum_t \left(\varepsilon_t\ \ + \langle t|\ \frac{\widehat{p}^2}{2M}\ |t\rangle\right)$$

➲ Crisis : Strong support for independent particle picture of nuclear systems but natural approach to map the many-body problem into a 1-body one fails

❷ Energy Density Functional approaches

C) Miraculous density dependence

✪ Origin of a density dependence

➲ Introduction of an explicit density dependence in the effective interaction

$$H_{eff} = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{v}|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

$$\longrightarrow \quad H_{eff}[\rho] = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{v}[\rho]|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

➲ Singular behavior of bare interaction leads to strong density dependence in the effective interaction

✪ Hard core potentials

➲ Diagrammatic definition of U is precisely obtained by formal variation of the approximate expression for the energy :

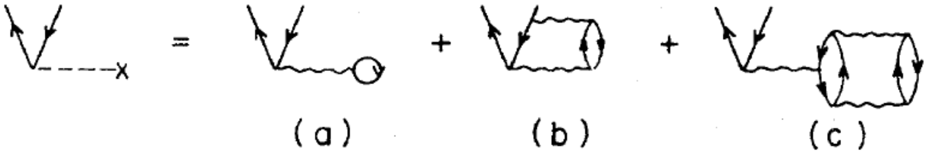
$$E = \sum_{\nu} \langle \nu | T | \nu \rangle + \tfrac{1}{2} \sum_{\nu\nu'} \langle \nu\nu' | G(\varepsilon_\nu + \varepsilon_{\nu'}) | \nu\nu' - \nu'\nu \rangle$$

Reaction matrix

$$G(W) = v - vQ \frac{1}{QTQ - W} QG(W) ,$$

$$\varepsilon_\nu = \langle \nu | T | \nu \rangle + \sum_{\nu'} \langle \nu\nu' | G(\varepsilon_\nu + \varepsilon_{\nu'}) | \nu\nu' - \nu'\nu \rangle$$

$$Q = \sum_{\rho\rho'} | \rho\rho' \rangle \langle \rho\rho' |$$



Davies et al, PRC 10, 2607 (1974)

✪ Origin of a density dependence

➲ Introduction of an explicit density dependence in the effective interaction

$$H_{eff} = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{v}|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

$$\longrightarrow \quad H_{eff}[\rho] = \sum_{ij} \langle i|T|j\rangle a_i^\dagger a_j + \frac{1}{4}\sum_{ij,kl} \langle ij|\tilde{v}[\rho]|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

➲ Singular behavior of bare interaction leads to strong density dependence in the effective interaction

➲ Effect of other degrees of freedom integrated out

❖ Partial restoration of chiral condensate with density ⇒ medium-dependent meson masses (Brown-Rho scaling)

❖ Model without mesons : 3-body interaction ≈ short range (linear) density dependent 2-body interaction at the mean-field level

✪ Effect of the density-dependence

➲ No rigorous physical argument justifying variational principle : convenient way for introducing rearrangement terms

$$E_{HF} = \sum_i \left\{ \varepsilon_{\alpha_i} - \frac{1}{2}\left[\left(U^{dir}\right)_{\alpha_i\alpha_i} + \left(U^{exc}\right)_{\alpha_i\alpha_i} \right] - \left(U^{rea}\right)_{\alpha_i\alpha_i} \right\}$$

$$B_{HF(A)} = B_{HF(A-1)} - \varepsilon_{\alpha_k} + \frac{1}{2}\left[\left(U^{dir}\right)_{\alpha_i\alpha_i} + \left(U^{exc}\right)_{\alpha_i\alpha_i} \right] + \left(U^{rea}\right)_{\alpha_i\alpha_i}$$

J.F. Berger (EJC 1991)	$-\sum_i \epsilon_{\alpha_i}$	$\frac{1}{2}\sum_i(\mathcal{U}^{DIR}_{HF})_{\alpha_i\alpha_i}$	$\frac{1}{2}\sum_i(\mathcal{U}^{ECH}_{HF})_{\alpha_i\alpha_i}$	$\sum_i(\mathcal{U}^{REA}_{HF})_{\alpha_i\alpha_i}$	B_{HF}
MeV	3186.9	-991.3	-2557.7	1297.7	935.5
$MeV/126$	25.3	-7.9	-20.3	10.3	7.4

➲ Modification of the HF relation between binding and s.p. energies : makes it possible to adjust global properties + obtain a sufficiently compressed s.p. spectrum

➲ Thermodynamics consistency (Hugenholtz-van Hove theorem)

$$T^{\mu\nu} \equiv -\eta^{\mu\nu}\,\mathcal{L} + \frac{\partial\,\mathcal{L}}{\partial\left(\partial_\mu \phi_i\right)}\partial^\nu\phi_i,\ \ \phi_i = \left\{\bar{\psi}, \psi, \sigma, \omega^\alpha, \vec{\rho}^\alpha, \vec{\pi}, A^\alpha\right\} \qquad \partial_\mu T^{\mu\nu} = 0$$

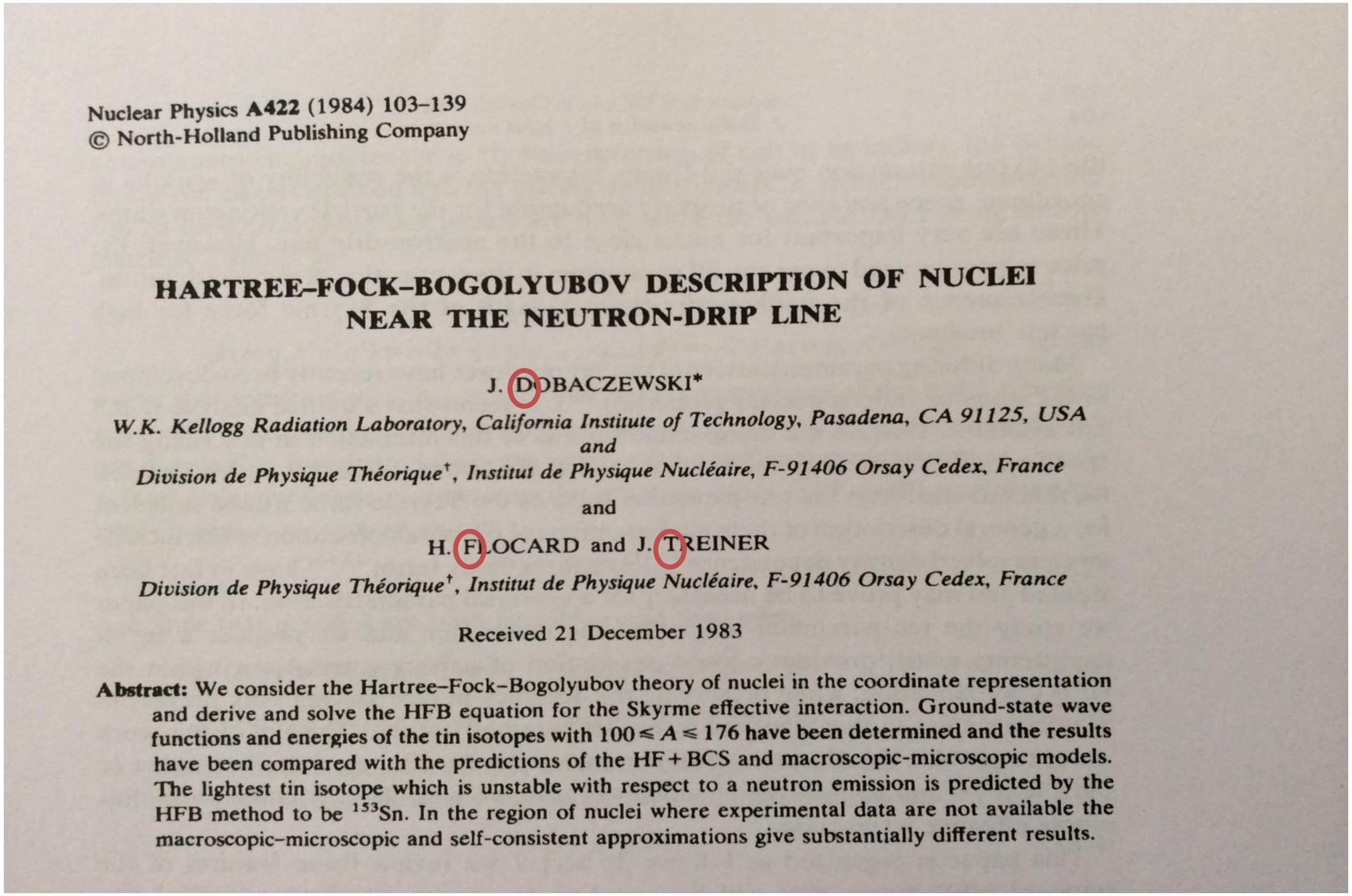
❷ Energy Density Functional approaches

D) Modern interpretation

✪ Density Functional Theory

- ➲ EDF : close in spirit to the DFT although conceptually completely different

- ➲ What is DFT ?



