Breaking and restoring symmetries with the nuclear EDF method

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Outline

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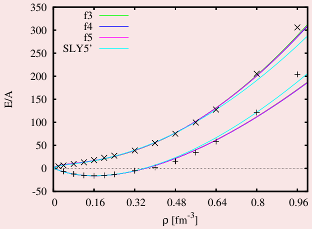
Towards a unified theoretical description of nucleonic matter

Extended matter $\rho \in [0, \sim 3\rho_{\text{sat}}]$

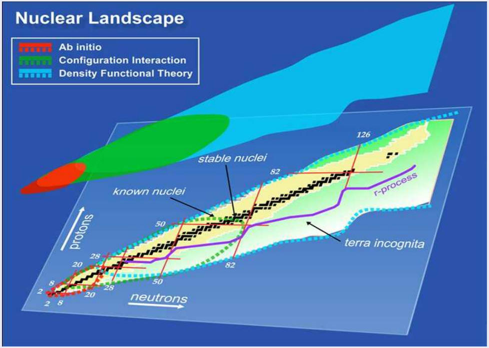


[T. Lesinski *et al.*, PRC74 (2006) 044315]

Theoretical methods

1. "Exact" (VMC, . . .)
2. Ab-initio (SCGF, BHF, . . .)
3. Effective (EDF)

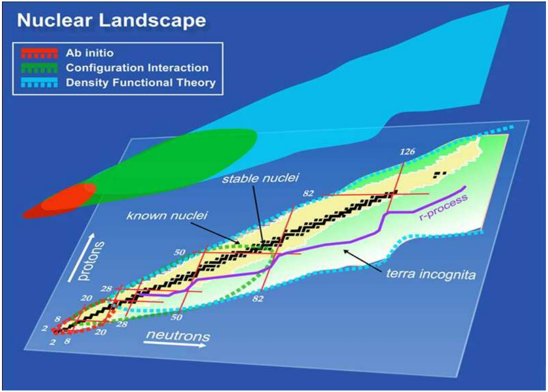
Finite nuclei $Z \in [0, 118+]$



Theoretical methods

1. "Exact" (GFMC, NCSM, . . .)
2. Ab-initio (CC, SCGF, IMSRG)
3. Effective (SM, EDF)

Playground versus theoretical methods



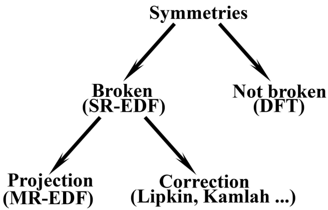
The nuclear Energy Density Functional method

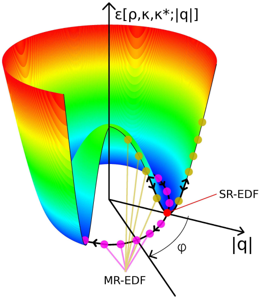
- Systematic quantal approach to medium- and heavy-mass nuclei
- Addresses both ground-state and spectroscopic properties
- Next generation of RIB facilities opens up EDF era
- EDF is meant to strongly overlap with ab-initio methods in the next 10 years

Key statements

Context

1. Two-step nuclear EDF method (i) single-reference (ii) multi-reference
2. Built by analogy with wave-function based methods (no existence theorem)
3. SR-EDF has both similarities and differences with (standard) DFT
4. Strongly relies on spontaneous symmetry breaking (SR) and restoration (MR)





Philosophy of the EDF method

Basic ingredients

1. Approach NOT based on $\{H; |\Psi\rangle\}$; i.e. $E = \langle\Psi|H|\Psi\rangle$ with $|\Psi\rangle \approx |\Psi_{\text{exact}}\rangle$
2. Key input is the off-diagonal energy kernel $\mathcal{E}_{qq'}$

$$\mathcal{E}_{qq'} \equiv \mathcal{E}[\langle\Phi_q|;|\Phi_{q'}\rangle] = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q\,*}]$$

which is a functional of one-body transition density matrices

$$\rho_{ij}^{qq'} \equiv \frac{\langle\Phi_q|a_j^\dagger a_i|\Phi_{q'}\rangle}{\langle\Phi_q|\Phi_{q'}\rangle} \quad ; \quad \kappa_{ij}^{qq'} \equiv \frac{\langle\Phi_q|a_j a_i|\Phi_{q'}\rangle}{\langle\Phi_q|\Phi_{q'}\rangle} \quad ; \quad \kappa_{ij}^{q'q\,*} \equiv \frac{\langle\Phi_q|a_i^\dagger a_j^\dagger|\Phi_{q'}\rangle}{\langle\Phi_q|\Phi_{q'}\rangle}$$

with $\{a_i^\dagger\}$ = arbitrary single-particle basis; e.g. $i = (\vec{r}, \sigma, \tau)$

- $|\Phi_q\rangle$ = product (Bogoliubov) state with collective label q
- EDF kernel re-sums bulk correlations through functional character

3. Approach relies on symmetry breaking and restoration $(J^2, N, Z, \Pi, \ldots)$
4. Empirical param. (Gogny, Skyrme,...) successful but lack predictive power

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Single-reference implementation

First level of implementation ("mean-field")

1. Invokes single state $|\Phi_q\rangle$ and diagonal energy kernel $\mathcal{E}_{qq} = \mathcal{E}[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}]$
2. $|\Phi_q\rangle$ may break symmetries and acquire finite order parameters $|q|\, e^{i\varphi_q}$
3. Provides first approx to BE, $\langle r^2_{\rm ch}\rangle$, $\rho_\tau(\vec{r})$, β_2 and ESPE $\{\epsilon_\alpha\}$

Single-particle basis $\{|\alpha\rangle\}$

- $a^\dagger_\alpha |0\rangle = |\alpha\rangle$
- $\psi_\alpha(\vec{r}\sigma\tau) \equiv \langle \vec{r}\sigma\tau|\alpha\rangle$

Diagonal density matrices

$$\rho_{\alpha\beta} \equiv \frac{\langle\Phi|a^\dagger_\beta a_\alpha|\Phi\rangle}{\langle\Phi|\Phi\rangle} = +\rho^*_{\beta\alpha}$$

$$\kappa_{\alpha\beta} \equiv \frac{\langle\Phi|a_\beta a_\alpha|\Phi\rangle}{\langle\Phi|\Phi\rangle} = -\kappa_{\beta\alpha}$$

Bogoliubov state (i)

1. Product of quasi-particle operators

$$|\Phi\rangle \equiv \prod_\mu \beta_\mu |0\rangle$$

$$\beta_\mu \equiv \sum_\alpha U^*_{\alpha\mu}\, a_\alpha + V^*_{\alpha\mu}\, a^+_\alpha$$

2. Unitary transformation $\begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix}$
3. Vacuum of quasi-particle operators

$$\beta_\mu |\Phi\rangle = 0 \ \forall\mu$$

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Bogoliubov state (ii)

1. Indefinite particle number $\kappa \neq 0$
2. Generalized density matrix

$$\mathcal{R} \equiv \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = \mathcal{R}^2$$

3. In basis $\{c^\dagger_\nu\}$ diagonalizing ρ

$$|\Phi\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, c^+_\nu\, c^+_{\bar{\nu}} \right) |0\rangle$$

BCS-like state with occupations $\rho_{\nu\nu} = v^2_\nu$

Outline

Ansatz

SR-EDF ansatz

- Diagonal energy kernel postulated as a functional $\mathcal{E} \equiv \mathcal{E}[\rho, \kappa, \kappa^*]$
- The energy results from the minimization of the diagonal kernel

$$E^{\mathrm{SR}} \equiv \mathrm{Min}_{\{|\Phi\rangle\}} \, \mathcal{E}[\rho, \kappa, \kappa^*]$$

within the manyfold spanned by product states $|\Phi\rangle$

- Bulk correlations, i.e. smoothly varying with (N, Z), resummed into $\mathcal{E}[\rho, \kappa, \kappa^*]$

Minimization and constraints

1. Independent variables are $\{\rho_{\alpha\beta}, \rho^*_{\alpha\beta}, \kappa_{\alpha\beta}, \kappa^*_{\alpha\beta} \quad \text{for} \quad \beta \leq \alpha\}$
2. The property that $\mathcal{R}^2 = \mathcal{R}$ must be enforced
   - ➡ Matrix Λ of Lagrange parameters (one per isospin τ)
3. Constrain $\langle\Phi|\hat{N}|\Phi\rangle = \mathrm{Tr}\{\rho\} = N$ as a free variation would lead to $E^{\mathrm{SR}} \rightarrow -\infty$
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Equation of motion

Minimization

1. Set $\delta_{\mathcal{R}}\left[\mathcal{E}[\rho,\kappa,\kappa^*]-\lambda\mathrm{Tr}\{\rho\}-\mathrm{Tr}\{\Lambda(\mathcal{R}^2-\mathcal{R})\}\right]=0$ leads to $[\mathcal{H},\mathcal{R}]=0$

$$\mathcal{H}\equiv\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}$$

where the effective one-body fields are defined through

$$h_{\alpha\gamma} \equiv \frac{\delta\mathcal{E}[\rho,\kappa,\kappa^*]}{\delta\rho_{\gamma\alpha}} \quad ; \quad \Delta_{\alpha\gamma}\equiv\frac{\delta\mathcal{E}[\rho,\kappa,\kappa^*]}{\delta\kappa^*_{\alpha\gamma}}$$

