Density-functionals and correlations

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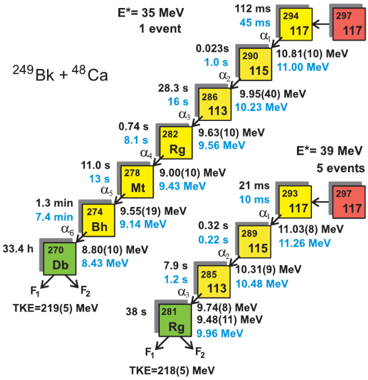
Outline

1. Alpha decay: correlations become important
2. Combining functionals with explicit correlations
   - A modified Skyrme interaction
3. Density functionals from systematic expansions
   - A method to build the functionals

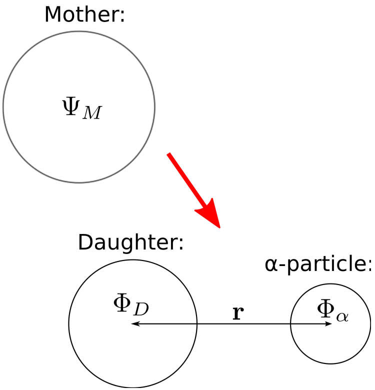
α-decay: Motivation

- Important decay mode in heavy nuclei.
- X-ray fingerprinting –> need α-decay rates to excited states
- First observation of excited states in the decay chain of $Z = 115$
  D.Rudolph *et al*, submitted to PRL



Yu.Ts. Oganessian, *et. al.* PRL 104, 142402 (2010)

Microscopic description of alpha decay



Decay width:

$$\Gamma = \hbar \frac{\ln 2}{T_{1/2}}.$$

- Strong dependence on energy Q_α.
- Nuclear structure:

$$\Gamma \sim \left| \langle \Phi_D \Phi_\alpha; r | \Psi_M \rangle \right|^2.$$

New for this work

- Skyrme-HFB wave functions.
- Convergence, large oscillator basis.
- Pairing prescriptions.

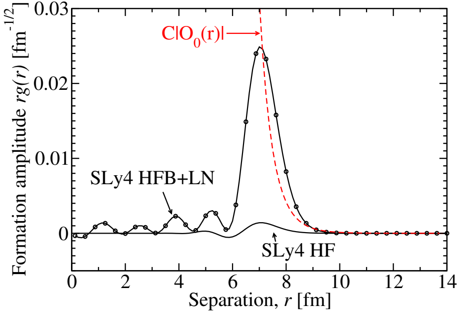
Microscopic description of alpha decay

- R-matrix formalism: Inner and outer solutions.
- Decay width: $\Gamma(r) = \hbar\sqrt{\frac{2Q_\alpha}{\mu}}\left|\frac{\langle\Phi_D\Phi_\alpha;r|\Psi_M\rangle}{O_0(Q_\alpha;r)}\right|^2.$
- Outgoing Coulomb wave function:

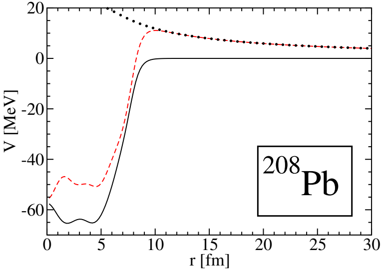
$$O_0(Q_\alpha;r).$$

- *Formation amplitude*:

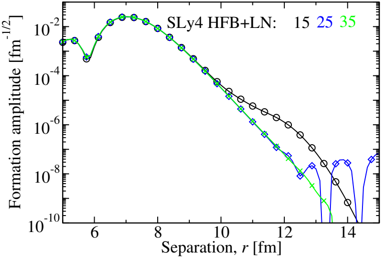
$$\langle\Phi_D\Phi_\alpha;r|\Psi_M\rangle$$