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HARTREE–FOCK–BOGOLYUBOV DESCRIPTION OF NUCLEI NEAR THE NEUTRON-DRIP LINE

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Received 21 December 1983

Abstract: We consider the Hartree–Fock–Bogolyubov theory of nuclei in the coordinate representation and derive and solve the HFB equation for the Skyrme effective interaction. Ground-state wave functions and energies of the tin isotopes with $100 \leqslant A \leqslant 176$ have been determined and the results have been compared with the predictions of the HF + BCS and macroscopic-microscopic models. The lightest tin isotope which is unstable with respect to a neutron emission is predicted by the HFB method to be ^{153}Sn. In the region of nuclei where experimental data are not available the macroscopic–microscopic and self-consistent approximations give substantially different results.

✪ Density Functional Theory – Existence theorem

➲ What is DFT ?

- ❖ Rigorous alternative to working with the many-body wave function
- ❖ Exact mapping of the interacting many-body problem to an easier to solve non interacting problem

➲ Hohenberg-Kohn theorem on existence

$$E_v[\rho] = \underbrace{F[\rho]}_{\textit{Universal functional}} + \int d\mathbf{x}\, \underbrace{v_{\text{ext}}}_{\textit{Static external potential}}(\mathbf{x})\rho(\mathbf{x})$$

- ❖ Energy functional of the density minimized at the **G.S. energy** with the **G.S. density**
- ❖ Offers no help in constructing F
- ❖ Rather gives a license to guess approximate energy functionals

Hohenberg & Kohn, Phys Rev 136 (1964)

✪ Density Functional Theory – Physical insight

➲ DFT **does not state** that all information about a quantum mechanical GS is contained in the constituent density, but rather that knowing the **most general response** of the GS to the perturbation of a source gives a **complete specification** of the many-body problem

"Wave function" treatment of the many-body problem

❖ Based on a single, fixed Hamiltonian $\widehat{H}$

❖ Variational calculation of GS : E stationary to variations in the relevant density matrices

$$E_{\mathrm{gs}} = \min_{\Psi} \langle \Psi | \widehat{H} | \Psi \rangle$$

DFT

❖ Family of Hamiltonians $\widehat{H}[v]$ with GS energy $E[v]$

❖ Legendre transformations

$$-F[\rho] = \min_{v}\{\int \mathrm{d}\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x}) - E[v]\}$$

$$E[v] = \min_{\rho}\{\int \mathrm{d}\mathbf{x}\, v(\mathbf{x})\rho(\mathbf{x}) + F[\rho]\} \equiv \min_{\rho}\{E_v[\rho]\}$$

❖ Response of the energy to a local source coupled to the density ⇒ GS energy as observable probed

✪ Density Functional Theory – Practical scheme

➲ Kohn-Sham procedure

❖ Introduces an auxiliary product state whose orbitals satisfy

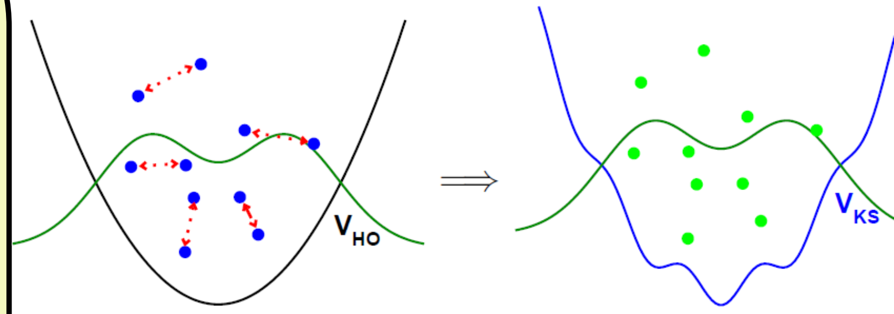
$$\left[-\frac{\nabla^2}{2m} + v_{\mathrm{KS}}(\mathbf{x})\right]\phi_i(\mathbf{x}) = \varepsilon_i\phi_i(\mathbf{x})$$

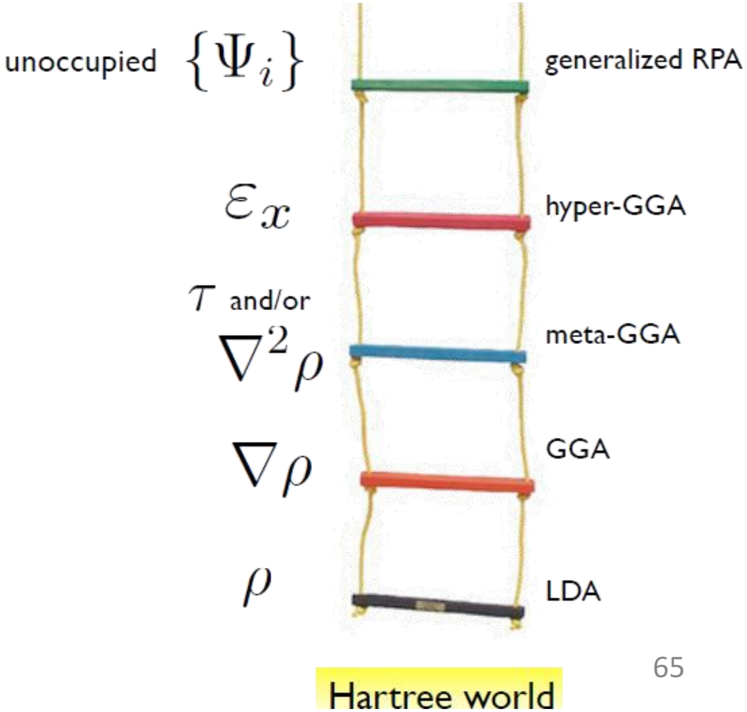
and from which one computes the density

$$\rho(\mathbf{x}) = \sum_i n_i\,|\phi_i(\mathbf{x})|^2$$

❖ KS potentials determined by

$$v_{\mathrm{KS}}(\mathbf{x}) = \delta(E_{\mathrm{ext}} + E_{\mathrm{H}} + E_{\mathrm{xc}})/\delta\rho(\mathbf{x})$$





Drut et al, Prog.Part.Nucl.Phys. 64:120 (2010)

✪ Nuclear Energy Density Functional

➲ Disquieting feature that there is no exterior potential for self-bound nuclei ⇒ existence of a functional has yet to be proven

➲ EDF relies heavily on the concept of symmetry breaking, outside the frame of HK theorem requiring that the minimum of the functional is reached for a local 1-body density that possesses **all** symmetries of the exact GS

➲ See T. Lesinski talk for connection between EDF and DFT

✪ *Spontaneous symmetry breaking : macroscopic case*

➲ SSB

❖ Classical mechanics : occurrence of SSB due to initial conditions (perturbations) breaking the symmetry

❖ Quantum mechanics of finite systems : tunneling between degenerate minima resulting a unique linear superposition GS ⇒ No SSB

❖ Quantum field theory : Suppression of the transition probabilities between degenerate vacuua partitioning Hilbert space into mutually inaccessible sectors built up over each GS

➲ In macroscopic systems broken-symmetry state can be safely taken as the effective GS

❖ Concept of generalized rigidity : heavy rigid rotor with a low-energy excitation spectrum $L^2/\mathscr{I}$

❖ spectrum above the GS (L=0) is essentially gapless ⇒ although GS possesses rotational symmetry, manifold of other degenerate states which can be recombined to give a very stable wave packet with the nature of the broken-symmetry state

❖ Macroscopic "heavyness" relaxation of the wave packet to the exact symmetrical GS exceedingly long

❖ Appropriately described by a set of non linear mean-field equation ⇒ bifurcations ⇒ emergent phenomena

Anderson, Basic Notions of Condensed Matter Physics

✪ *Spontaneous symmetry breaking and quantum correlations*

➲ Qualitative division of correlations

- ❖ Bulk of correlations (varying smoothly with A) re-summed into EDF kernel. Amount for ~ 8 A MeV

