

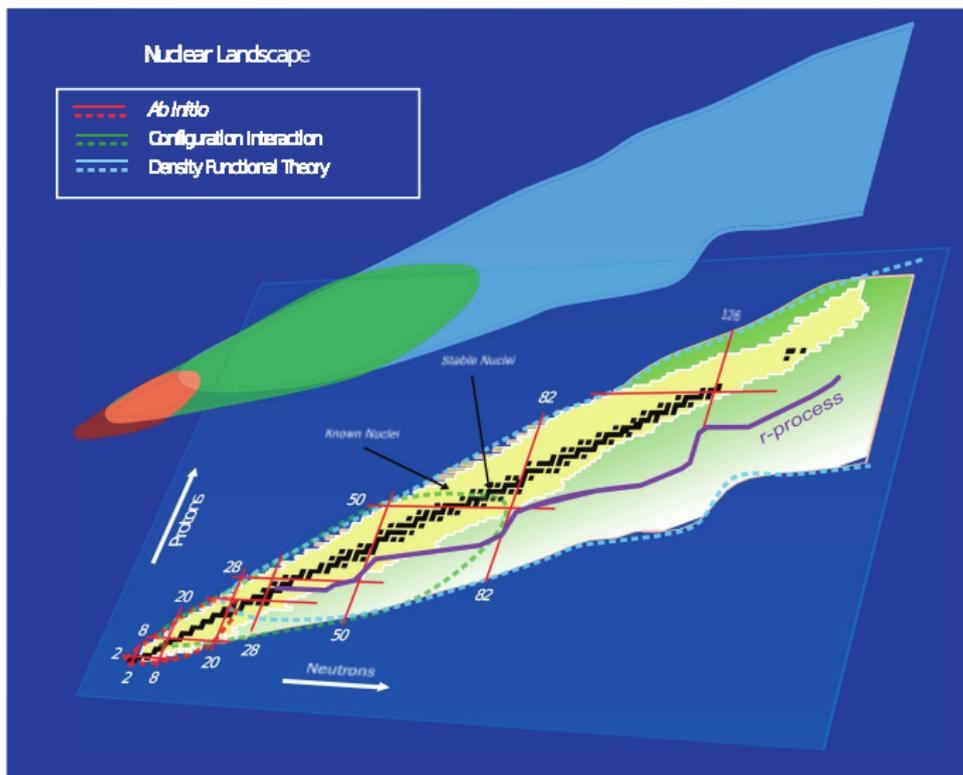
Two ideas for nuclear DFT (and friends)

Thomas Lesinski

Dept. of Physics & Institute for Nuclear Theory
University of Washington, Seattle

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“The Extreme Matter Physics of Nuclei: From Universal Properties to
Neutron-Rich Extremes”

Nuclear structure: methods



Outline

- 1 Separable approximations of few-nucleon forces
 - Introduction
 - $V_{\text{low } k}$, NN, particle-hole channel
 - Chiral V_{3N} at N3LO, particle-hole channel
- 2 DFT with configuration mixing
 - Hohenberg-Kohn scheme
 - Form of the functional
- 3 Summary

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Separable V_{NN}

■ Principle

$$v_{ijkl} = \sum_a \lambda_a g_{ij}^{a*} g_{kl}^a = \sum_a \lambda'_a g_{ik}^{/a} g_{jl}^{/a}$$

■ If $\lambda_a \ll \lambda_1$ for $a > n$: truncate

■ HF: $\Gamma_{ij} = \sum_a g_{ij}^{/a} \lambda'_a \check{\rho}_a$, with $\check{\rho}_a = \sum_{ij} g_{ij}^{/a} \rho_{ij}$

■ HFB: $\Delta_{ij} = \sum_a g_{ij}^a \lambda_a \check{\kappa}_a$, with $\check{\kappa}_a = \sum_{ij} g_{ij}^a \kappa_{ij}$

■ Cost $\mathcal{O}(nN)$ down from $\mathcal{O}(N^2) = \mathcal{O}(n_o^4)$

■ The story so far

■ K. Hebeler, T. Duguet, TL, A. Schwenk,
Phys. Rev. C 80 044321 (2009)

■ Y. Tian, Z. Ma, P. Ring Phys. Rev. C 79 064301 (2009)

■ T. Nikšić, P. Ring, D. Vretenar, Yuan Tian and Zhong-yu Ma,
Phys. Rev. C 81, 054318 (2010)