Convergence



Need convergence for $r > 9$



Fulfilled with $N_{max} > 20$

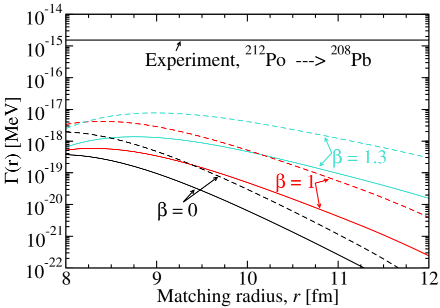
R-matrix decay width

Decay width:

$$\Gamma(r) = \hbar\sqrt{\frac{2Q_\alpha}{\mu}}\left|\frac{\langle\Phi_D\Phi_\alpha; r|\Psi_M\rangle}{O(Q_\alpha; r)}\right|^2$$

Pairing interaction:

$$V_{pair}(\mathbf{r},\mathbf{r}') = V_\beta\left[1-\beta\frac{\rho(\mathbf{r})}{\rho_c}\right]\delta(\mathbf{r}-\mathbf{r}')$$



- More surface peaked pairing →larger decay width

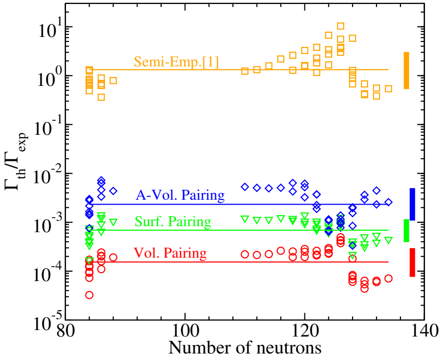
Skyrme HFB

- Weak dependence on Skyrme parameters.
  SLy4, SKM*, SKX
- Strong dependence on pairing strength.
- Approx. particle number projection increases formation.

Comparison experiment

all available data from spherical nuclei

- Γ_{th} evaluated at touching radius
- HFB+LN results systematically too small.
- relative values are well described.

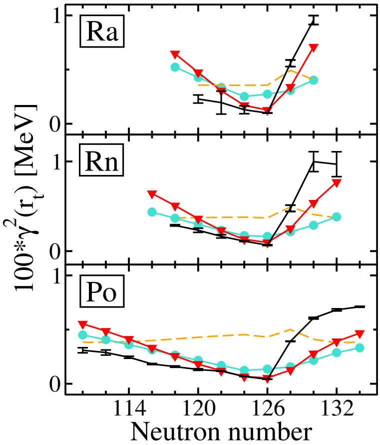


[1] C. Qi *et al*, PRC 80, 044326 (2009).

Comparison of reduced widths γ^2

Lets assume that missing correlations scales all formation amplitudes with the same constant

reduced widths: γ^2
orange: empirical formula
red: surface pairing
cyan: volume pairing



D. Ward, B.G. Carlsson and S. Åberg, manuscript in preparation

Conclusions part 1/3

- Convergence possible in oscillator basis
- Skyrme-HFB underestimates α clustering
- Reduced widths reproduced by adding 1 phenomenological parameter

Can we do better by going beyond HFB ? configuration mixing, proton-neutron correlations etc.

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Skyrme's interaction

In momentum space Skyrme's interaction looks like:

$$\bar{v}\left(\vec{k}',\vec{k}\right) \propto t_0\left(1+x_0 P^\sigma\right)+\frac{1}{2}t_1\left(1+x_1 P^\sigma\right)\left(k'^2+k^2\right) + t_2\left(1+x_2 P^\sigma\right)\vec{k}'\cdot\vec{k}+iW_0\left(\vec{\sigma}_1+\vec{\sigma}_2\right)\cdot\vec{k}'\times\vec{k}$$

T.H.R. Skyrme 1959: "...this form is unrealistic for large momentum transfers, so that its not suitable for the discussion of second-order effects, unless some momentum cut-off is introduced"

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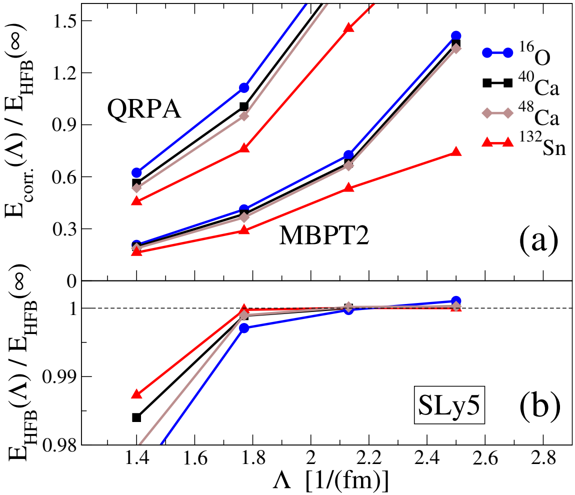
Lets introduce a momentum cut-off:

$$\bar{v}^{(\Lambda)}\left(\vec{k}',\vec{k}\right) = \bar{v}\left(\vec{k}',\vec{k}\right)\theta\left(\Lambda - k'\right)\theta\left(\Lambda - k\right)$$

and study correlations using the RPA interaction

$$\begin{aligned}
\tilde{v}_{pmqn} &= \left.\frac{\partial^2 E_{HF}}{\partial\rho_{qp}\partial\rho_{nm}}\right|_{\rho=\rho_0} \\
&= v_{pmqn}[\rho] \\
&+ \sum_{jl}\rho_{lj}\left(\frac{\partial v_{mjnl}[\rho]}{\partial\rho_{qp}} + \frac{\partial v_{pjql}[\rho]}{\partial\rho_{nm}}\right) \\
&+ \left.\frac{1}{2}\sum_{ijkl}\rho_{ki}\frac{\partial v_{ijkl}[\rho]}{\partial\rho_{nm}\partial\rho_{qp}}\rho_{lj}\right|_{\rho=\rho_0} .
\end{aligned}$$

Correlation energy

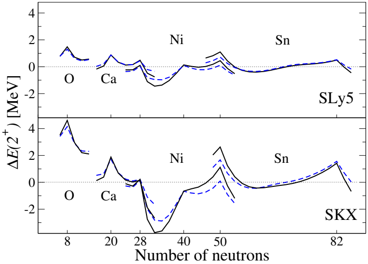


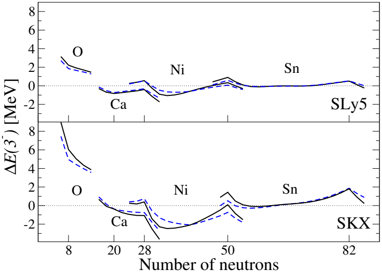
Fluctuating part of the correlation energy

$$\Delta E = E^{(2)}_{MBPT} - E_{LD}$$

where

$$E_{LD} = a_{vol}A + a_{surf}A^{2/3} + a_{sym}\frac{(N-Z)^2}{A}$$





B.G. Carlsson, J.Toivanen and U. von Barth, Phys. Rev. C.87 054303 (2013)

Conclusions part 2/3

Good things:

- Λ regularization => finite results for correlation energies
- Gives the possibility to use a many-body method of choice (QRPA, MBPT, CI etc)
- Refits of the interaction needed

Bad things:

- Computationally intensive => approximations needed

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Motivation

Has the Skyrme interaction reached its limit of precision ?

Lets try to extend it beyond the current standard form

The HF direct term

Lets consider a simple expansion of the Hartree-Fock direct term

$$V_{dir} = \frac{1}{2} \int \int v(|\vec{r}_1 - \vec{r}_2|) \rho(\vec{r}_1) \rho(\vec{r}_2) d\vec{r}_1 d\vec{r}_2.$$

Taylor expansion in powers of $\vec{r} = \vec{r}_1 - \vec{r}_2$ around $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$

$$\rho(\vec{r}_1) = \rho\left(\vec{R} + \frac{\vec{r}}{2}\right) = \sum_n \left\{ \frac{1}{n!} \left(\frac{\vec{r}}{2} \cdot \vec{\nabla}_{r'} \right)^n \rho(\vec{r'}) \right\}_{\vec{r}'=\vec{R}}.$$

Expanding both densities and recoupling, a term in the series takes the form

$$v(r) \left\{ \left[\left[\left[\vec{r}^{\,n+m} \right]_{j_1} \left[\vec{\nabla}^n_{r'} \right]_{j_2} \right]_{j_3} \rho(\vec{r'}), \left[\vec{\nabla}^m_{r''} \right]_{j_3} \rho(\vec{r''}) \right]_0 \right\}_{\vec{r}'=\vec{r}''=\vec{R}}$$