✪ *Spontaneous symmetry breaking and quantum correlations*

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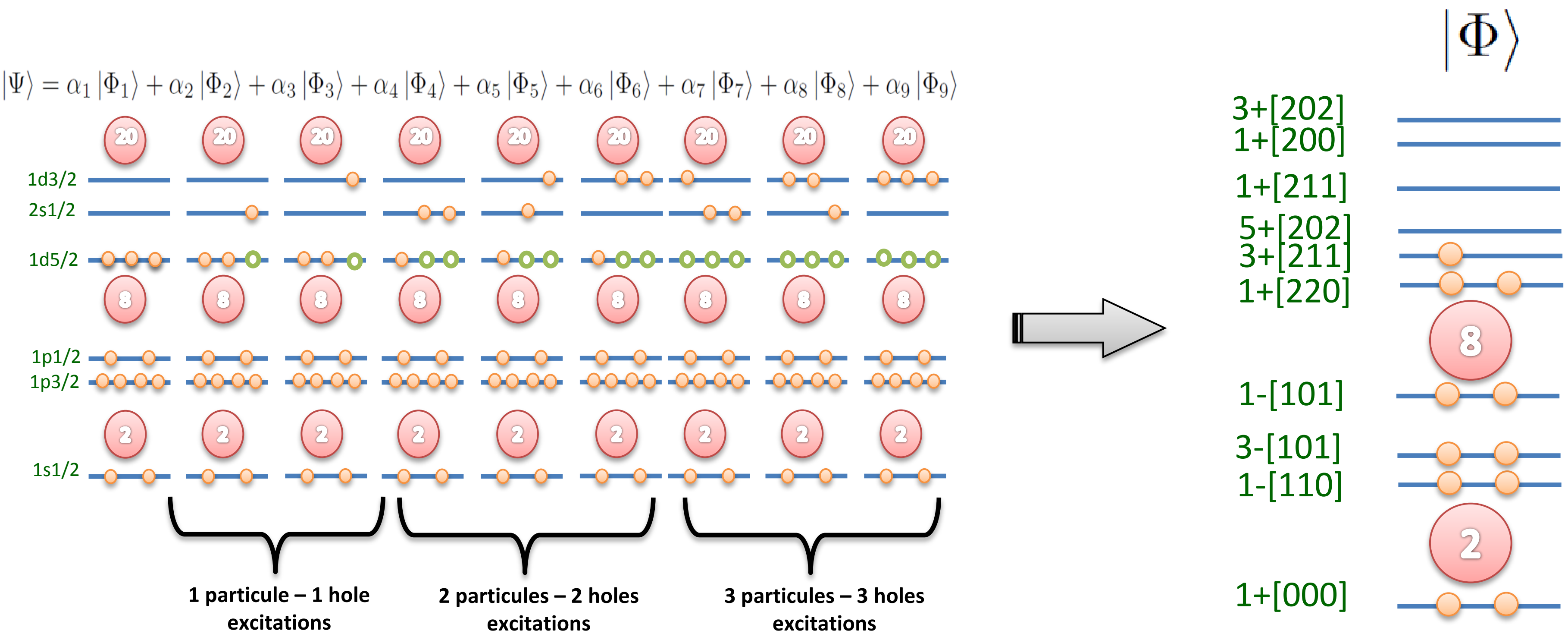
- ❖ Bulk of correlations (varying smoothly with A) re-summed into EDF kernel. Amount for ~ 8 A MeV
- ❖ Static collective correlations (quickly varying with the filling of nuclear shells) accounted for through symmetry breaking ⇒ allow to grasp correlations while retaining the simplicity inherent to a 1-body problem



$$|\Psi\rangle = \alpha_1\,|\Phi_1\rangle + \alpha_2\,|\Phi_2\rangle + \alpha_3\,|\Phi_3\rangle + \alpha_4\,|\Phi_4\rangle + \alpha_5\,|\Phi_5\rangle + \alpha_6\,|\Phi_6\rangle + \alpha_7\,|\Phi_7\rangle + \alpha_8\,|\Phi_8\rangle + \alpha_9\,|\Phi_9\rangle$$

✪ Spontaneous symmetry breaking and quantum correlations

➲ Qualitative division of correlations

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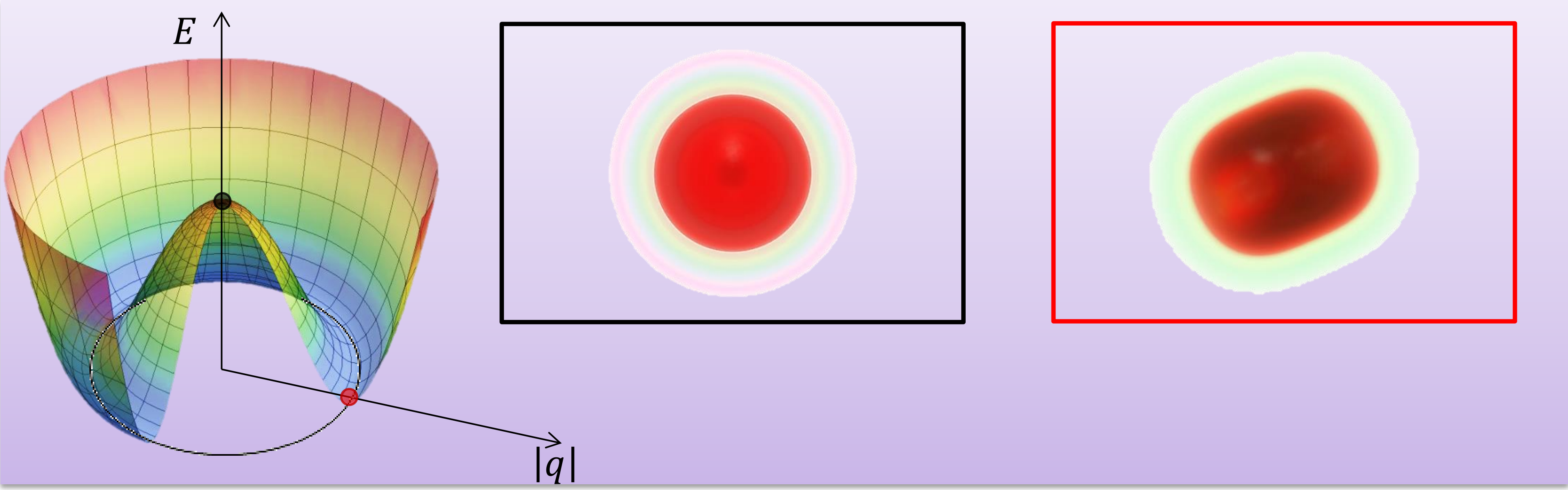
- ❖ Static collective correlations (quickly varying with the filling of nuclear shells) accounted for through symmetry breaking ⇒ allow to grasp correlations while retaining the simplicity inherent to a 1-body problem. Few tens of MeV

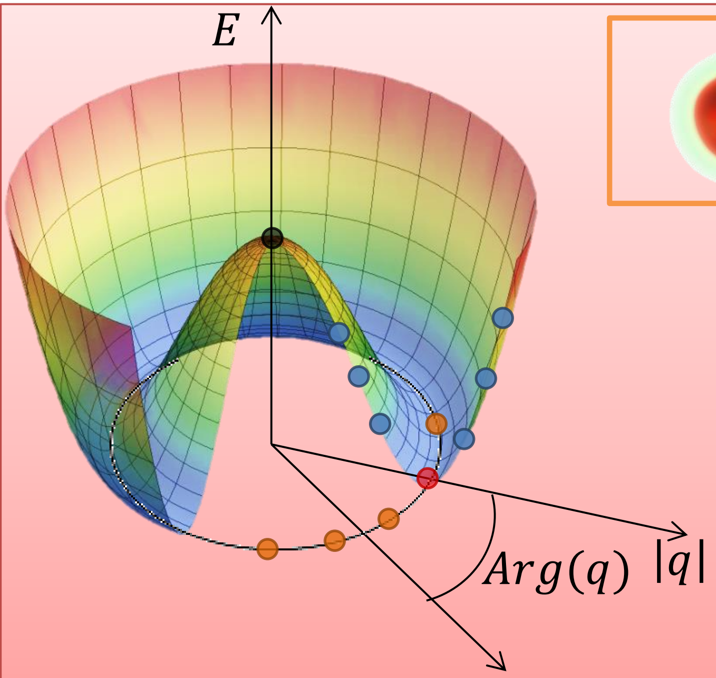


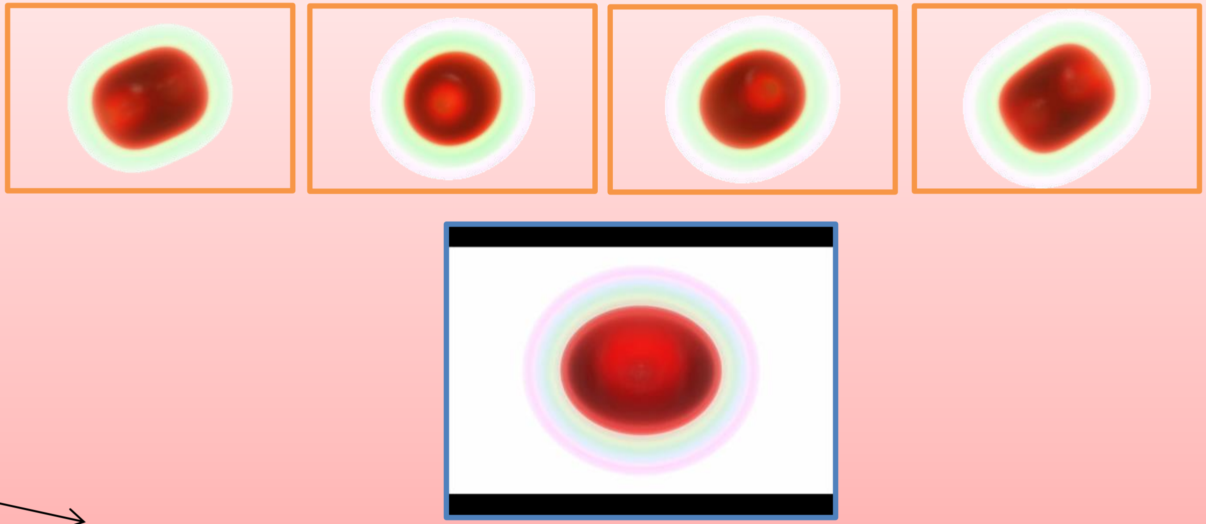
➲ SR-EDF equations are nonlinear ⇒ SSB associated of appearance of bifurcations in total energies

✪ Spontaneous symmetry breaking and quantum correlations

➲ Qualitative division of correlations

- ❖ Bulk of correlations (varying smoothly with A) re-summed into EDF kernel. Amount for ~ 8 A MeV
- ❖ Static collective correlations (quickly varying with the filling of nuclear shells) accounted for through symmetry breaking ⇒ allow to grasp correlations while retaining the simplicity inherent to a 1-body problem. Few tens of MeV
- ❖ Finiteness of the system ⇒ quantum fluctuations cannot be neglected ⇒ dynamic collective correlations (quickly varying with the filling of nuclear shells) accounted for through restoration of broken at the MR-EDF step. Few MeV