■ L. M. Robledo, Phys. Rev. C 81, 044312 (2010)

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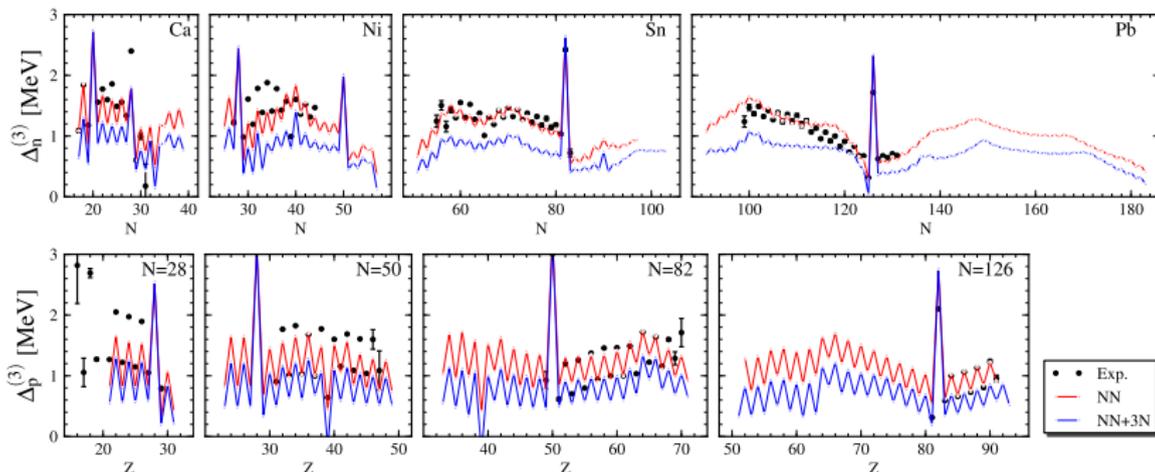
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J. Phys. G 39 015108 (2012)

Separable V_{NN} : pairing systematics



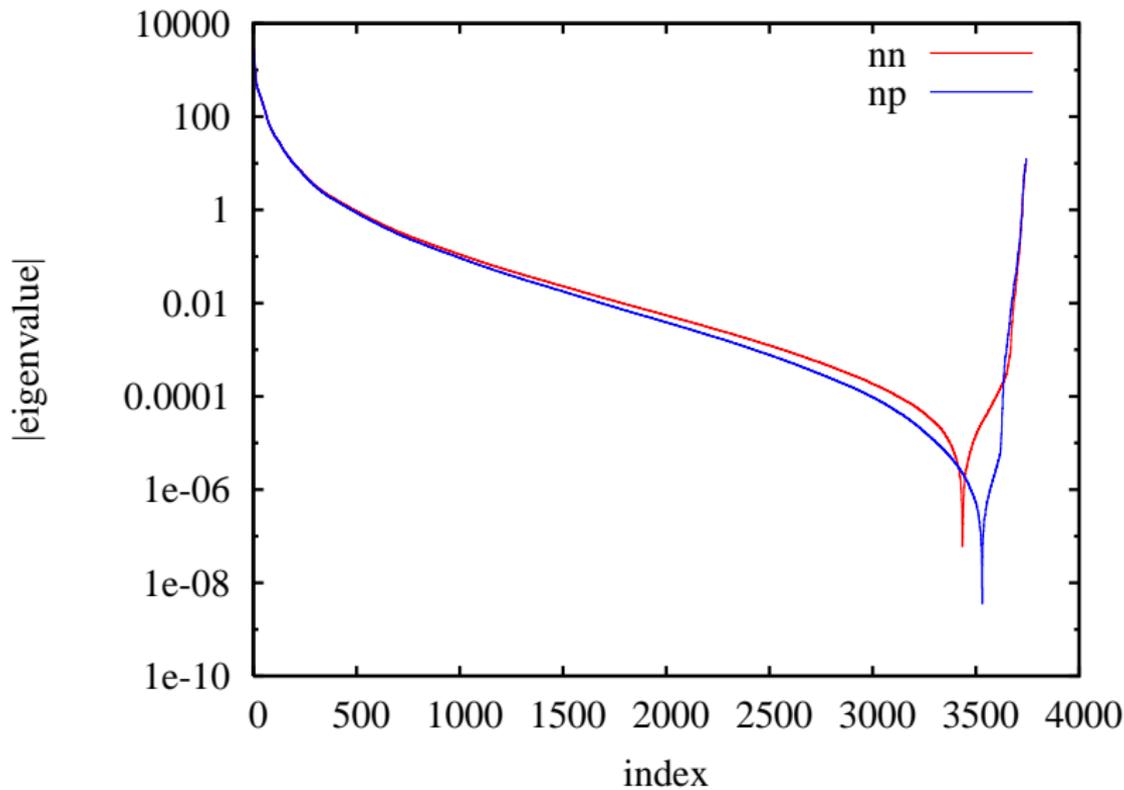
TL, K Hebeler, T Duguet and A Schwenk,
 J. Phys. G 39 015108 (2012)