2. This is equivalent to solving a Bogoliubov-De-Gennes eigenvalue problem

$$\mathcal{H}\begin{pmatrix} U \\ V \end{pmatrix}_{\mu} = E_{\mu}\begin{pmatrix} U \\ V \end{pmatrix}_{\mu}$$

where $\{(U,V)_{\mu}\}$ and $\{E_{\mu}\}$ denote quasi-particle states and energies

3. h drives the effective shell structure while Δ drives the pair scattering

4. Iterative procedure $\mathcal{H}[\{(U,V)^{[n]}_{\mu}\}]\rightarrow\{(U,V)^{[n+1]}_{\mu}\}\rightarrow\mathcal{H}[\{(U,V)^{[n+1]}_{\mu}\}]\rightarrow\ldots$

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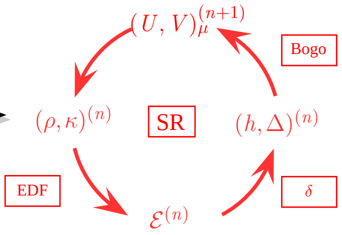
Iterative procedure and self-consistency

In

1. $\mathcal{E} \equiv \mathcal{E}[\rho, \kappa, \kappa^*]$
2. N, Z
3. $|\alpha\rangle^{(0)}$
4. $(U, V)_\mu^{(0)}$

$\Longrightarrow$



$\Longrightarrow$

Out

- E^{SR}
- $(U, V)_\mu$
- E_μ
- $\rho(\vec{r}), r_{\mathrm{ch}}^2$
- ...

Outline

Symmetries

Symmetries of H and quantum numbers

- In nuclear physics $[X, H] = 0$ for $\{X\} = \{N, Z, \vec{P}, J^2, J_z, \Pi, \mathcal{T}^2\}$
- ➡ Solutions $|\Psi_i^x\rangle$ are eigenstates of $\{X\}$ and labeled by quantum numbers $\{x\}$
- The nuclear part of H also nearly commutes with isospin operators (T^2, T_z)

In which space do we actually vary $|\Phi\rangle/\{\rho, \kappa\}$ when minimizing $\mathcal{E}[\rho, \kappa, \kappa^*]$?

- Natural to vary such that $|\Phi\rangle$ carries the same quantum numbers $\{x\}$ as $|\Psi_i^x\rangle$
- ➡ Too constraining for simple product states
- ➡ Let $|\Phi\rangle$ span several irreducible representations of the symmetry group $\mathcal{G}$

$$|\Phi\rangle \quad \equiv \quad \sum_x c_x \, |\Theta^x\rangle$$

- ✔ E^{SR} lower than for a symmetry-conserving variation
- ✘ E^{SR} does not access the ground-state energy but the one of a wave-packet

$$E^{\text{SR}} \quad = \quad \sum_x |c_x|^2 \, E^x$$

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Physical content and patterns

Origin and manifestation of spontaneous symmetry breaking

	Group		Correlations	
	Label	Casimir	V^{NN}	Internal motion
Translation $\vec{a}$	$T(3)$	$\hat{P}$	Short range	Spatial localization
Rotation φ	$U(1)$	$\hat{N}$	S-wave virtual state	Pairing
Rotation α,β,γ	$SO(3)$	$\hat{J}^2$	Quadrup.-quadrup.	Angular localization

Nuclei and spontaneous symmetry breaking

	Nuclei	Excitation pattern
Translation $\vec{a}$	All of them	Surface vibrations
Rotation φ	All but doubly-magic ones	Energy gap
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- Symmetries are enforced or relaxed according to which nucleus is studied
- Enforcing symmetries leads to a great gain in CPU time

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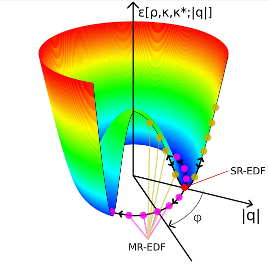
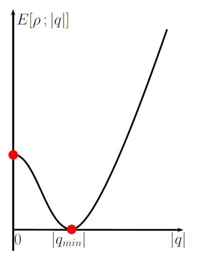
Minimization and correlation energy

Order parameter and energy minimization





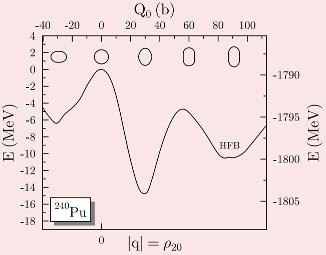
1. Symmetry breaking monitored by an order parameter $q \equiv |q|\, e^{i\mathrm{Arg}(q)}$
2. E^{SR} is independent of $\mathrm{Arg}(q)$ such that $\mathcal{E}_{qq} = \mathcal{E}_{|q||q|}$
3. The magnitude $|q|$ may vary when minimizing $\mathcal{E}_{qq}$
   1. Variation at fixed $|q| = 0$ provides symmetry-conserving solution
   2. Free variation ($|q| \neq 0$) may provide a lower solution in the larger space
   3. Constrained variation via Lagrange $(-\lambda_q \langle \Phi_q | \hat{Q} | \Phi_q \rangle)$ to access PES

Minimization and correlation energy

Breaking of $S0(3)$ and spatial deformation

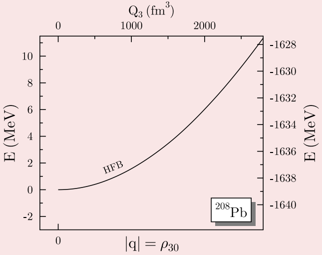
1. Order parameter relates to
   1. The non-zero multipoles of the density distribution, i.e. $|q| \equiv \rho_{\lambda\mu}$
   2. The orientation of the density distribution, i.e. $\text{Arg}(q) \equiv (\alpha, \beta, \gamma)$
2. Captures static long-range multipole-multipole correlations

Quadrupole ($\not J = 0$) correlation $\Delta E_{\rho_{20}}$



[M. Bender, private communication]

Octupole ($\not J^{\pi} = 0^+$) correlation $\Delta E_{\rho_{30}}$



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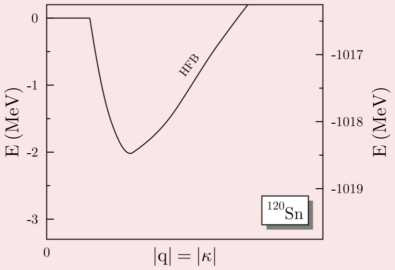
Minimization and correlation energy

Breaking of $U(1)$ and pairing deformation

1. Order parameter relates to
   1. The non-zero anomalous density, i.e. $|q| \equiv |\kappa|$
   2. The orientation of κ in gauge space, i.e. $\mathrm{Arg}(q) \equiv \alpha$
2. Captures static long-range pairing correlations

Pairing ($\not{N} = 70$) correlation $\Delta E_{||\kappa||}$



Data from [M. Bender, T.D., IJME16 (2007) 222]

Pairing correlations

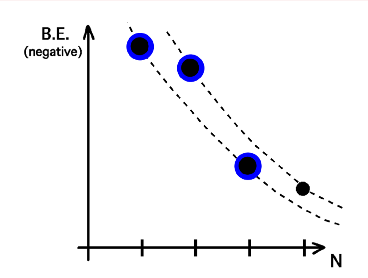
- Weak symmetry breaking
- $|\Delta E_{||\kappa||}| \ll \Delta E_{\rho_{20}}$
- $|\Delta E_{||\kappa||}| \geq$ needed accuracy
- Sharp collapse for $||\kappa|| \leq ||\kappa||_{\mathrm{crit.}}$

Minimization and correlation energy

Fingerprint at finite density of n-n virtual state in vacuum

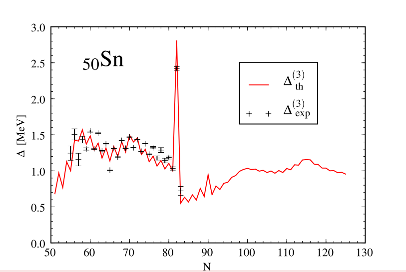
- Additional ground-state correlations
- Odd-even mass staggering (OEMS)
- Gap opens up in individual excitation spectrum
- Moment of inertia $\nearrow$ with J $\Longleftrightarrow$ Meissner effect in superconductors

Odd-even mass staggering



From [S. Baroni, private communication]

Gap extracted from the OEMS



Data from [T. D., T. Lesinski, arXiv:0907.1043]