Linear properties of the equation recovered

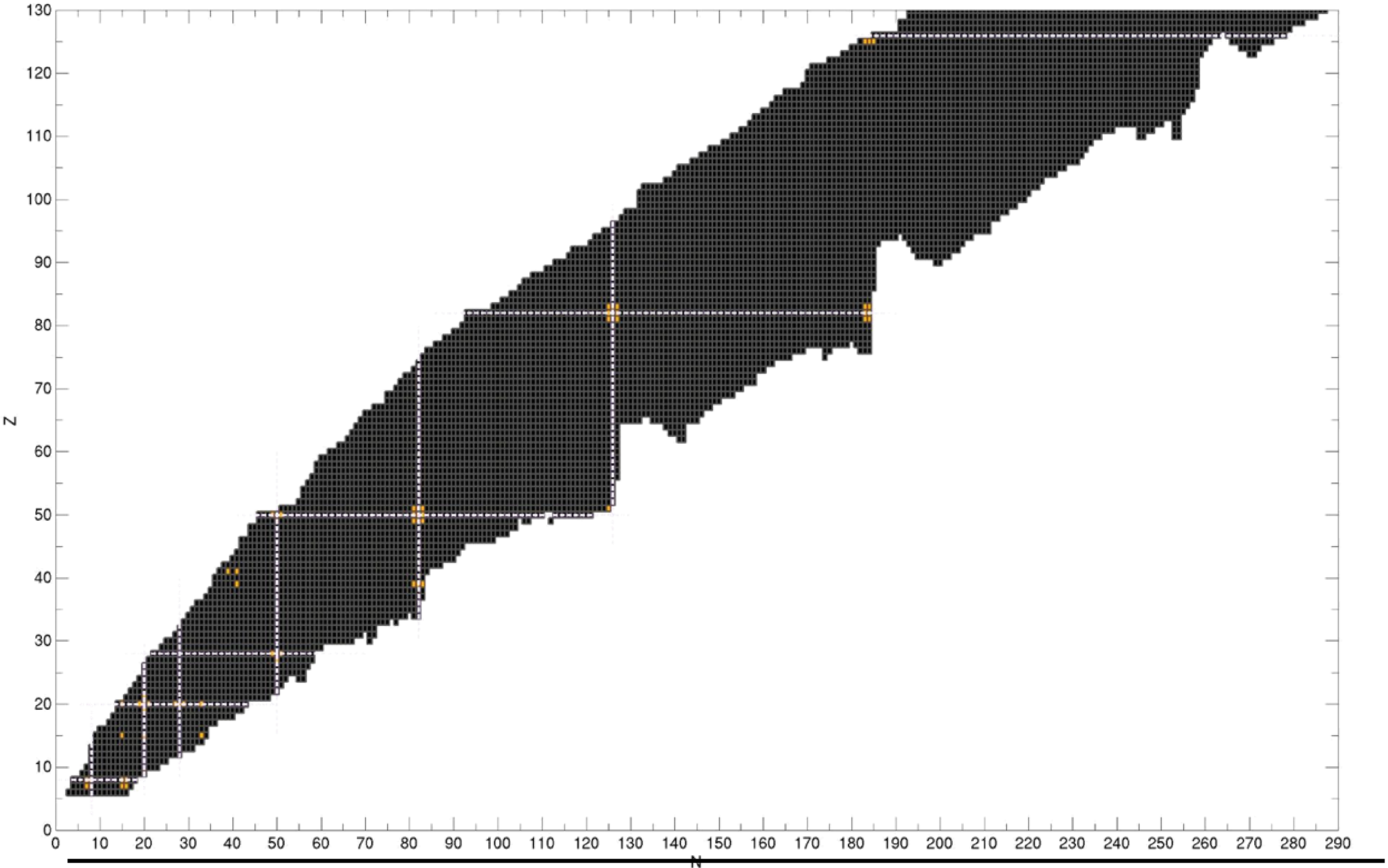
✪ *Spontaneous symmetry breaking and quantum correlations*

➲ Why bother with the SR-EDF step if symmetries are ultimately fulfilled ?

  - ❖ Allow a first description of nuclear systems at cheap cost

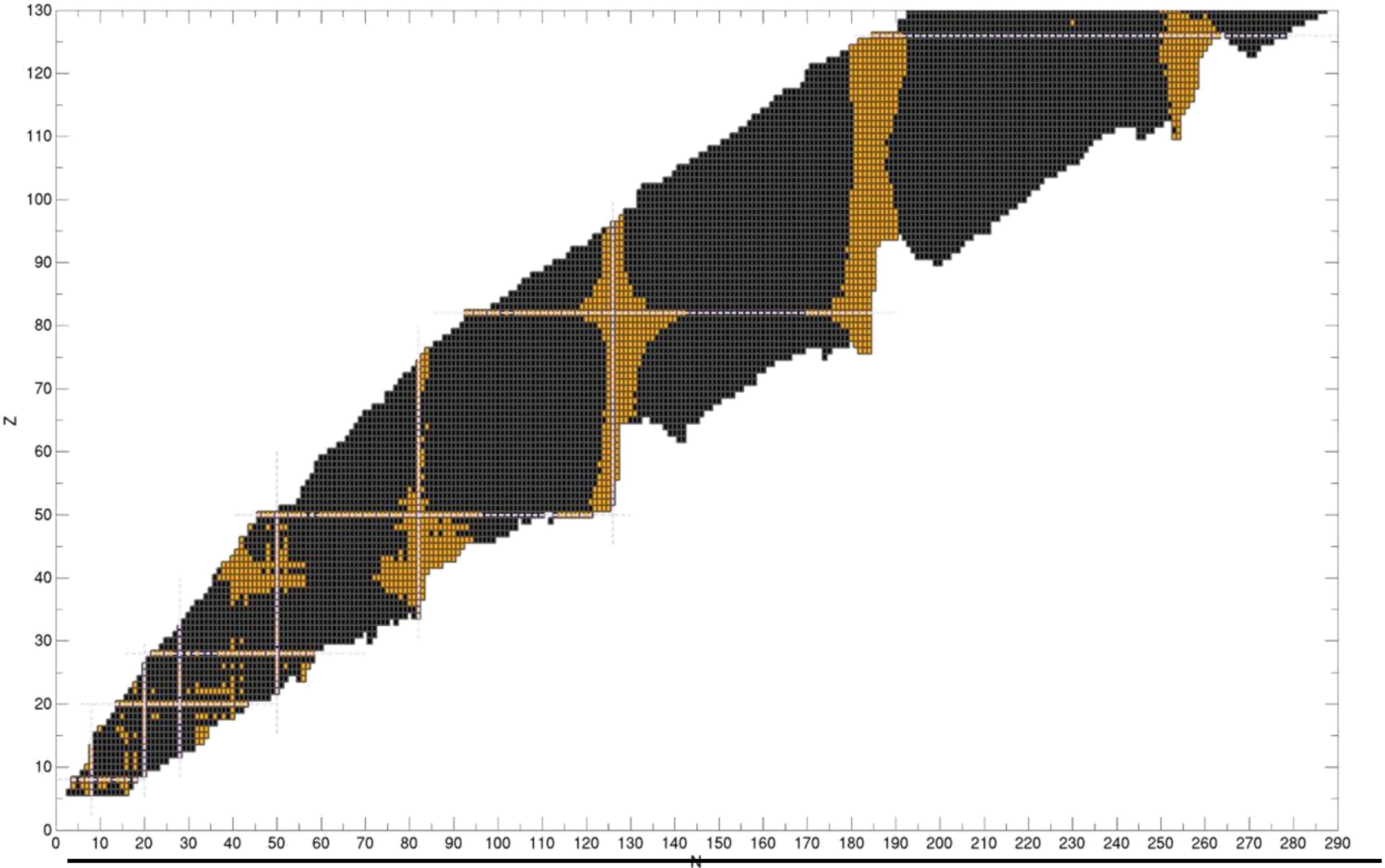
✪ Spontaneous symmetry breaking and quantum correlations