$V_{\text{low } k}$, NN, ($\Lambda = 2.0 \text{ fm}^{-1}$) particle-hole channel

- Basis: spherical Bessel, $R_{\text{box}} = 18 \text{ fm}$, $k_{\text{cut}} = 2.5 \text{ fm}^{-1}$, $l_{\text{cut}} = 20$
- $N = 3744$ for $J^\pi = 0^+$
- Obtain ph-separable form

$$\begin{aligned} & \langle n_1 l_1 j_1 (n'_1 l'_1 j'_1)^{-1} | \bar{V}_{\text{NN}, T_z} | (n_2 l_2 j_2)^{-1} n'_2 l'_2 j'_2 \rangle^{(J)} \\ &= \sum_a \lambda_a^{JT_z} g_{(n_1 l_1 j_1, n'_1 l'_1 j'_1)}^{JT_z, a} g_{(n_2 l_2 j_2, n'_2 l'_2 j'_2)}^{JT_z, a} \end{aligned}$$

- Eigenvalue decomposition: ScaLAPACK PDSYEV

$V_{\text{low } k}$, NN, particle-hole channel

V_{3N} ?

- Can we use a similar technique for 3N forces ?

Higher-Order Singular Value Decomposition (HOSVD)

- L. De Lathauwer, B. De Moor and J. Vandewalle, SIAM J. Matrix Anal. Appl. 21, 1253 (2000)
- For a symmetric rank-3 tensor: $T_{pqr} = \sum_{stu} S_{stu} U_{sp} U_{tq} U_{ur}$ with
 - U an orthogonal (unitary) matrix
 - All-orthogonality: $\sum_{rs} S_{prs}^* S_{qrs} = \sigma_p^2 \delta_{pq}$
 - Ordering: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N$

- ph and pp factorizations: HF scaling $\mathcal{O}(N^3) = \mathcal{O}(n_o^6) \rightarrow \mathcal{O}(n^3) + \mathcal{O}(nN)$

$$v_{ijklmn}^{(3)} = \sum_{abc} \lambda_{abc} g_{ij}^{a*} g_{lm}^b g_{kn}^{c'} = \sum_{abc} \lambda'_{abc} g_{il}^{a'} g_{jm}^{b'} g_{kn}^{c'}$$

- ① Define $A_{pI} = T_{pqr}$, with $I = (q, r)$ and SVD $A_{pI} = \sum_s U_{ps} \sigma_s V_{Is}^*$

- ② Core tensor:

- Use $S_{pqr} = \sum_{stu} U_{ps}^* U_{qt}^* U_{ru}^* T_{stu}$, cost $\mathcal{O}(N^5)$
- Invert $\sum_{stu} U_{sp} U_{tq} U_{ur} S_{stu} = T_{pqr}$, cost $\mathcal{O}(n^9)$