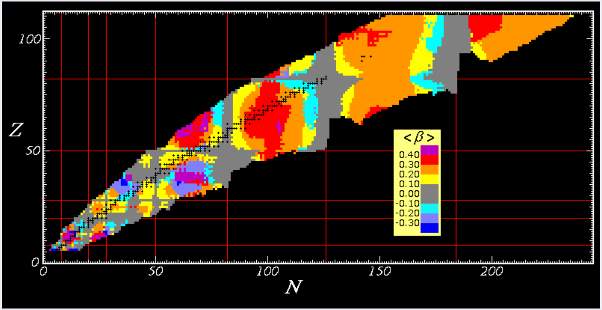
Outline

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Ground-state properties over the nuclear chart



- Large-scale deformed calculations in one day
- Masses, deformation, radii, s.p.e energies...
- Tables for experimentalists/astrophysics
- Ex: http://www-phynu.cea.fr/HFB-Gogny.htm

[S. Hilaire and M. Girod, Eur. Phys. J. **A33** (2007) 237]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
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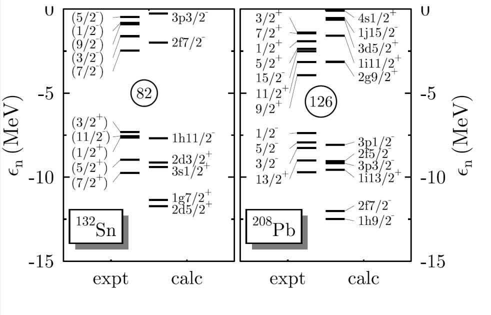
7. Reactions

Spherical shell-structure in Sn and Pb isotopes

- $h \varphi_{nlj\tau} = \epsilon_{nlj\tau} \varphi_{nlj\tau}$
- $\epsilon_{nlj\tau} \equiv$ centroid of one-nucleon separation energies

[T. D., J. Sadoudi, (2011) unpublished]



- Too spread out to anticipate correlations
- Current interest focuses on $N-Z$ behavior

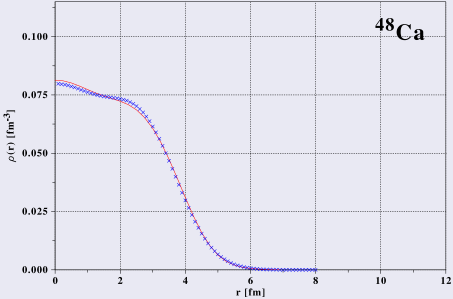
[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Charge density distribution in ^{48}Ca



- $\rho_{\mathrm{ch}}(\vec{r}) \approx \rho_p(\vec{r})$
- Saturation density $\rho_{sat} = 2\rho_p(0) \approx 0.16\ \mathrm{fm}^{-3}$
- Stable nuclei = good reproduction of data
- No measure yet in unstable nuclei

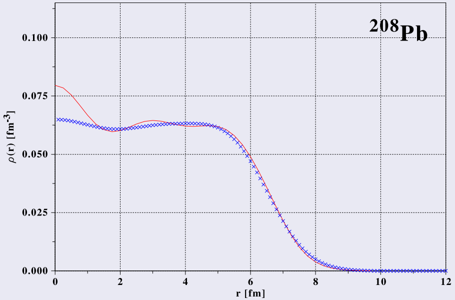
[V. Rotival and T. D., unpublished]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Charge density distribution in ^{208}Pb



- $\rho_{\rm ch}(\vec{r})$
- Saturation density $\rho_{sat} \approx 2\rho_p(0) \approx 0.16 \text{ fm}^{-3}$
- Sensitive to shell effects
- Sensitive to correlations

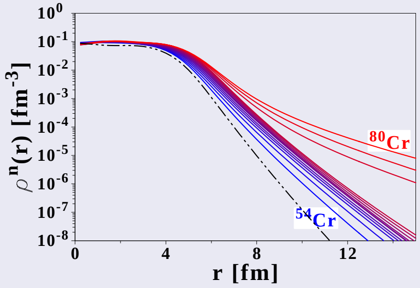
[V. Rotival and T. D., unpublished]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Halos in medium-mass nuclei



- Nuclei with anomalous extensions
- Predictions done over the nuclear chart
- Can only exist very close to neutron drip-line
- Best candidates are Cr and Fe isotopes

[V. Rotival, T. D., PRC79 (2009) 054308]

[V. Rotival, K. Bennaceur, T. D., PRC79 (2009) 054309]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
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5. Radii
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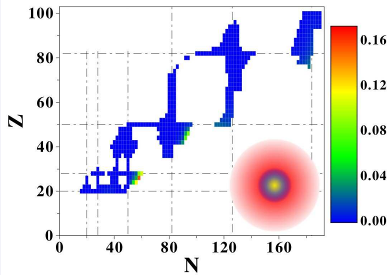

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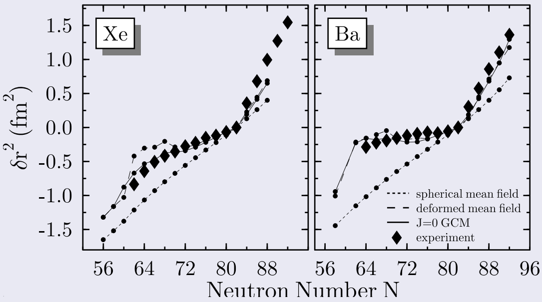
[V. Rotival, K. Bennaceur, T. D., PRC79 (2009) 054309]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Charge radii in Xe and Ba isotopes



- Good reproduction of data
- Correct $N-Z$ dependence
- Importance of static deformation

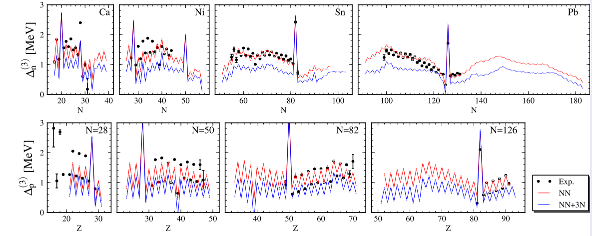
[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]

Typical results from SR-EDF calculations

Calculations

1. Systematics
2. Shells
3. Densities
4. Halos
5. Radii
6. Superfluidity
7. Reactions

Systematic of pairing gap in semi-magic nuclei



- The nucleus is superfluid
- Odd-even mass staggering is a measure of Δ_τ
- All low-energy nuclear properties impacted

[T. Lesinski, K. Hebeler, T. D., A. Schwenk, JPG (2011) in press]

Typical results from SR-EDF calculations

Calculations

1. Systematics
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4. Halos
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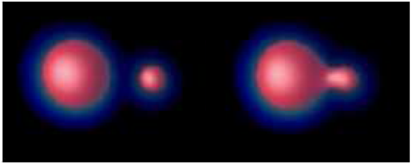
6. Superfluidity
7. Reactions

Reactions from time-dependent EDF calculations



- Ex: fusion at the Coulomb barrier ($^{16}O+^{208}Pb$)
- Pre-transfer, barrier distribution. . .
- Note: full EDF essential to solve old problems

[C. Simenel and B. Avez, arXiv:0711.0934]

Outline

Outline

Building $\mathcal{E}_{qq'} = \mathcal{E}[\langle\Phi_q|;|\Phi_{q'}\rangle] = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

The mathematical form

1. It can be as elaborate and as complicated as one finds empirically necessary
   - ➨ It can be a very non-local functional in space, i.e.

$$\mathcal{E}_{qq'} = \sum_{\sigma_1\ldots\sigma_n,\tau_1\ldots\tau_n} \int \cdots \int d\vec{r}_1 \ldots d\vec{r}_n \; \mathcal{E}(\rho^{qq'}_{\vec{r}_1\sigma_1\tau_1\vec{r}_2\sigma_2\tau_2}, \ldots, \kappa^{qq'}_{\vec{r}_{n-1}\sigma_{n-1}\tau_{n-1}\vec{r}_n\sigma_n\tau_n})$$

   - ➨ One tries to limit the complexity and the number of free parameters
2. The form is constrained as $\mathcal{E}_{qq'}$ (implicitly) relates to the *scalar* operator H

$$\mathcal{E}[\langle\Phi_q|R^\dagger(g); R(g)|\Phi_{q'}\rangle] \quad = \quad \mathcal{E}[\langle\Phi_q|;|\Phi_{q'}\rangle] \quad \text{for any} \quad R(g) \in \mathcal{G}$$

Fitting its free parameters (so far done at the SR level)

1. Use empirical knowledge of Infinite Nuclear Matter equation of state
   - ➨ $e_{\rm sat}, \rho_{\rm sat}, K_\infty, m^*_0, a_{\rm sym}$ + various $\rho_{\rm inst}$
2. Use a selected set of finite nuclei properties
   - ➨ $BE, r^2_{\rm ch}, \Delta\epsilon_{j=l\mp1/2}, \Delta E^{\rm fission}_{\rm isomer}, \cdots$

Building $\mathcal{E}_{qq'} = \mathcal{E}[\langle\Phi_q|;|\Phi_{q'}\rangle] = \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}]$