The HF direct term

The integration over relative coordinates gives

$$\int v(r)\left[\vec{r}^{\,n+m}\right]_{j_1} d\vec{r} = \frac{\delta_{j_1,0}\delta_{q,0}4\pi}{\left(-\sqrt{3}\right)^{(n+m)/2}} \int v(r) r^{n+m+2} dr = C,$$

the HF direct term turns into an integral of the local energy density

$$V_{dir} = \frac{1}{2}\int \sum_{n,m,j} C_{n,m,j} \left[[\vec{\nabla}^n]_j \rho(\vec{R}), [\vec{\nabla}^m]_j \rho(\vec{R})\right]_0 d\vec{R}$$

with constants related to moments of the force.

The HF exchange term

$$-\frac{1}{2}\int\int\rho\left(\vec{r}_1,\vec{r}_2\right)\rho\left(\vec{r}_2,\vec{r}_1\right)v(|\vec{r}_1-\vec{r}_2|)d\vec{r}_1d\vec{r}_2$$

expanded in a Taylor series

$$\begin{aligned}\rho\left(\vec{r}_1,\vec{r}_2\right) &= \rho\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right)\\ &= \sum_n\left\{\frac{1}{n!}\left(\frac{\vec{r}}{2}\cdot 2i\vec{k}\right)^n\rho\left(\vec{r}',\vec{r}''\right)\right\}_{\vec{r}'=\vec{r}''=\vec{R}}.\end{aligned}$$

Where $\vec{k}=\frac{\vec{\nabla}_{\vec{r}'}-\vec{\nabla}_{\vec{r}''}}{2i}$. Leads to

$$-\frac{1}{2}\int\sum_{nmj}C_{nmj}\,(2i)^{n+m}\left\{\left[[\vec{k}^n]_j\rho(\vec{r}',\vec{r}'),[\vec{k}^m]_j\rho(\vec{r}',\vec{r}'')\right]_0\right\}_{\vec{r}'=\vec{r}''=\vec{R}}d\vec{R}$$

General non-local interaction

Local densities

$$\rho_{nLvJ}(\vec{r}) = \left\{[[\vec{k}^n]_L, \rho_v(\vec{r},\vec{r}')]_J\right\}_{\vec{r}'=\vec{r}}$$

A general term in the EDF can be written

$$T^{m'I',n'L'v'J'}_{mI,nLvJ,Q}(\vec{r}) = C\left[\left[[\vec{\nabla}^{m'}]_{I'}, \rho_{n'L'v'J'}(\vec{r})\right]_Q \left[[\vec{\nabla}^{m}]_{I}, \rho_{nLvJ}(\vec{r})\right]_Q\right]_0$$

With density-independent coupling-constants P.I gives

$$T^{n'L'v'J'}_{mI,nLvJ}(\vec{r}) = C[\rho_{n'L'v'J'}(\vec{r}),[[\vec{\nabla}^m]_I\rho_{nLvJ}(\vec{r})]_{J'}]_0$$

Method

1. Construct all possible terms of this form going up to 6th order in derivatives (equivalent to extending Skyrmes expansion to higher orders in momentum or higher partial waves)

1. Consider only those terms which has symmetries consistent with the nuclear interaction

1. Derive all relations among such terms resulting from imposing additional symmetries (e.g. Galilean invariance)

Symmetries

Basic symmetries we require from the model:

- quadratic in densities
- time reversal invariant
- space-inversion invariant
- invariant with respect to rotations in space
- invariant with respect to rotations in iso-space

Additional symmetries we have investigated:

- Galilean invariance
- Local gauge invariance
- Pseudopotential

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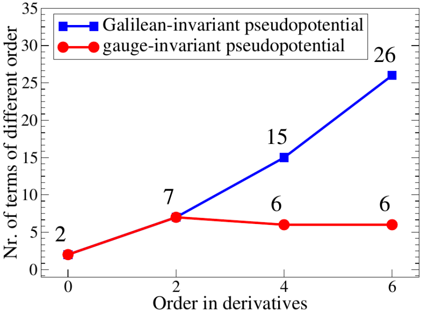
Number of coupling constants

- 2th order results corresponds to Skyrme's standard interaction
- 4th order results contains Skyrme's suggested additional D-wave term (Skyrme 1959)
- Psudopotential symmetry reduces the number of C's by a factor of 2



B.G. Carlsson, J. Dobaczewski, M. Kortelainen, Phys.Rev.C78:044326, (2008)

F. Raimondi, B. G. Carlsson, J. Dobaczewski, Phys.Rev.C83:054311, (2011)

How can this be used ?