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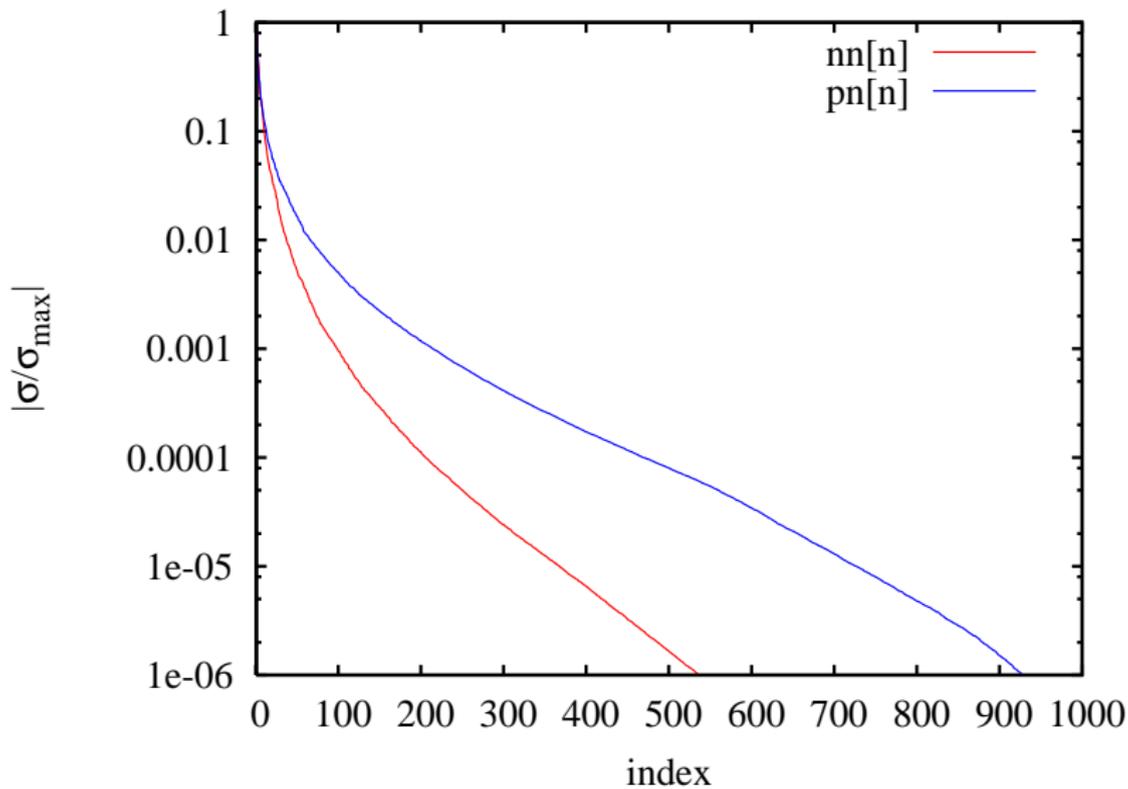
V_{3N} ?

- Define $A_{pI} = T_{pqr}$, with $I = (q, r)$ and SVD $A_{pI} = \sum_s U_{ps} \sigma_s V_{Is}$
- Use EVD of $\sum_I A_{pI} A_{qI}^* = \sum_s U_{ps} \sigma_s^2 U_{qs}^*$
- Choose convenient representation

$$\sum_I A_{pI} A_{qI}^* = \sum_{IJK} A_{pI} W_{JI}^* W_{JK} A_{qK}^*$$

$$\langle \vec{k}_1 \sigma_1 \vec{k}_2 \sigma_2 (\vec{k}'_1 \sigma'_1)^{-1} (\vec{k}'_2 \sigma'_2)^{-1} | V_{3N} | (l_3 j_3 n_3)^{-1} l'_3 j'_3 n'_3 \rangle^{(J)}$$

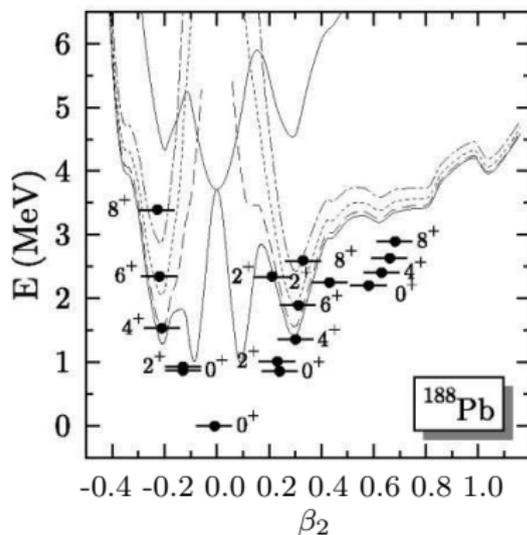
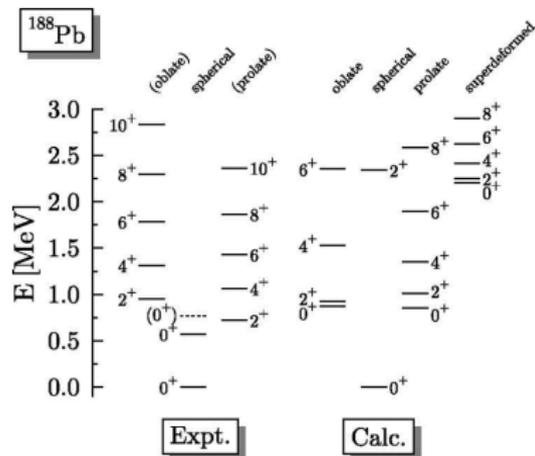
- Basis: spherical Bessel, $R_{\text{box}} = 15 \text{ fm}$, $k_{\text{cut}} = 2.5 \text{ fm}^{-1}$, $l_{\text{cut}} = 12$
 - $N = 1909$ for $J^\pi = 0^+$
- V_{3N} chiral N2LO, $\Lambda_\chi = 700 \text{ MeV}$, $\Lambda_{3N} = 2.0 \text{ fm}^{-1}$
 $(c_1 = -0.76, c_3 = -4.78, c_4 = 3.96, c_D = -2.785, c_E = -0.822)$