➲ no static long-range correlation



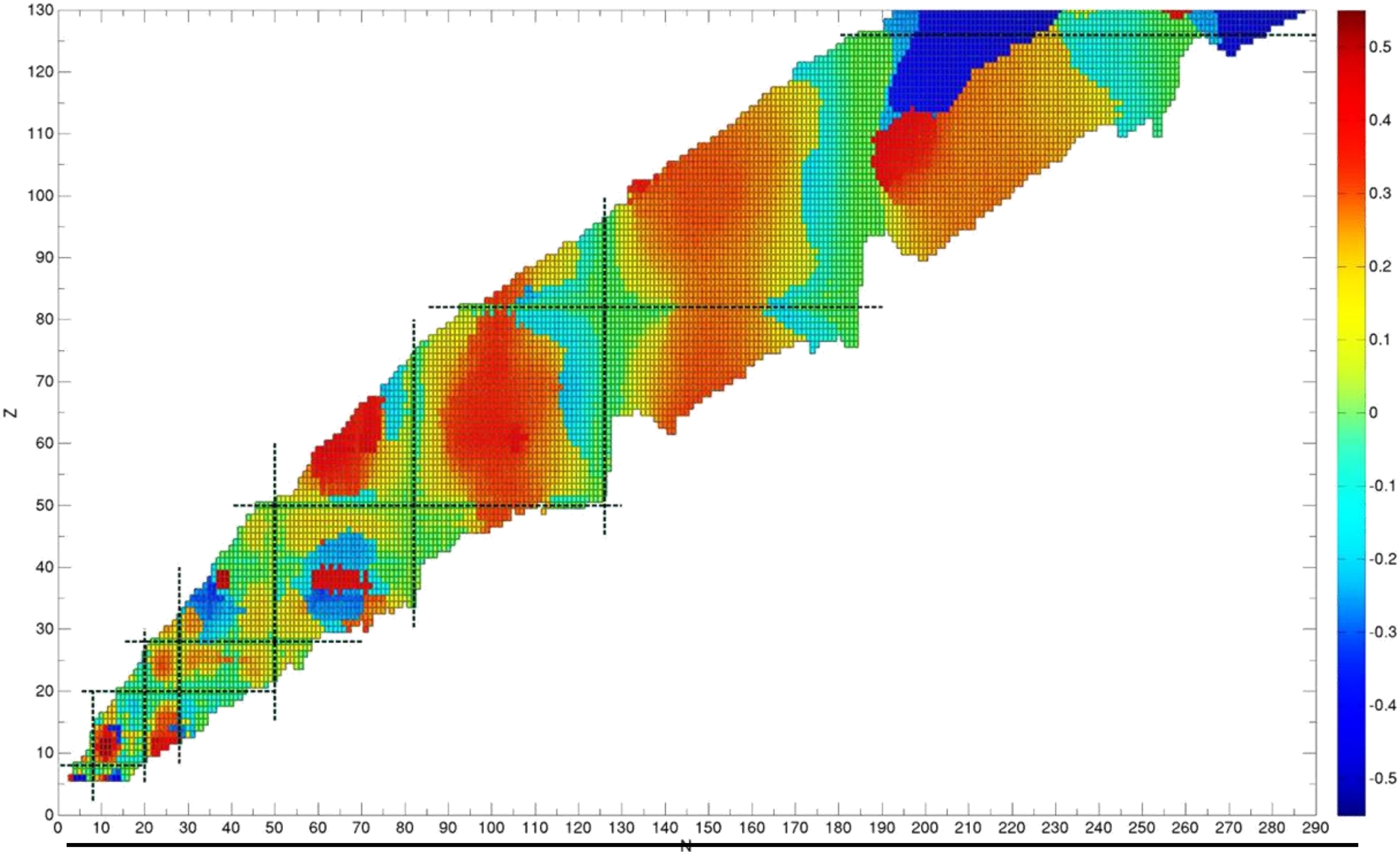
✪ Spontaneous symmetry breaking and quantum correlations

➲ Pairing correlation through U(1) symmetry breaking



✪ *Spontaneous symmetry breaking and quantum correlations*

➲ Quadrupole correlations through breaking of rotational symmetry



✪ *Spontaneous symmetry breaking and quantum correlations*

➲ Why bother with the SR-EDF step if symmetries are ultimately fulfilled ?

- ❖ Allow a first description of nuclear systems at cheap cost
- ❖ Lower symmetry properties do not disappear, instead they are hidden. Can be revealed e.g. via inspection of conditional probability distribution
- ❖ Further signatures in excitation spectra pattern

✪ SR-EDF

➲ The most basic input of EDF in the off-diagonal energy kernel E[q',q] involving two product states possibly carrying different values of the order parameters

➲ SR-EDF invokes the diagonal part of the Energy kernel.

➲ See T. Duguet lecture for a discussion of EDF starting from E[q',q]

➲ Energy functional $\mathcal{E}\left[\rho, \kappa^*, \kappa\right]$

$$\rho_{ji} = \langle\Phi| b_i^\dagger b_j |\Phi\rangle \;\; ; \;\; \kappa_{ji} = \langle\Phi| b_i b_j |\Phi\rangle$$

$$|\Phi\rangle \equiv \prod_{i=1}^{A} \beta_i |0\rangle \;\; ; \;\; \beta_i \equiv \sum_i U_{ji}^* b_j + V_{ji}^* b_j^\dagger$$

$$\mathcal{R} \equiv \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

✪ SR-EDF

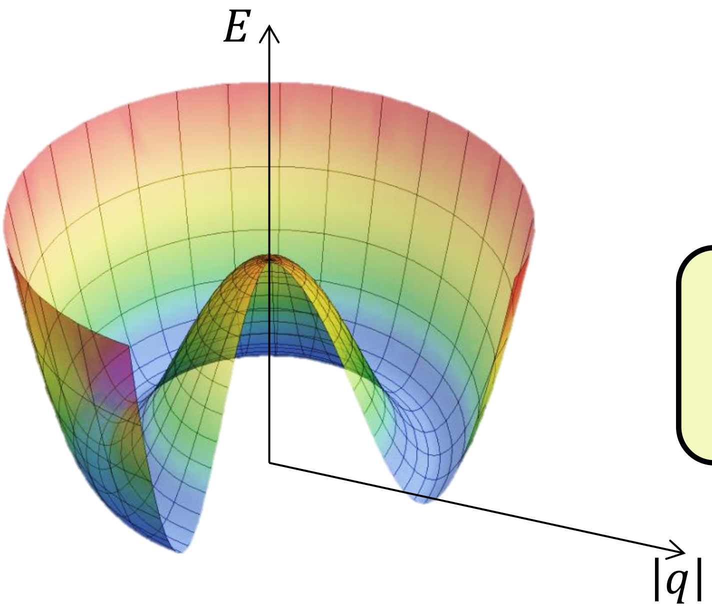
➲ Minimization of the functional yield HFB-like equation

$$\delta\left(\mathcal{E}\left[\rho,\kappa^{*},\kappa\right]-\frac{1}{2}\lambda\left[Tr\left(\rho\right)+Tr\left(\rho^{*}\right)\right]-Tr\left(\Lambda\left[\mathcal{R}^{2}-\mathcal{R}\right]\right)\right)=0$$

$$\mathcal{H}^{HFB}\begin{pmatrix}U\\V\end{pmatrix}_{\mu}\equiv\begin{pmatrix}h-\lambda & \Delta\\-\Delta^{*} & -h^{*}+\lambda\end{pmatrix}\begin{pmatrix}U\\V\end{pmatrix}_{\mu}=E_{\mu}\begin{pmatrix}U\\V\end{pmatrix}_{\mu}$$

$$h_{ij}\equiv\frac{\delta\,\mathcal{E}}{\delta\rho_{ji}}\equiv t_{ij}+\sum_{kl}\bar{v}^{ph}_{ijkl}\rho_{lk}$$

$$\Delta_{ij}\equiv\frac{\delta\,\mathcal{E}}{\delta\kappa^{*}_{ij}}\equiv\frac{1}{2}\sum_{kl}\bar{v}^{pp}_{ijkl}\kappa_{kl}$$



➲ SR-EDF only depends on $|q| \bar{=} \langle\bar{\Phi}|\,Q\,|\Phi\rangle$

➲ Constrained SR-EDF calculations : $-\lambda_{|q|}\left[Tr\left(\rho Q\right)-|q|\right]$

✪ Skyrme functionals

➲ Skyrme functional constructed from bilinear combinations of local densities and their gradient upt to some order that respect the symmetries of the nuclear Hamiltonian

$$\mathcal{E}\left[\rho,\kappa^*,\kappa\right] = \mathcal{E}_{kin}\left[\rho\right] + \mathcal{E}_{Skyrme}\left[\rho\right] + \mathcal{E}_{pair}\left[\rho,\kappa^*,\kappa\right] + \mathcal{E}_{Coul}\left[\rho\right] + \mathcal{E}_{c.o.m.}\left[\rho\right]$$

$$\begin{aligned}
\mathcal{E}_{Skyrme}\left[\rho\right] = \quad & \sum_q \int d^3r A^{\rho\rho}\rho^q\rho^q + A^{\rho\Delta\rho}\rho^q\Delta\rho^q + A^{\rho\tau}\left(\rho^q\tau^q - \vec{j}^q.\vec{j}^q\right) \\
& + A^{ss}\vec{s}^q.\vec{s}^q + A^{s\Delta s}\vec{s}^q.\Delta\vec{s}^q + A^{\rho\nabla J}\left(\rho^q\vec{\nabla}.\vec{J}^q + \vec{j}^q.\vec{\nabla}\times\vec{s}^q\right) \\
& + A^{\nabla s\nabla s}\left(\vec{\nabla}.\vec{s}^q\right)\left(\vec{\nabla}.\vec{s}^q\right) + A^{JJ}\left(\sum_{\mu\nu} J^q_{\mu\nu}J^q_{\mu\nu} - \vec{s}^q.\vec{T}^q\right) \\
& + A^{JJ}\left[\left(\sum_\mu J^q_{\mu\mu}\right)\left(\sum_\mu J^q_{\mu\mu}\right) + \sum_{\mu\nu} J^q_{\mu\nu}J^q_{\nu\mu} - 2\vec{s}^q.\vec{F}^q\right] \\
+ \quad & \sum_{q\neq q'} \int d^3r B^{\rho\rho}\rho^q\rho^{q'} + B^{\rho\Delta\rho}\rho^q\Delta\rho^{q'} + B^{\rho\tau}\left(\rho^q\tau^{q'} - \vec{j}^q.\vec{j}^{q'}\right) \\
& + B^{ss}\vec{s}^q.\vec{s}^{q'} + B^{s\Delta s}\vec{s}^q.\Delta\vec{s}^{q'} + B^{\rho\nabla J}\left(\rho^q\vec{\nabla}.\vec{J}^{q'} + \vec{j}^q.\vec{\nabla}\times\vec{s}^{q'}\right) \\
& + B^{\nabla s\nabla s}\left(\vec{\nabla}.\vec{s}^q\right)\left(\vec{\nabla}.\vec{s}^{q'}\right) + B^{JJ}\left(\sum_{\mu\nu} J^q_{\mu\nu}J^{q'}_{\mu\nu} - \vec{s}^q.\vec{T}^{q'}\right) \\
& + B^{JJ}\left[\left(\sum_\mu J^q_{\mu\mu}\right)\left(\sum_\mu J^{q'}_{\mu\mu}\right) + \sum_{\mu\nu} J^q_{\mu\nu}J^{q'}_{\nu\mu} - 2\vec{s}^q.\vec{F}^{q'}\right]
\end{aligned}$$