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   - $BE, r^2_{\text{ch}}, \Delta\epsilon_{j=l\mp1/2}, \Delta E^{\text{fission}}_{\text{isomer}}, \ldots$

Outline

Quasi-local form of $\mathcal{E} = \mathcal{E}[\rho, \kappa, \kappa^*]$

Strategy followed below

1. Diagonal kernel $\mathcal{E}_{qq} \equiv \mathcal{E}[\rho, \kappa, \kappa^*]$
2. Focus on the ρ dependence

Scalar and vector non-local densities

$$\rho_\tau(\vec{r}, \vec{r}\,') \equiv \sum_{\sigma\sigma'} \rho_{\vec{r}\sigma\tau\vec{r}\,'\sigma'\tau} \, 1^{\sigma'\sigma}$$

$$s_{\tau,\nu}(\vec{r}, \vec{r}\,') \equiv \sum_{\sigma\sigma'} \rho_{\vec{r}\sigma\tau\vec{r}\,'\sigma'\tau} \, \sigma_\nu^{\sigma'\sigma}$$

Time-even local densities

$$\rho_\tau(\vec{r}) \equiv \rho_\tau(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Matter density

$$\tau_\tau(\vec{r}) \equiv \sum_{\mu} \nabla_\mu \nabla'_\mu \rho_\tau(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Kinetic density

$$J_{\tau,\mu\nu}(\vec{r}) \equiv \frac{i}{2} \left(\nabla'_\mu - \nabla_\mu\right) s_{\tau,\nu}(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Spin-current tensor density

$$J_{\tau,\kappa}(\vec{r}) \equiv \sum_{\mu,\nu=x}^{z} \epsilon_{\kappa\mu\nu} \, J_{\tau,\mu\nu}(\vec{r})$$ Spin-orbit density

Quasi-local form of $\mathcal{E} = \mathcal{E}[\rho, \kappa, \kappa^*]$

Strategy followed below

1. Diagonal kernel $\mathcal{E}_{qq} \equiv \mathcal{E}[\rho, \kappa, \kappa^*]$
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Scalar and vector non-local densities

$$\rho_\tau(\vec{r}, \vec{r}\,') \equiv \sum_{\sigma\sigma'} \rho_{\vec{r}\sigma\tau\vec{r}\,'\sigma'\tau} \, 1^{\sigma'\sigma}$$

$$s_{\tau,\nu}(\vec{r}, \vec{r}\,') \equiv \sum_{\sigma\sigma'} \rho_{\vec{r}\sigma\tau\vec{r}\,'\sigma'\tau} \, \sigma_\nu^{\sigma'\sigma}$$

Time-odd local densities

$$s_{\tau,\nu}(\vec{r}) \equiv s_{\tau,\nu}(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Spin density

$$T_{\tau,\nu}(\vec{r}) \equiv \sum_\mu \nabla_\mu \nabla'_\mu \, s_{\tau,\nu}(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Spin-kinetic density

$$F_{\tau,\mu}(\vec{r}) \equiv \frac{1}{2} \sum_\nu \left(\nabla_\mu \nabla'_\nu + \nabla_\nu \nabla'_\mu\right) s_{\tau,\nu}(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Tensor-kinetic density

$$j_{\tau,\mu}(\vec{r}) \equiv \frac{i}{2} \left(\nabla'_\mu - \nabla_\mu\right) \rho_\tau(\vec{r}, \vec{r}\,')|_{\vec{r}=\vec{r}\,'}$$ Current density

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Building procedure

1. *Local* bilinear form up to two gradients and two Pauli matrices
2. Form scalars
3. Couplings $C^{ff'}_{\tau\tau'}$ may further depend on $\vec{r} \equiv$ higher-order terms

Skyrme energy density functional

$$
\begin{aligned}
\mathcal{E}[\rho,\kappa,\kappa^*] \;=\; & \sum_{\tau} \int d\vec{r}\, \frac{\hbar^2}{2m} \tau_\tau \\
& + \sum_{\tau\tau'} \int d\vec{r} \Big[C^{\rho\rho}_{\tau\tau'}\, \rho_\tau\, \rho_{\tau'} + C^{\rho\Delta\rho}_{\tau\tau'}\, \rho_\tau \Delta \rho_{\tau'} + C^{\rho\tau}_{\tau\tau'} \left(\rho_\tau\, \tau_{\tau'} - \vec{j}_\tau \cdot \vec{j}_{\tau'} \right) \\
& + C^{ss}_{\tau\tau'}\, \vec{s}_\tau \cdot \vec{s}_{\tau'} + C^{s\Delta s}_{\tau\tau'}\, \vec{s}_\tau \cdot \Delta \vec{s}_{\tau'} + C^{\rho\nabla J}_{\tau\tau'} \left(\rho_\tau \vec{\nabla} \cdot \vec{J}_{\tau'} + \vec{j}_\tau \cdot \vec{\nabla} \times \vec{s}_{\tau'} \right) \\
& + C^{\nabla s \nabla s}_{\tau\tau'} \left(\nabla \cdot \vec{s}_\tau \right) \left(\nabla \cdot \vec{s}_{\tau'} \right) + C^{JJ}_{\tau\tau'} \left(\sum_{\mu\nu} J_{\tau,\mu\nu}\, J_{\tau',\mu\nu} - \vec{s}_\tau \cdot \vec{T}_{\tau'} \right) \\
& + C^{J\bar{J}}_{\tau\tau'} \left(\sum_{\mu\nu} J_{\tau,\mu\mu}\, J_{\tau',\nu\nu} + J_{\tau,\mu\nu}\, J_{\tau',\nu\mu} - 2\, \vec{s}_\tau \cdot \vec{F}_{\tau'} \right) \Big] + \text{terms in} [\kappa, \kappa^*]
\end{aligned}
$$

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Building procedure

1. *Local* bilinear form up to two gradients and two Pauli matrices
2. Form scalars with respect to (i) Galilean transformation
3. Couplings $C^{ff'}_{\tau\tau'}$ may further depend on $\vec{r}$ ≡ higher-order terms

Skyrme energy density functional

$$
\begin{aligned}
\mathcal{E}[\rho,\kappa,\kappa^*] \;=\; & \sum_{\tau}\int d\vec{r}\,\frac{\hbar^2}{2m}\tau_\tau \\
& + \sum_{\tau\tau'}\int d\vec{r}\,\Big[C^{\rho\rho}_{\tau\tau'}\,\rho_\tau\,\rho_{\tau'} + C^{\rho\Delta\rho}_{\tau\tau'}\,\rho_\tau\Delta\rho_{\tau'} + C^{\rho\tau}_{\tau\tau'}\left(\rho_\tau\,\tau_{\tau'} - \vec{j}_\tau\cdot\vec{j}_{\tau'}\right) \\
& + C^{ss}_{\tau\tau'}\,\vec{s}_\tau\cdot\vec{s}_{\tau'} + C^{s\Delta s}_{\tau\tau'}\,\vec{s}_\tau\cdot\Delta\vec{s}_{\tau'} + C^{\rho\nabla J}_{\tau\tau'}\left(\rho_\tau\vec{\nabla}\cdot\vec{J}_{\tau'} + \vec{j}_\tau\cdot\vec{\nabla}\times\vec{s}_{\tau'}\right) \\
& + C^{\nabla s\nabla s}_{\tau\tau'}\,(\nabla\cdot\vec{s}_\tau)\,(\nabla\cdot\vec{s}_{\tau'}) + C^{JJ}_{\tau\tau'}\left(\sum_{\mu\nu} J_{\tau,\mu\nu}\,J_{\tau',\mu\nu} - \vec{s}_\tau\cdot\vec{T}_{\tau'}\right) \\
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\end{aligned}
$$

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Building procedure

1. *Local* bilinear form up to two gradients and two Pauli matrices
2. Form scalars with respect to (ii) space rotation
3. Couplings $C^{ff'}_{\tau\tau'}$ may further depend on $\vec{r}$ ≡ higher-order terms

Skyrme energy density functional

$$
\begin{aligned}
\mathcal{E}[\rho,\kappa,\kappa^*] \; = \; & \sum_{\tau} \int d\vec{r}\, \frac{\hbar^2}{2m} \tau_\tau \\
& + \sum_{\tau\tau'} \int d\vec{r} \Big[C^{\rho\rho}_{\tau\tau'} \rho_\tau \rho_{\tau'} + C^{\rho\Delta\rho}_{\tau\tau'} \rho_\tau \Delta \rho_{\tau'} + C^{\rho\tau}_{\tau\tau'} \left(\rho_\tau \tau_{\tau'} - \vec{j}_\tau \cdot \vec{j}_{\tau'} \right) \\
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Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Building procedure

1. *Local* bilinear form up to two gradients and two Pauli matrices
2. Form scalars with respect to (iii) time reversal
3. Couplings $C^{ff'}_{\tau\tau'}$ may further depend on $\vec{r} \equiv$ higher-order terms