- Better long-range properties
- Better spectroscopic properties

Two routes to finding the coupling constants:

- Fit C's to observables
- Derive C's from an interaction (e.g. DME)

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Computer code for the new functionals

- The program HOSPHE (v1.00)

Solves HF equations for spherical symmetry

B.G. Carlsson, J. Dobaczewski, J. Toivanen, P. Vesely,
Comp. Phys. Commun. 181, 1641 (2010)

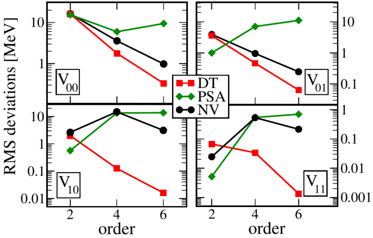
- The program HOSPHE (v2.00)

Additions: HFB, iterative-QRPA, iterative-pnQRPA ,
Lipkin-Nogami, Broyden method, Finite range forces, etc ..

B.G. Carlsson, J. Toivanen, J. Dobaczewski, P. Vesely, Y. Gao and D. Ward
manuscript in preparation

Some first results

Gogny force in DME expansion



B.G. Carlsson and J. Dobaczewski Phys.Rev.Lett.105:122501,(2010)

Developments:

- Nuclear matter equations
- Landau parameters (D. Davesne et. al.)

Preliminary full fits to data indicate:

- Improvements to fitted observables (masses,radii, sp-energies)
- Bad extrapolation properties

Lots of data and few parameters needed to make the fits work

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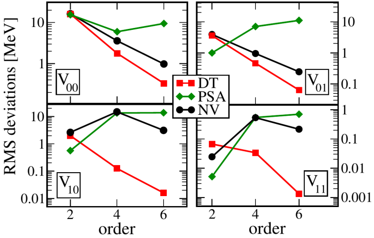

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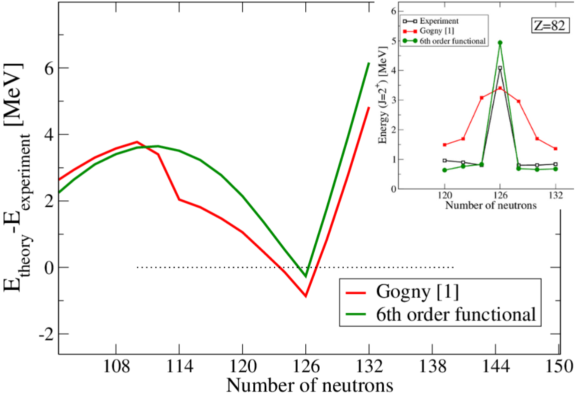
Calculations with many derivatives

Do higher-order terms make the model unstable ?



[1] J.P. Delaroche, Phys.Rev.C81:014303,(2010)

Higher order terms does not cause convergence problems.

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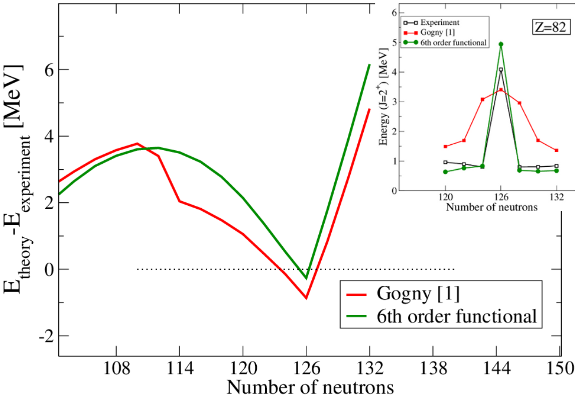

[1] J.P. Delaroche, Phys.Rev.C81:014303,(2010)

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Summary

- The description of some observables seem to require treating correlations beyond HFB
- Rigorous treatments remains a challenge
- Generalized functionals may improve accuracy but can be tricky to fit

Thank you for your attention!