$$\rho^0(\vec{r},\vec{r}') = \sum_i Tr_{\sigma q}\left[\varphi_i^\dagger(\vec{r}')\varphi_i(\vec{r})\right]$$

$$\rho^1(\vec{r},\vec{r}') = \sum_i Tr_{\sigma q}\left[\varphi_i^\dagger(\vec{r}')\tau_z\varphi_i(\vec{r})\right]$$

$$\vec{s}^0(\vec{r},\vec{r}') = \sum_i Tr_{\sigma q}\left[\varphi_i^\dagger(\vec{r}')\vec{\sigma}\varphi_i(\vec{r})\right]$$

$$\vec{s}^1(\vec{r},\vec{r}') = \sum_i Tr_{\sigma q}\left[\varphi_i^\dagger(\vec{r}')\vec{\sigma}\tau_z\varphi_i(\vec{r})\right]$$

$$\rho^q(\vec{r}) \equiv \rho^q(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'} \qquad \vec{s}^q(\vec{r}) \equiv \vec{s}^q(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

$$\tau^q(\vec{r}) \equiv \vec{\nabla}.\vec{\nabla}'\rho^q(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

$$T^q_\mu(\vec{r}) \equiv \vec{\nabla}.\vec{\nabla}'s^q_\mu(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

$$\vec{j}^q(\vec{r}) \equiv -\frac{\imath}{2}\left(\vec{\nabla}-\vec{\nabla}'\right)\rho^q(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

$$J^q_{\mu\nu}(\vec{r}) \equiv -\frac{\imath}{2}\left(\nabla_\mu-\nabla'_\mu\right)s^q_\nu(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

$$F^q_\mu(\vec{r}) \equiv \frac{1}{2}\sum_\nu\left(\nabla_\mu\nabla'_\nu+\nabla'_\mu\nabla_\nu\right)s^q_\nu(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'}$$

✪ Skyrme functionals

➲ One can derive the Skyrme functional from an effective vertex

$$v_{Skyrme}(\vec{R},\vec{r},\overrightarrow{k},\overleftarrow{k}') = \left[v_{centr}+v_{LS}+v_{tens}\right](\vec{R},\vec{r},\overrightarrow{k},\overleftarrow{k}')$$

$$\begin{aligned} v_{centr}(\vec{R},\vec{r},\overrightarrow{k},\overleftarrow{k}') = \quad & t_0\,(1+x_0P_\sigma)\,\delta(\vec{r}) \\ & +\frac{1}{2}t_1\,(1+x_1P_\sigma)\left[\overleftarrow{k}'^2\delta(\vec{r})+\delta(\vec{r})\,\overrightarrow{k}^2\right] \\ & +t_2\,(1+x_2P_\sigma)\,\overleftarrow{k}'.\delta(\vec{r})\,\overrightarrow{k} \\ & +\frac{1}{6}t_3\,(1+x_3P_\sigma)\,\rho^\alpha(\vec{R})\delta(\vec{r}) \end{aligned}$$

$$v_{LS}(\vec{r},\overrightarrow{k},\overleftarrow{k}') = \imath W_0\left[\vec{\sigma}_1+\vec{\sigma}_2\right].\overleftarrow{k}'\times\delta(\vec{r})\,\overrightarrow{k}$$

$$\begin{aligned} v_{tens}(\vec{r},\overrightarrow{k},\overleftarrow{k}') = \quad & \frac{1}{2}t_e\left\{\left[3\left(\vec{\sigma}_1.\overleftarrow{k}'\right)\left(\vec{\sigma}_2.\overleftarrow{k}'\right)-(\vec{\sigma}_1.\vec{\sigma}_2)\,\overleftarrow{k}'^2\right]\delta(\vec{r})\right. \\ & \left.+\,\delta(\vec{r})\left[3\left(\vec{\sigma}_1.\overrightarrow{k}\right)\left(\vec{\sigma}_2.\overrightarrow{k}\right)-(\vec{\sigma}_1.\vec{\sigma}_2)\,\overrightarrow{k}^2\right]\right\} \\ & +t_o\left[3\left(\vec{\sigma}_1.\overleftarrow{k}'\right)\delta(\vec{r})\left(\vec{\sigma}_2.\overrightarrow{k}\right)-(\vec{\sigma}_1.\vec{\sigma}_2)\,\overleftarrow{k}'.\delta(\vec{r})\,\overrightarrow{k}\right] \end{aligned}$$

✪ Skyrme functionals

➲ Particle-particle channel

$$\mathcal{E}_{pair}\left[\rho,\kappa^*,\kappa\right] = \int d^3r\,A^{\kappa\kappa}\sum_q |\kappa^q|_2(\vec{r})$$

$$A^{\kappa\kappa} = \frac{\tilde{t}_0}{4}\left[1-\eta\left(\frac{\rho_0}{\rho_{sat}}\right)^{\alpha}\right]$$

➲ Effective vertex

$$v_{p-p}(\vec{R},\vec{r}) = \tilde{t}_0\left(\frac{1-P_\sigma}{2}\right)\left[1-\eta\left(\frac{\rho_0(\vec{R})}{\rho_{sat}}\right)^{\alpha}\right]\delta(\vec{r})$$

✪ *Gogny functionals*

➲ One can derive the Gogny functional from an effective vertex

$$\begin{aligned} v_{D1X}(\vec{R},\vec{r},\overrightarrow{k},\overleftarrow{k}') = \quad & \sum_{i=1}^{2}\left[W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau\right] e^{-\frac{r^2}{\mu_i^2}} \\ & + t_0\left(1 + x_0 P_\sigma\right)\rho^\alpha(\vec{R})\delta(\vec{r}) \\ & + \imath W_{LS}\left(\vec{\sigma}_1 + \vec{\sigma}_2\right)\overleftarrow{k}' \times \delta(\vec{r})\overrightarrow{k} \end{aligned}$$

✪ Covariant functionals

➲ Covariant functional : elementary building blocks :

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \qquad \mathcal{O}_\tau \in \{1, \tau_i\} \qquad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

$$\begin{aligned}
j_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\psi_k \ , \\
\vec{j}_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\vec{\tau}\psi_k \ , \\
\rho_S &= \langle\phi_0|\overline{\psi}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\psi_k \ , \\
\vec{\rho}_S &= \langle\phi_0|\overline{\psi}\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\vec{\tau}\psi_k
\end{aligned}$$

✪ Covariant functionals

➲ Functional can be deduced from a pseudo Lagrangian

$$\begin{aligned}\mathcal{L}_{int} = \; & -g_\sigma(\rho_v)\bar{\psi}\sigma\psi - g_\omega(\rho_v)\bar{\psi}\gamma_\mu\omega^\mu\psi - g_\rho(\rho_v)\bar{\psi}\gamma_\mu\vec{\rho}^\mu.\vec{\tau}\psi \\ & -\frac{f_\pi(\rho_v)}{m_\pi}\bar{\psi}\gamma_5\gamma_\mu\partial^\mu\vec{\pi}.\vec{\tau}\psi - e\bar{\psi}\gamma_\mu A^\mu\left(\frac{1-\tau_3}{2}\right)\psi\end{aligned}$$

$$\begin{aligned}\mathcal{L}_{PC}^{Int} = \; & -\frac{1}{2}\alpha_S(\bar{\psi}\psi)^2 - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\ & -\frac{1}{2}\alpha_{TS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) - \frac{1}{2}\alpha_{TV}(\bar{\psi}\gamma_\mu\vec{\tau}\psi)(\bar{\psi}\gamma^\mu\vec{\tau}\psi)\end{aligned}$$

✪ SR-EDF

➲ Pseudo potentials

$$\mathcal{E}_{SR}\left[\rho,\kappa,\kappa^*\right]=\sum t_{ii}\rho_{ii}+\frac{1}{2}\sum\overline{v}^{\rho\rho}_{ijij}\rho_{ii}\rho_{jj}+\frac{1}{4}\sum\overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\kappa^*_{i\bar{i}}\kappa_{j\bar{j}}$$

➲ Spurious self-interaction : Pauli principle enforce $v^{\rho\rho}_{ijkk}$=0 thus a relation between the parameters of the functional that is not fulfilled