Skyrme energy density functional

$$
\begin{aligned}
\mathcal{E}[\rho,\kappa,\kappa^*] \;=\; & \sum_{\tau}\int d\vec{r}\,\frac{\hbar^2}{2m}\tau_\tau \\
& + \sum_{\tau\tau'}\int d\vec{r}\Big[C^{\rho\rho}_{\tau\tau'}\,\rho_\tau\,\rho_{\tau'} + C^{\rho\Delta\rho}_{\tau\tau'}\,\rho_\tau\Delta\rho_{\tau'} + C^{\rho\tau}_{\tau\tau'}\left(\rho_\tau\,\tau_{\tau'} - \vec{j}_\tau\cdot\vec{j}_{\tau'}\right) \\
& + C^{ss}_{\tau\tau'}\,\vec{s}_\tau\cdot\vec{s}_{\tau'} + C^{s\Delta s}_{\tau\tau'}\,\vec{s}_\tau\cdot\Delta\vec{s}_{\tau'} + C^{\rho\nabla J}_{\tau\tau'}\left(\rho_\tau\vec{\nabla}\cdot\vec{J}_{\tau'} + \vec{j}_\tau\cdot\vec{\nabla}\times\vec{s}_{\tau'}\right) \\
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&+ C^{J\bar{J}}_{\tau\tau'} \left(\sum_{\mu\nu} J_{\tau,\mu\mu} J_{\tau',\nu\nu} + J_{\tau,\mu\nu} J_{\tau',\nu\mu} - 2\, \vec{s}_\tau \cdot \vec{F}_{\tau'} \right) \Big] + \text{terms in } [\kappa,\kappa^*]
\end{aligned}
$$

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Historically: kernel derived from a pseudo-Hamiltonian H^{pseudo}

1. Quasi zero-range two-body pseudo-potential with 9 parameters

$$V_{\text{skyrme}} \equiv V_{\text{cent}} + V_{\text{ls}} + V_{\text{tens}}$$

$$\begin{aligned}
V_{\text{cent}} &= t_0\,(1 + x_0 P_\sigma)\,\delta(\vec{r}) \\
&+ \frac{t_1}{2}\,(1 + x_1 P_\sigma)\left[\delta(\vec{r})\,\overrightarrow{k}^2 + \overleftarrow{k'}^2\,\delta(\vec{r})\right] \\
&+ t_2\,(1 + x_2 P_\sigma)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k} \\
V_{\text{ls}} &= i\,W_0\,(\vec{\sigma_1} + \vec{\sigma_2})\,\overleftarrow{k'}\wedge\delta(\vec{r})\,\overrightarrow{k} \\
V_{\text{tens}} &= \frac{t_e}{2}\left\{\left[3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,(\vec{\sigma}_2\cdot\overleftarrow{k'}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}^2\right]\delta(\vec{r})\right. \\
&\quad \left. +\delta(\vec{r})\left[3\,(\vec{\sigma}_1\cdot\overrightarrow{k})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overrightarrow{k}^2\right]\right\} \\
&+ t_o\left\{3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,\delta(\vec{r})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k}\right\}
\end{aligned}$$

2. $\mathcal{E}_H[\rho,\kappa,\kappa^*] \equiv \langle\Phi|T + V_{\text{skyrme}}|\Phi\rangle \iff$ *Effective* Hartree-Fock

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

Historically: kernel derived from a pseudo-Hamiltonian H^{pseudo}

1. Quasi zero-range two-body pseudo-potential with 9 parameters

$$V_{\text{skyrme}} \equiv V_{\text{cent}} + V_{\text{ls}} + V_{\text{tens}}$$

$$\begin{aligned}
V_{\text{cent}} &= t_0\,(1 + x_0 P_\sigma)\,\delta(\vec{r}) \\
&+ \frac{t_1}{2}\,(1 + x_1 P_\sigma)\left[\delta(\vec{r})\,\overrightarrow{k}^{\,2} + \overleftarrow{k'}^{\,2}\,\delta(\vec{r})\right] \\
&+ t_2\,(1 + x_2 P_\sigma)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k} \\
V_{\text{ls}} &= i\,W_0\,(\vec{\sigma_1} + \vec{\sigma_2})\,\overleftarrow{k'}\wedge\delta(\vec{r})\,\overrightarrow{k} \\
V_{\text{tens}} &= \frac{t_e}{2}\left\{\left[3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,(\vec{\sigma}_2\cdot\overleftarrow{k'}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}^{\,2}\right]\delta(\vec{r})\right. \\
&\qquad \left. +\delta(\vec{r})\left[3\,(\vec{\sigma}_1\cdot\overrightarrow{k})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overrightarrow{k}^{\,2}\right]\right\} \\
&+ t_o\left\{3\,(\vec{\sigma}_1\cdot\overleftarrow{k'})\,\delta(\vec{r})\,(\vec{\sigma}_2\cdot\overrightarrow{k}) - (\vec{\sigma}_1\cdot\vec{\sigma}_2)\,\overleftarrow{k'}\cdot\delta(\vec{r})\,\overrightarrow{k}\right\}
\end{aligned}$$

2. $\mathcal{E}_H[\rho, \kappa, \kappa^*] \equiv \langle\Phi|T + V_{\text{skyrme}}|\Phi\rangle \iff$ *Effective* Hartree-Fock

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

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1. $\langle\Phi|H^{\text{pseudo}}_{\text{skyrme}}|\Phi\rangle$ = purely bilinear Skyrme-type EDF
2. Correlations induced among the 18 EDF couplings = Pauli principle

$$
\begin{aligned}
\mathcal{E}_H[\rho,\kappa,\kappa^*] = & \sum_\tau \int d\vec{r}\, \frac{\hbar^2}{2m}\tau_\tau \\
& + \sum_{\tau\tau'} \int d\vec{r} \Big[C^{\rho\rho}_{\tau\tau'}\, \rho_\tau \rho_{\tau'} + C^{\rho\Delta\rho}_{\tau\tau'}\, \rho_\tau \Delta\rho_{\tau'} + C^{\rho\tau}_{\tau\tau'} \left(\rho_\tau\tau_{\tau'} - \vec{j}_\tau\cdot\vec{j}_{\tau'}\right) \\
& + C^{ss}_{\tau\tau'}\, \vec{s}_\tau\cdot\vec{s}_{\tau'} + C^{s\Delta s}_{\tau\tau'}\, \vec{s}_\tau\cdot\Delta\vec{s}_{\tau'} + C^{\rho\nabla J}_{\tau\tau'} \left(\rho_\tau \vec{\nabla}\cdot\vec{J}_{\tau'} + \vec{j}_\tau\cdot\vec{\nabla}\times\vec{s}_{\tau'}\right) \\
& + C^{\nabla s\nabla s}_{\tau\tau'}\, (\nabla\cdot\vec{s}_\tau)(\nabla\cdot\vec{s}_{\tau'}) + C^{JJ}_{\tau\tau'} \left(\sum_{\mu\nu} J_{\tau,\mu\nu} J_{\tau',\mu\nu} - \vec{s}_\tau\cdot\vec{T}_{\tau'}\right) \\
& + C^{J\bar{J}}_{\tau\tau'} \left(\sum_{\mu\nu} J_{\tau,\mu\mu} J_{\tau',\nu\nu} + J_{\tau,\mu\nu} J_{\tau',\nu\mu} - 2\,\vec{s}_\tau\cdot\vec{F}_{\tau'}\right) \Big] + \text{terms in}\,[\kappa,\kappa^*]
\end{aligned}
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➡ Not enough (i) powers of the densities and (ii) freedom to fix the $C^{ff'}_{\tau\tau'}$

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Historically: kernel derived from a *density-dependent* effective pseudo-potential

1. Step towards EDF philosophy by adding a density dependence to "V_{skyrme}"

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"V_{\text{cent}}" &= t_0\,(1 + x_0 P_\sigma)\,\delta(\vec{r}) \\
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&+ \frac{1}{6}\,t_3\,(1 + x_3 P_\sigma)\,\rho_0^\alpha(\vec{r})\,\delta(\vec{r})
\end{aligned}
$$

2. Compute $\mathcal{E}_{"H"}[\rho,\kappa,\kappa^*] \equiv \langle\Phi|\,T + "V_{\text{skyrme}}"|\Phi\rangle$

   ➡ Only $C^{\rho\rho}_{\tau\tau'}$ further depend on $\vec{r}$ via $\rho_0^\alpha(\vec{r})$

3. Modern EDF approach = exploit full freedom offered by EDF kernel
   - Bypass "V_{skyrme}" entirely to parameterize $\mathcal{E}[\rho,\kappa,\kappa^*]$ directly
   - Freedom to use any functional form; e.g. Padé, exponential...
   - Relax constraints between EDF couplings

   ➡ Is that free from any difficulty?