V_{3N} (PRELIMINARY)

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MR-EDF: Capabilities



M. Bender, P. Bonche, T. Duguet, and P.-H. Heenen, PRC 69, 064303 (2004)

- Describe 188-body correlations
- + Fission, reactions, neutron star crusts, etc., etc...

DFT for nuclei: (0) Hohenberg-Kohn-Sham scheme

- Consider a system with Hamiltonian $H = T + U + V$

$$F[V] = \min_{\Psi} \langle \Psi | T + U + V | \Psi \rangle$$

- Legendre transform with $\rho = \partial E / \partial V$

$$\begin{aligned} E[\rho] &= \min_V \left[F[V] - \int d^3\vec{r} V \rho \right] \\ &= \min_{\Psi \rightarrow \rho} \langle \Psi | T + U | \Psi \rangle \end{aligned}$$

- $E[\rho]$ “universal” w.r.t choice of V
- Kohn-Sham scheme: write

$$E[\rho] = E_T[\rho] + E_H[\rho] + E_{xc}[\rho]$$

DFT for nuclei: (1) Definitions

- Consider a system of N particles with Hamiltonian $H = T + U + V$

$$\mathbf{R} = (\vec{r}_1, \dots, \vec{r}_N), \quad d^{3N} \mathbf{R} = d^3 \vec{r}_1 \dots d^3 \vec{r}_N$$

- Now consider real functions $Q_\alpha(\vec{r})$, $\alpha = 1 \dots n$, $\underline{q} = (q_1, \dots, q_n)$

$$Q_\alpha(\mathbf{R}) = \sum_i Q_\alpha(\vec{r}_i)$$

$$P(\underline{q}, \mathbf{R}) = \prod_\alpha \delta(Q_\alpha(\mathbf{R}) - q_\alpha)$$

- Define the generalized density...

$$D(\underline{q}, \vec{r}) = N \int d^{3N} \mathbf{R} \delta^{(3)}(\vec{r} - \vec{r}_1) P(\underline{q}, \mathbf{R}) \Psi^*(\mathbf{R}) \Psi(\mathbf{R})$$

- ...the collective wave function...

$$f(\underline{q}) = \eta(\underline{q}) \left[N^{-1} \int d^3 \vec{r} D(\underline{q}, \vec{r}) \right]^{1/2}$$

- ...and the \underline{q} -dependent density

$$d(\underline{q}, \vec{r}) = [f^*(\underline{q})f(\underline{q})]^{-1} D(\underline{q}, \vec{r})$$

DFT for nuclei: (2) Properties

■ Normalisation

$$\int d^n \underline{q} f^*(\underline{q}) f(\underline{q}) = 1$$

$$\int d^3 \vec{r} d(\underline{q}, \vec{r}) = N$$

$$\int d^n \underline{q} D(\underline{q}, \vec{r}) = \rho(\vec{r})$$

$$\int d^n \underline{q} \int d^3 \vec{r} D(\underline{q}, \vec{r}) = N$$

■ Verify that

$$\int d^3 \vec{r} Q_\alpha(\vec{r}) d(\underline{q}, \vec{r}) = q_\alpha$$

DFT for nuclei: (3) External potential

- \underline{q} -dependent wave function (“slice”)

$$\Psi(\underline{q}, \mathbf{R}) = f^{-1}(\underline{q}) P(\underline{q}, \mathbf{R}) \Psi(\mathbf{R})$$

$$\int d^{3N} \mathbf{R} \Psi^*(\underline{q}, \mathbf{R}) \Psi(\underline{q}', \mathbf{R}) = \delta^{(n)}(\underline{q} - \underline{q}')$$