➲ Spurious self-pairing : Idem but because if interrelation $v^{\rho\rho}_{ijkl} = v^{\kappa\kappa}_{ijkl}$

➲ Not noticeable repercussions at the SR level

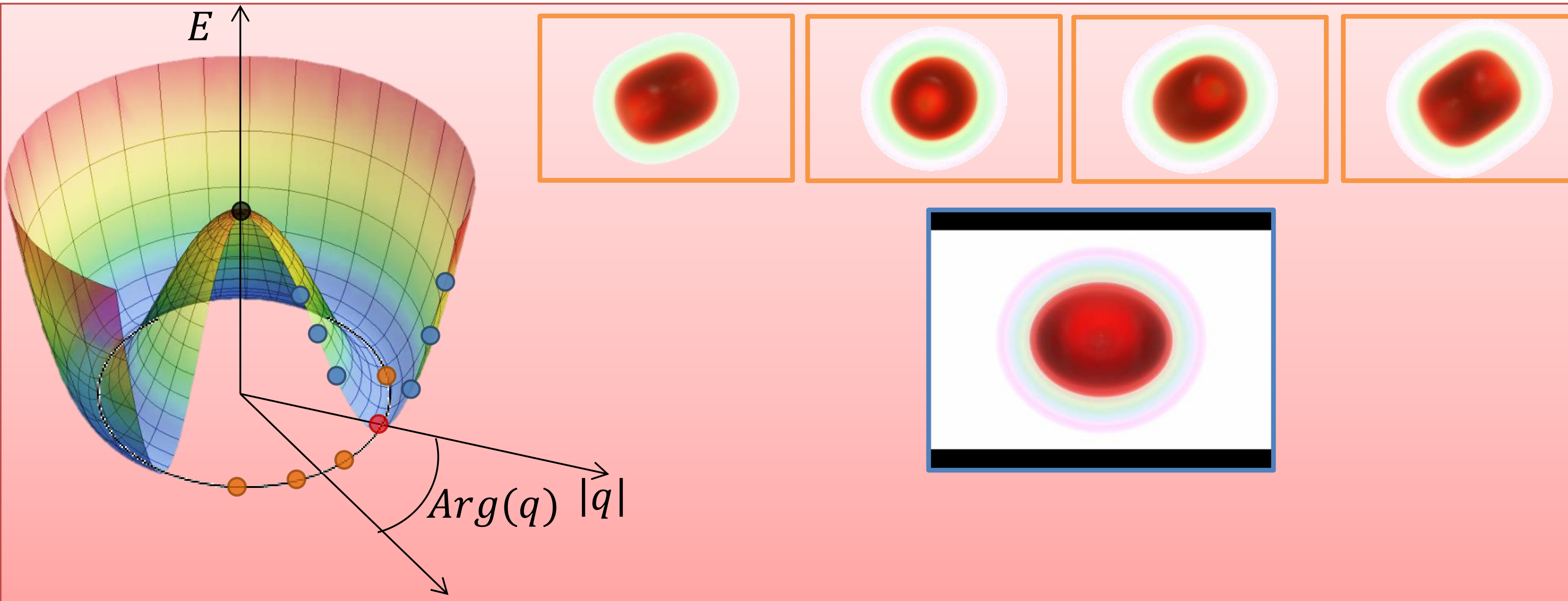
✪ MR-EDF

➲ Configuration mixing of SR states

$$|\Psi_k\rangle = \int dq \, |\Phi(q)\rangle \, f_k(q)$$

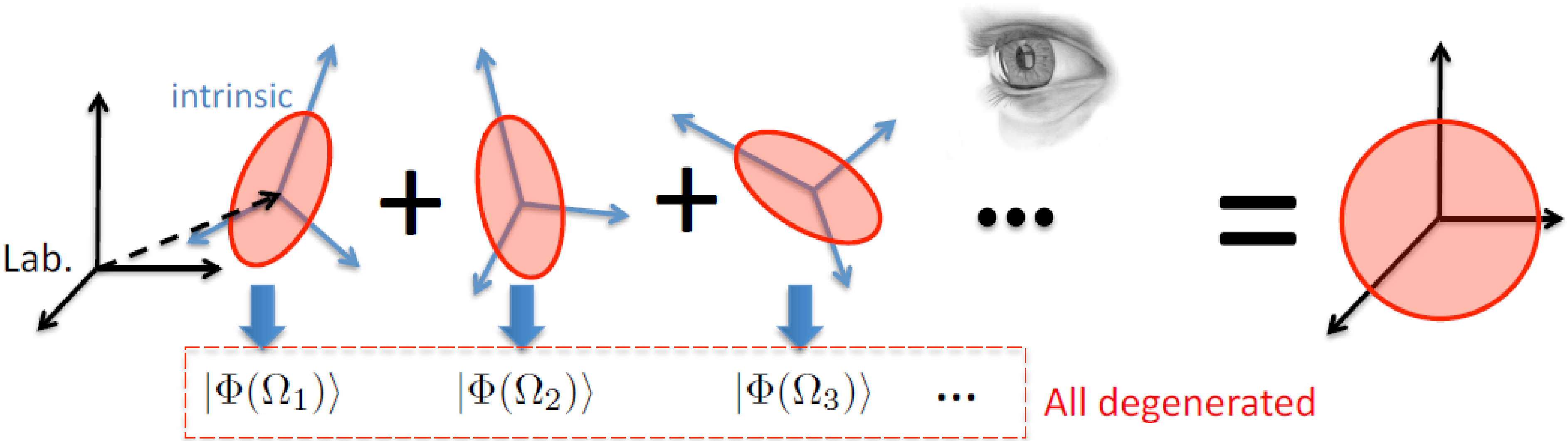
$$\int dq' \left[\mathcal{H}(q,q') - E_k \, \mathcal{I}(q,q')\right] f_k(q') = 0$$

$$\mathcal{H}(q,q') = \langle\Phi(q)| \, H \, |\Phi(q')\rangle$$
$$\mathcal{I}(q,q') = \langle\Phi(q) \, |\Phi(q')\rangle$$



➲ Restoration of broken symmetries : from the intrinsic to the lab frame

Symmetry Restoration : the rotation case



D. Lacroix EJC 2011

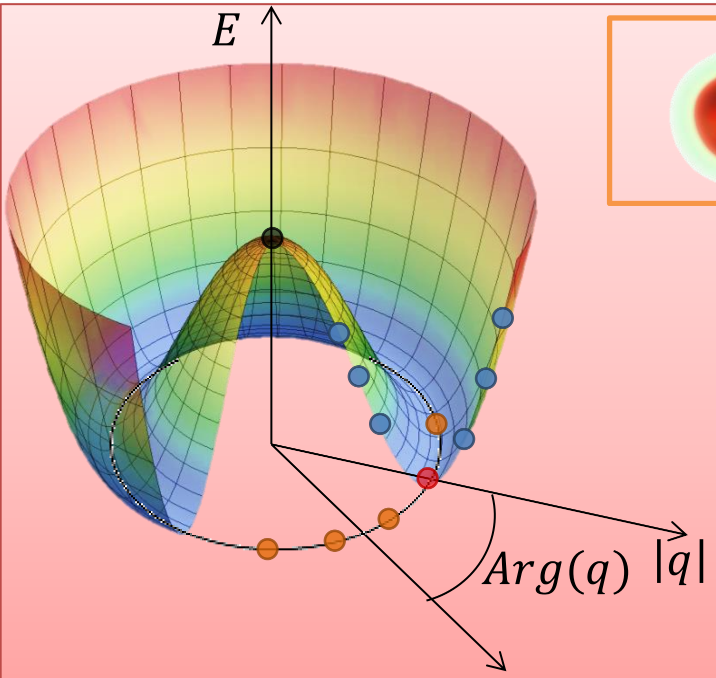
✪ MR-EDF

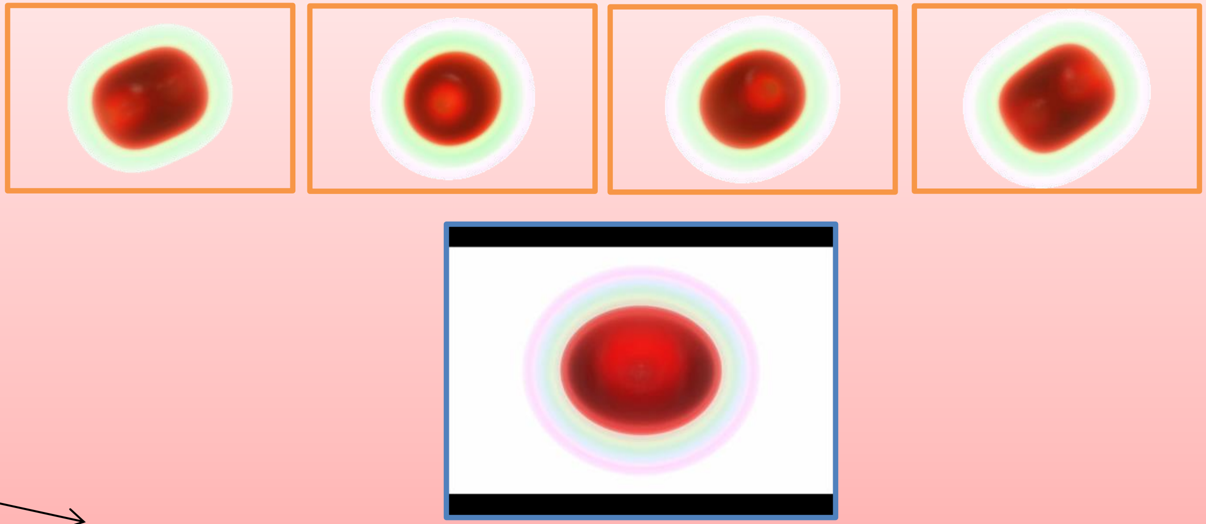
➲ Configuration mixing of SR states

$$|\Psi_k\rangle = \int dq\, |\Phi(q)\rangle\, f_k(q)$$

$$\int dq' \left[\mathcal{H}(q,q') - E_k\, \mathcal{I}(q,q')\right] f_k(q') = 0$$

$$\mathcal{H}(q,q') = \langle\Phi(q)|\, H\, |\Phi(q')\rangle$$
$$\mathcal{I}(q,q') = \langle\Phi(q)\, |\Phi(q')\rangle$$