Quasi-local form of $\mathcal{E}_{qq'} = \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

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Limitations of the single-reference method

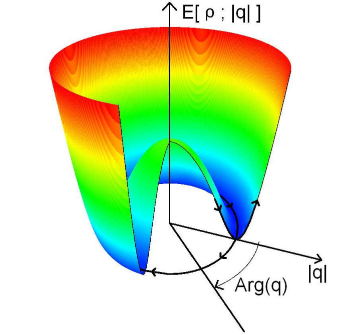
Using a single reference state $|\Phi_q\rangle$

- Casimir operator A, i.e. J^2, of $\mathcal{G}$

  $A\,|\Phi_{q_{\min}}\rangle \neq a|\Phi_{q_{\min}}\rangle$ with $a \equiv \text{Irrep}(a)$

➡ Zero-energy mode at any $|q| \neq 0$

Collective landscape



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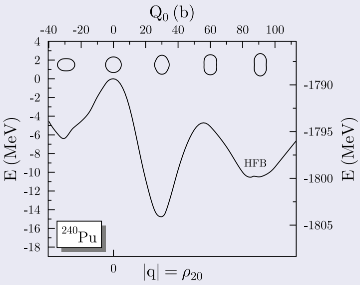
Different categories of nuclei (1) Stiff



[M. Bender, private communication]

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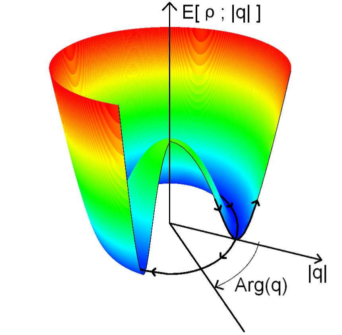

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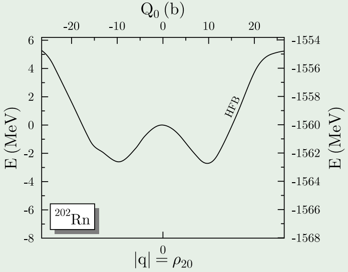
- ➡ Soft mode as a function of $|q|$?

Different categories of nuclei (2) Soft



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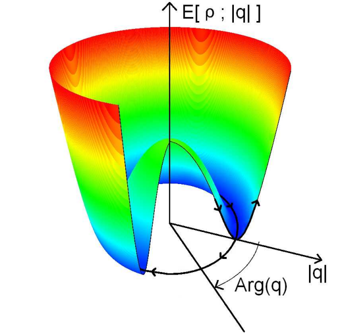

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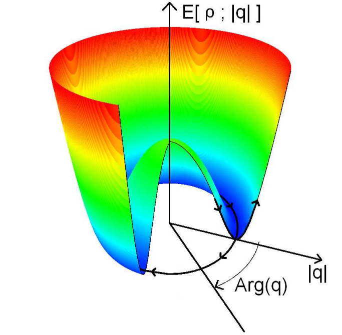


How to improve on that consistently?

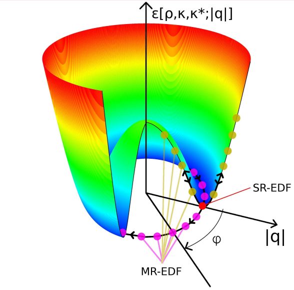
- Go beyond $|\Phi_q\rangle$ at fixed q
- ➡ Mixing in $|q|$ and $\text{Arg}(q)$
- ➡ Add dynamical correlations
- ➡ Provide excitations

Multi-reference implementation in a nutshell

Second level of implementation

- Mixes off-diagonal energy kernels associated with MR set $\{|\Phi_q\rangle\}$

$$E_k^{\text{MR}} \equiv \text{Min}_{\{f_q^k\}} \frac{\sum_{q,q'\in\text{MR}} f_q^{k*} f_{q'}^k \, \mathcal{E}_{qq'} \, \langle\Phi_q|\Phi_{q'}\rangle}{\sum_{q,q'\in\text{MR}} f_q^{k*} f_{q'}^k \, \langle\Phi_q|\Phi_{q'}\rangle}$$



- Treats collective vibrations = mixing along $|q|$
  - $\{f_q^k\}$ obtained via minimization
- Restores broken symmetries = mixing along φ_q
  - $\{f_q^k\}$ fixed by symmetry-group structure

- Large-amplitude quantum fluctuations
  1. Includes G.S. correlations
  2. Provides associated collective excitations
- Common approximation schemes
  1. QRPA = harmonic fluctuations
  2. Bohr-Hamiltonian = GOA

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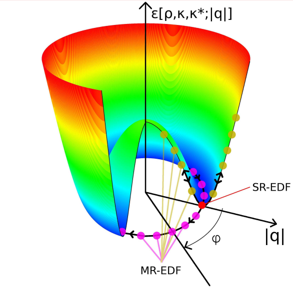

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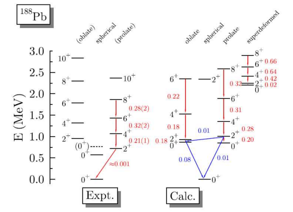

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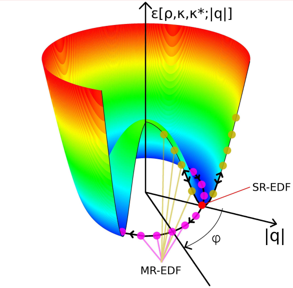

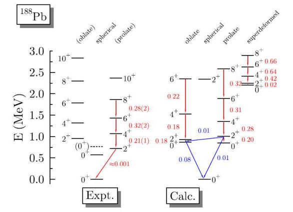

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Outline

Symmetry group $\mathcal{G}$ of H

Symmetry group $\mathcal{G} = \{\mathcal{R}(g)\}$

1. Continuous, non-abelian, compact, Lie group
   - Parameterized by $g \equiv \{g_i \in D_i\,;\, i = 1, \ldots, r\} \equiv \text{Arg}(g)$
   - Invariant measure $dm(g)$ and volume $v_{\mathcal{G}} \equiv \int_{\mathcal{G}} dm(g)$
   - Infinitesimal generators $\mathcal{C} = \{\mathcal{C}_i\,;\, i = 1, \ldots, r\}$ and Casimir Λ
2. Represented on Fock space by $R(g)$ with Irreps of dimension d_λ

$$S^{\lambda}_{ab}(g) \equiv \langle \Theta^{\lambda a} |\, R(g)\, | \Theta^{\lambda b} \rangle \quad \text{where } (a, b) \text{ run over } d^2_\lambda \text{ values}$$

3. Unitarity of Irreps and combination of transformations

$$\sum_c S^{\lambda\,*}_{ca}(g')\, S^{\lambda}_{cb}(g) = \sum_c S^{\lambda}_{ac}(-g')\, S^{\lambda}_{cb}(g) = S^{\lambda}_{ab}(g - g')$$

4. Decomposition of function $f(g)$ over volume of $\mathcal{G}$

$$f(g) \equiv \sum_{\lambda ab} f^{\lambda}_{ab}\, S^{\lambda}_{ab}(g)$$

Symmetry group $\mathcal{G}$ of H

Ex1: Space rotation $SO(3) = \{\mathcal{R}(\Omega)\}$

1. Continuous, non-abelian, compact, Lie group
   - Parameterized by three Euler angles $\Omega = (\alpha, \beta, \gamma) \in ([0, 2\pi], [0, \pi], [0, 2\pi])$
   - Invariant measure $d\Omega = \sin\beta \, d\alpha \, d\beta \, d\gamma$ and volume $v_{SO(3)} \equiv 16\pi^2$
   - Infinitesimal generators $\vec{J}$ and Casimir J^2
2. On Fock space $R(\Omega) = e^{-i\alpha J_z} \, e^{-i\beta J_y} \, e^{-i\gamma J_z}$ with Irreps of $d_J = 2J + 1$

   $$\langle JM | \, R(\Omega) \, | J' M' \rangle \equiv \mathcal{D}^J_{MM'}(\Omega) \, \delta_{JJ'} \text{ with } 2J \in \mathbb{N} \; ; \; -2J \leq 2(M, M') \leq +2J \in \mathbb{Z}$$
3. Unitarity of Irreps and combination of transformations

   $$\sum_{M''} \mathcal{D}^{J\,*}_{M''M}(\Omega') \, \mathcal{D}^J_{M''M'}(\Omega) = \sum_{M''} \mathcal{D}^J_{MM''}(-\Omega') \, \mathcal{D}^J_{M''M'}(\Omega) = \mathcal{D}^J_{MM'}(\Omega - \Omega')$$
4. Decomposition of function $f(\Omega)$ over volume of $SO(3)$

   $$f(\Omega) \equiv \sum_{JMM'} f^J_{MM'} \, \mathcal{D}^J_{MM'}(\Omega)$$

Symmetry group $\mathcal{G}$ of H

Ex2: Gauge rotation $U(1) = \{\mathcal{R}(\varphi)\}$

1. Continuous, abelian, compact, Lie group
   - Parameterized by a gauge angle $\varphi \in [0, 2\pi]$
   - Invariant measure $d\varphi$ and volume $v_{U(1)} \equiv 2\pi$
   - Infinitesimal generator N and Casimir N^2
2. On Fock space $R(\varphi) = e^{i\varphi N}$ with Irreps of $d_N = 1$

$$\langle N|\, R(\varphi)\, |N'\rangle \equiv R_N(\varphi)\, \delta_{NN'} = e^{iN\varphi}\, \delta_{NN'} \text{ with } N \in \mathbb{Z}$$