- Let $w(\underline{q}, \vec{r})$ be a real function and

$$w(\underline{q}, \mathbf{R}) = \sum_i w(\underline{q}, \vec{r}_i) \quad W(\mathbf{R}) = \int d^n \underline{q} w(\underline{q}, \mathbf{R}) P(\underline{q}, \mathbf{R})$$

- We have

$$\langle \Psi | W | \Psi \rangle = \int d^n \underline{q} \int d^3 \vec{r} w(\underline{q}, \vec{r}) D(\underline{q}, \vec{r})$$

DFT for nuclei: (4) Energy functional

- Define the functional

$$F[w] = \min_{\Psi} \langle \Psi | T + U + W | \Psi \rangle$$

- then

$$\begin{aligned} E[D] &= \min_w \left[F[w] - \int d^n \underline{q} \int d^3 \vec{r} w(\underline{q}, \vec{r}) D(\underline{q}, \vec{r}) \right] \\ &= \min_{\Psi \rightarrow D} \langle \Psi | T + U | \Psi \rangle \end{aligned}$$

- f and d can be recovered from D (see (1))

$$E[D] = E[f, d]$$

- Universality: V is a special case of W ($w(\underline{q}, \vec{r}) = v(\vec{r})$)

DFT for nuclei: (5) Form of the functional

- Assume local U

$$E[f, d] = \int d^n \underline{q} f^*(\underline{q}) \left[\sum_{\alpha\beta} \partial_\alpha \mathcal{B}_{\alpha\beta}(\underline{q}) \partial_\beta + \mathcal{U}(\underline{q}) \right] f(\underline{q})$$

$$\mathcal{B}_{\alpha\beta}(\underline{q}) = -\frac{1}{\langle \Psi | \delta^{(n)}(\underline{q} - \underline{q}') | \Psi \rangle} \\ \times \int d^{3N} \mathbf{R} P(\underline{q}, \mathbf{R}) \Psi^*(\mathbf{R}) \nabla Q_\alpha(\mathbf{R}) \circ \nabla Q_\beta(\mathbf{R}) \Psi(\mathbf{R})$$

$$\mathcal{U}(\underline{q}) = \frac{1}{\langle \Psi | \delta^{(n)}(\underline{q} - \underline{q}') | \Psi \rangle} \\ \times \int d^{3N} \mathbf{R} P(\underline{q}, \mathbf{R}) \left[-\Psi^*(\mathbf{R}) \Delta \Psi(\mathbf{R}) + \Psi^*(\mathbf{R}) U(\mathbf{R}) \Psi(\mathbf{R}) \right]$$

- E.g. $(Q_\alpha(\vec{r}))$ isomorphic to $(\beta, \gamma, \alpha_1, \alpha_2, \alpha_3)$: Bohr Hamiltonian

DFT for nuclei: (6) Form cont'd

- Assume...
 - f given by symmetry
 - $d(\underline{q}, \vec{r})$ and $d(\underline{q}', \vec{r})$ related by sym. transformation
- ... then $E[f, d] = E[\rho_{\text{int}}]$, with $\rho_{\text{int}}(\vec{r}) = d(\underline{0}, \vec{r})$
 - Functional of the density of “pinned down” wf
 - $(Q_1, Q_2, Q_3)(\vec{r}) = \frac{1}{N}(x, y, z)$: CoM DFT
 - J. Messud, M. Bender, E. Suraud, Phys.Rev.C 80 054314 (2009)

- General case: introduce $\{\phi_{i,\underline{q}}(\vec{r})\}$ for each \underline{q} : \mathcal{B}, \mathcal{U} ?

- ??? Pairing ???
 - D. Lacroix, G. Hupin, arXiv:1005.0300
 - G. Hupin, D. Lacroix, M. Bender, Phys.Rev.C 84 014309 (2011)

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Summary and outlook

- Separable approximations to V_{NN} and V_{3N} may offer significant speedup
 - ➔ Use them more !
 - TODO: multipoles, HFB, axial, publish codes+data, OEP

- We can write a **DFT** allowing for symmetry breaking and configuration mixing
 - ➔ May be simpler than ad-hoc formulation...