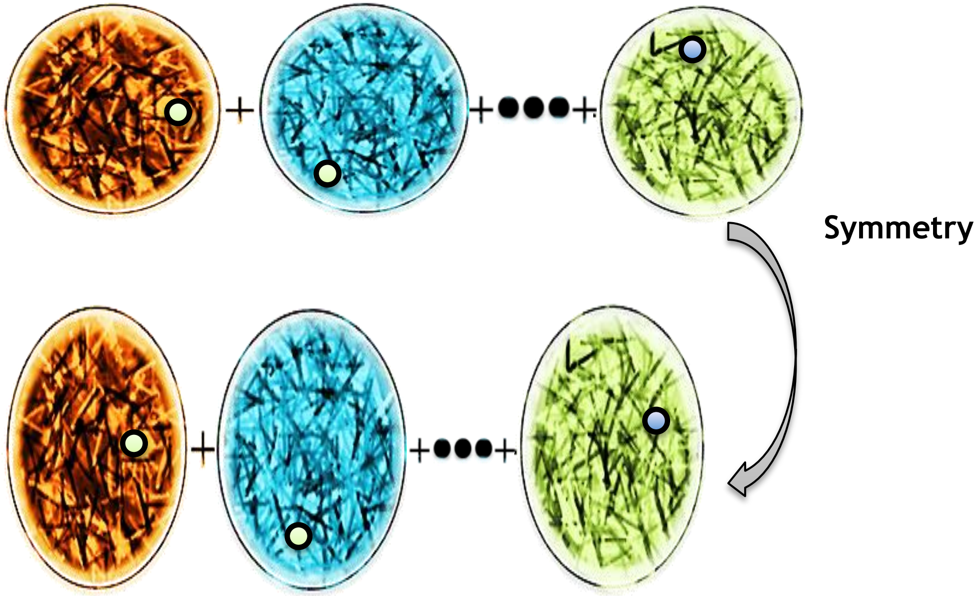


Conclusion

Conclusion

➲ **E.D.F.**

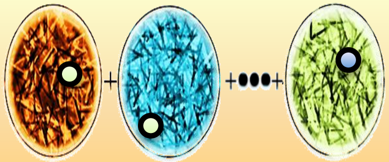
➊ Static correlations → SR-EDF



Conclusion

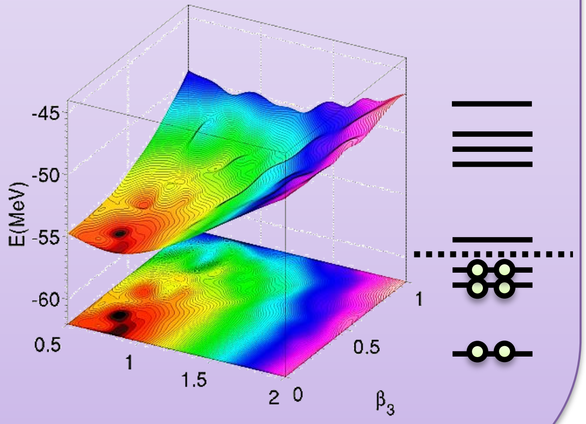
➲ E.D.F.

❶ Static correlations → SR-EDF



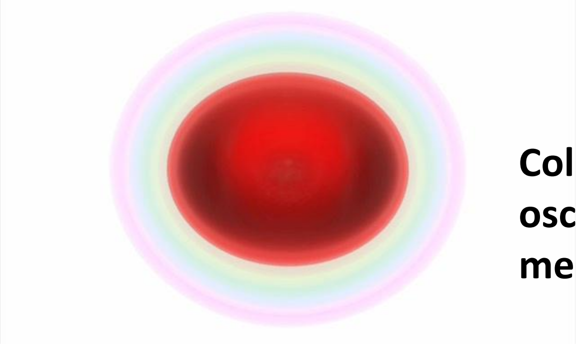
➲ Results

GS observables in intrinsic frame



G.S.

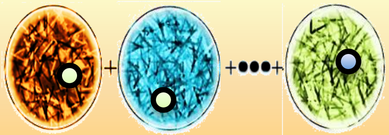
Conclusion



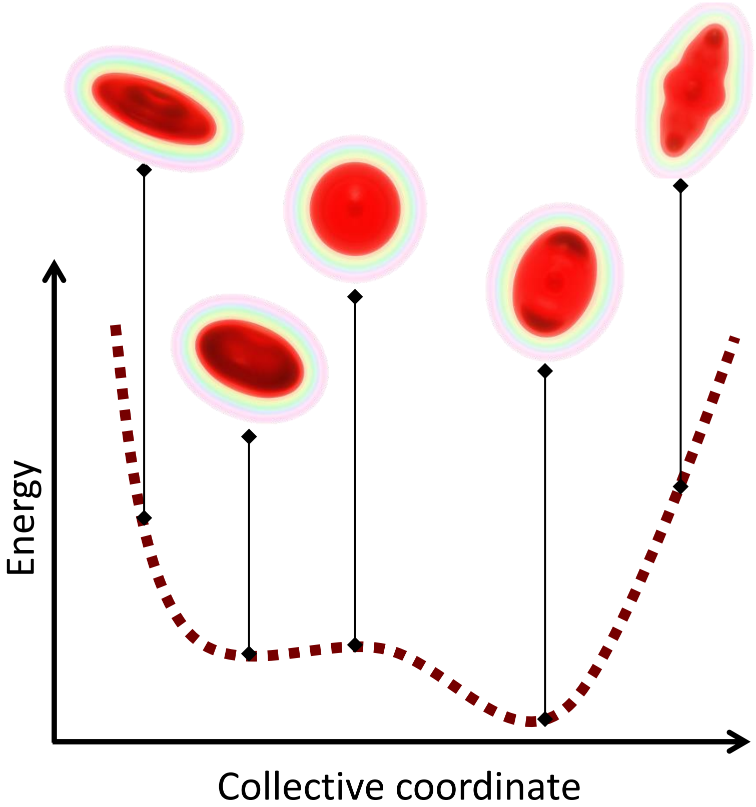
Collective oscillation of the mean-field

➲ **E.D.F.**

❶ Static correlations → SR-EDF



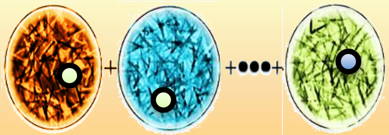
❷ Dynamical correlations→ MR-EDF



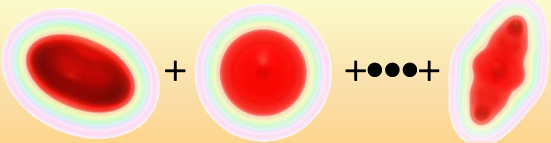
Conclusion

➲ **E.D.F.**

➊ Corrélations statiques → HFB

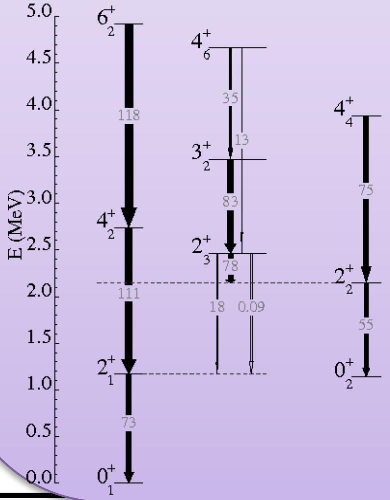


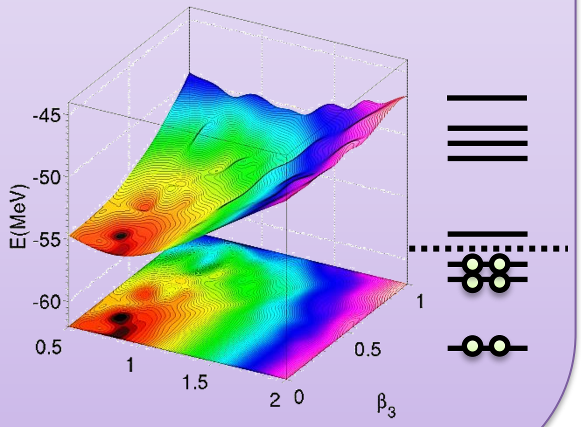
➋ Corrélations oscillations collectives → QRPA-(TD)GCM



➲ **Results**

Refinement of the results in step ➊
+ lab frame + Spectroscopy





Thank you !!

Back up