3. Unitarity of Irreps and combination of transformations

$$[e^{i\varphi' N}]^* \, e^{i\varphi N} = e^{i(-\varphi')N} \, e^{i\varphi N} = e^{i(\varphi - \varphi')N}$$

4. Decomposition, i.e. Fourier expansion, of function $f(\varphi)$ over volume of $U(1)$

$$f(\varphi) \equiv \sum_{N \in \mathbb{Z}} f^N \, e^{i\varphi N}$$

Symmetry restored MR-EDF energy

Symmetry-restored energies E_λ^{MR}

1. Single-reference state $|\Phi_0\rangle \equiv \sum_{\lambda a} c_{\lambda a} |\Theta^{\lambda a}\rangle$ with $|\Theta^{\lambda a}\rangle \in$ Irrep λ
2. MR set $\{|\Phi_g\rangle \equiv R(g)\,|\Phi_0\rangle\}$ and energy kernel $\mathcal{E}_{g'g} \equiv \mathcal{E}[\langle\Phi_{g'}|;|\Phi_g\rangle]$
3. Decomposition of kernels over Irreps of $\mathcal{G}$

$$\mathcal{E}[\langle\Phi_{g'}|;|\Phi_g\rangle]\,\langle\Phi_{g'}|\Phi_g\rangle \equiv \sum_{\lambda ab} E^\lambda_{ab}\, S^\lambda_{ab}(g-g')$$

$$\langle\Phi_{g'}|\Phi_g\rangle = \sum_{\lambda ab} c^*_{\lambda a}\, c_{\lambda b}\, S^\lambda_{ab}(g-g')$$

whose coefficients, e.g. E^λ_{ab}, can be extracted through

$$E^\lambda_{ab} = \left(\frac{d_\lambda}{v_{\mathcal{G}}}\right)^2 \int\!\!\int_{\mathcal{G}} dm(g')\, dm(g)\; S^\lambda_{ca}(g')\, S^{\lambda\,*}_{cb}(g)\; \mathcal{E}[\langle\Phi_{g'}|;|\Phi_g\rangle]\, \langle\Phi_{g'}|\Phi_g\rangle$$

4. Real and scalar symmetry-restored MR energy defined through

$$E^{\mathrm{MR}}_\lambda \equiv E^\lambda_{ab}/c^*_{\lambda a}\, c_{\lambda b}$$

Symmetry restored MR-EDF energy

Pseudo-potential-based EDF method

1. Non-diagonal kernel $\mathcal{E}_H[\langle\Phi_{g'}|;|\Phi_g\rangle] \equiv \langle\Phi_{g'}|H^{\text{pseudo}}|\Phi_g\rangle = \mathcal{E}_H[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'\,*}]$

➨ In general $\mathcal{E}[\langle\Phi_{g'}|;|\Phi_g\rangle]$ CANNOT be factorized as $\langle\Phi_{g'}|H^{\text{pseudo}}|\Phi_g\rangle$

2. Transfer operator

$$P^{\lambda}_{ab} \equiv \frac{d_\lambda}{v_{\mathcal{G}}} \int_{\mathcal{G}} \frac{dm(g)}{c_{\lambda b}} S^{\lambda\,*}_{ab}(g)\, R(g) \qquad \text{such that} \qquad |\Theta^{\lambda a}\rangle = P^{\lambda}_{ab}|\Phi_0\rangle$$

3. Decomposition of the energy kernel becomes

$$\mathcal{E}_H[\langle\Phi_{g'}|;|\Phi_g\rangle]\,\langle\Phi_{g'}|\Phi_g\rangle \quad = \quad \sum_{\lambda ab} c^{*}_{\lambda a}\, c_{\lambda b}\, E^{\lambda}\, S^{\lambda}_{ab}(g-g')$$

4. Symmetry-restored MR energy reads

$$E^{\text{MR}}_{\lambda} \quad \equiv \quad \frac{E^{\lambda}_{ab}}{c^{*}_{\lambda a}\, c_{\lambda b}} = E^{\lambda} = \langle\Theta^{\lambda a}|H^{\text{pseudo}}|\Theta^{\lambda a}\rangle$$

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Symmetry restored MR-EDF energy

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Is that difference with the general case of any importance?

$$\mathcal{E}_H[\langle\Phi_{g'}|;|\Phi_g\rangle]\,\langle\Phi_{g'}|\Phi_g\rangle = \sum_{\lambda ab} c^{*}_{\lambda a}\, c_{\lambda b}\, E^{\lambda}\, S^{\lambda}_{ab}(g-g')$$

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Outline

Consistency requirements on the EDF kernel

Key question

What are the authorized analytical forms of $\mathcal{E}_{q'q}$?

Inspiration: pseudo-potential-based EDF kernel

From Generalized Wick Theorem $\mathcal{E}_{q'q} \equiv \langle \Phi_{q'} | H^{\text{pseudo}} | \Phi_q \rangle = \mathcal{E}_H[\rho^{q'q}, \kappa^{q'q}, \kappa^{qq'\,*}]$

Set of consistency requirements [L. Robledo, IJMP E16 (2007) 337; JPG 37 (2010) 064020]

1. $\mathcal{E}_\lambda^{\text{MR}}$ must be real and a scalar under all transformations of $\mathcal{G}$
2. Consistency of MR and SR schemes
   1. $\mathcal{E}_\lambda^{\text{MR}} = \mathcal{E}^{\text{SR}}$ when the MR set $\{|\Phi_q\rangle\}$ reduces to a single state $|\Phi_q\rangle$
   2. Chemical potential λ must be recovered from Kamlah expansion of $\mathcal{E}_N^{\text{MR}}$
   3. QRPA must be recovered through harmonic limit of $\mathcal{E}_\lambda^{\text{MR}}$

Conclusion: kernel must involve $\langle \Phi_{q'}|$ and $|\Phi_q\rangle$ only

---

Diagonal SR kernel	$\leftrightarrows$	**Off-diagonal MR kernel**
$\mathcal{E}[\rho^{\mathbf{qq}}, \kappa^{\mathbf{qq}}, \kappa^{\mathbf{qq}\,*}]$	GWT-inspired connection Is it always a viable option?	$\mathcal{E}[\rho^{\mathbf{qq}'}, \kappa^{\mathbf{qq}'}, \kappa^{\mathbf{q}'\mathbf{q}\,*}]$

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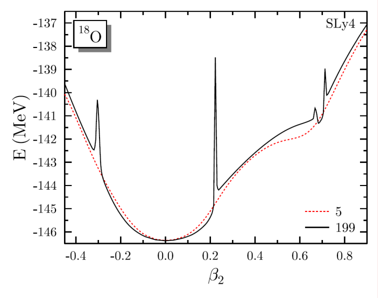
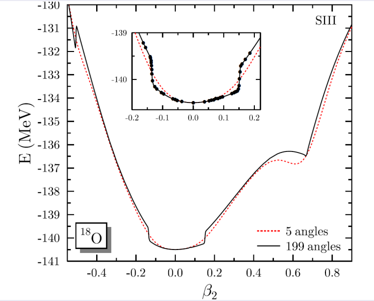
Unexpected pathologies

$\mathcal{E}^{MR}_{Z=8,N=10}$ vs ρ_{20} for $\mathcal{E}[\rho\rho\rho^{1/6}]$



[M. Bender *et al.*, PRC79 (2009) 044319]

$\mathcal{E}^{MR}_{Z=8,N=10}$ vs ρ_{20} for $\mathcal{E}[\rho\rho\rho]$



[M. Bender *et al.*, PRC79 (2009) 044319]

1. Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
2. Non-analyticity of $\mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]$ over $\mathbb{C}^*$-plane with $e^{i\varphi} \equiv z$
3. $\mathcal{E}^{MR}_N \neq 0$ for $N \leq 0$!! [M. Bender, T.D., D. Lacroix, PRC79 (2009) 044319]
4. Similar problems for other MR modes, e.g. angular momentum restoration

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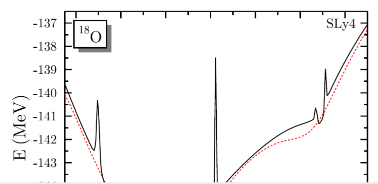

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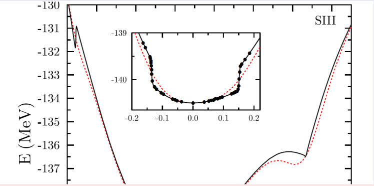

[M. Bender *et al.*, PRC79 (2009) 044319]

Absent from pseudo-potential-based method

Pauli principle is fulfilled, i.e. no self-interaction/self-pairing

1. Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
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4. Similar problems for other MR modes, e.g. angular momentum restoration

What to do about that?

Related topics covered during the workshop

1. Design a regularization method $\mathcal{E}^{\text{REG}}_{q'q} \equiv \mathcal{E}[\rho^{q'q}, \kappa^{q'q}, \kappa^{qq'*}] - \mathcal{E}_C[\langle\Phi_{q'}|;|\Phi_q\rangle]$

   [D. Lacroix, M. Bender, L. Robledo]

2. Build a pseudo-potential-based kernel $\mathcal{E}^{H}_{q'q} \equiv \langle\Phi_{g'}|H^{\text{pseudo}}_{\text{Skyrme}}|\Phi_g\rangle$

   [J. Sadoudi]

3. Use spuriosity-free approximations to $\mathcal{E}_{q'q}$

   [J. Libert, D. Vretenar, P.-G. Reinhard, N. Hinohara]

4. Bypass the MR-EDF step altogether

   [J. Messud, J. Dobaczewski, G. Hupin]

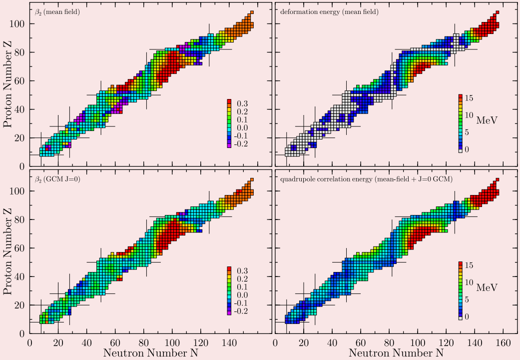
Outline

Typical results from MR-EDF calculations

Calculations

1. Binding
2. Shells
3. Radii
4. Resonances
5. Spectroscopy
6. Fission

Systematic of quadrupole correlations



1. Static deformation dominate in heavy nuclei
2. Fluctuations dominate in light nuclei
3. MR correlations improve binding energies

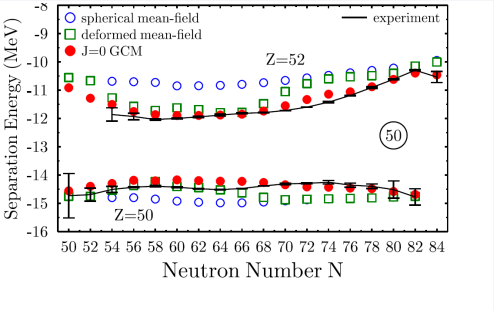
[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]

Typical results from MR-EDF calculations

Calculations

1. Binding
2. Shells
3. Radii
4. Resonances
5. Spectroscopy
6. Fission

$Z = 50$ magic gaps in Sn isotopes



- From difference of $-S_{2p}(Z) = E_0^Z - E_0^{Z+2}$
- Importance of correlations to reproduce data
- Current focus on evolution with $N-Z$

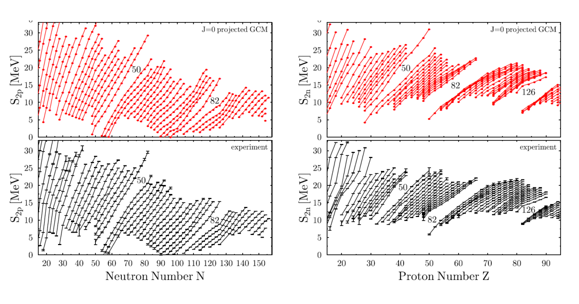
[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC78 (2008) 054312]

Typical results from MR-EDF calculations

Calculations

1. Binding
2. Shells
3. Radii
4. Resonances
5. Spectroscopy
6. Fission

Systematic of S_{2q} and magic gaps



- Visible (e.g. $N = 50$) shell quenching
- Collective correlations are essential
- Shell effects too pronounced in heavy nuclei

[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC78 (2008) 054312]

Typical results from MR-EDF calculations

Calculations

1. Binding
2. Shells
3. Radii
4. Resonances
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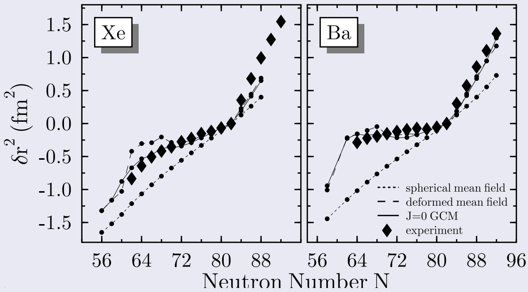
6. Fission

Charge radii in Xe and Ba isotopes



- Good reproduction of data
- Correct $N-Z$ dependence
- Importance of correlations

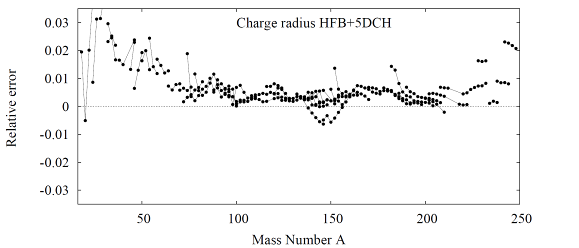
[M. Bender, G. F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]

Typical results from MR-EDF calculations

Calculations

1. Binding
2. Shells
3. Radii
4. Resonances
5. Spectroscopy
6. Fission

Systematic of charge radii



- Good agreement ($\leq 3\%$)
- More difficult to extract r_n^2 experimentally
- Neutron skin $\sqrt{r_n^2} - \sqrt{r_p^2}$ of importance
- New interest triggered by JLAB exp. on ^{208}Pb

[J. P. Delaroche *et al.*, unpublished]

Typical results from MR-EDF calculations

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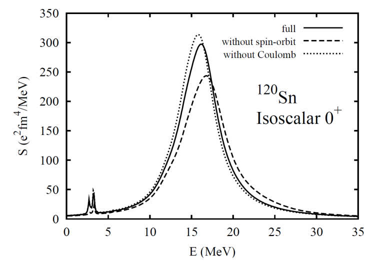
Isoscalar giant monopole resonance in ^{120}Sn



- QRPA = harmonic approximation of MR-EDF
- Strength distribution

$$S_\lambda(E) = \sum_i \left| \langle \Psi_0^A | F_\lambda | \Psi_i^A \rangle \right|^2 \delta(E_i^A - E_0^A)$$

- Resonances for all $\lambda = L^\pi$ and $T = 0, 1$ with $L \leq 3$
- Test features of EDF (K_∞, m^*_τ, a_{sym}, pairing...)

[J. Engel, unpublished]

Typical results from MR-EDF calculations

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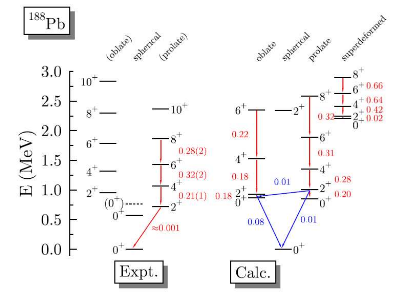
1. Binding
2. Shells
3. Radii
4. Resonances
5. Spectroscopy
6. Fission

Low-lying collective spectroscopy of ^{186}Pb



- Complex nucleus displaying shape coexistence
- Good overall picture: bands, in/out $B(E2)$s
- Too spread out spectra and too large $E0$

➡ Extensions needed

[M. Bender *et al.*, PRC69 (2004) 064303]

Typical results from MR-EDF calculations

Calculations

1. Binding
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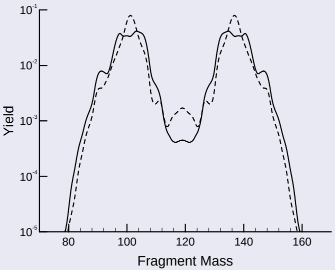
Nuclear fission of ^{238}Pu



- Fission fragments properties: A, E_{kin} distrib.
- SR-EDF ⇒ static paths for asymmetric fission
- Bohr Hamiltonian ⇒ fission dynamics
- Need exp. Z distrib., $T_{1/2}$, n/γ with $N - Z$

[H. Goutte *et al.*, PRC71 (2005) 024316]

Outline

SR-EDF numerical codes

Some published SR-EDF (Skyrme) codes

1. 1D code with spherical symmetry HFBRAD

   [K. Bennaceur, J. Dobaczewski, Comp. Phys. Comm. **168** (2005) 96]

   http://www.sciencedirect.com/science/article/pii/S0010465505002304

2. 2D code with axial symmetry HFBTHO

   [M. V. Stoitsov, J. Dobaczewski, W. Nazarewicz, P. Ring, Comp. Phys. Comm. **167** (2005) 43]

   http://www.sciencedirect.com/science/article/pii/S0010465505000305

3. 3D code with 3 symmetry planes ev8

   [P. Bonche, H. Flocard, P.-H. Heenen, Comp. Phys. Comm. **171** (2005) 49]

   http://www.sciencedirect.com/science/article/pii/S0010465505002821

4. 3D code with no symmetry HFODD

   [J. Dobaczewski *et al.*, Comp. Phys. Comm. **180** (2009) 2361]

   http://www.sciencedirect.com/science/article/pii/S0010465509002598

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- J. Dobaczewski *et al.*,
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