Recent progress in nuclear DFT

Nobuo Hinohara

Center for Computational Sciences
University of Tsukuba

筑波大学 University of Tsukuba

Dec. 7, 2022

YITP workshop “Fundamentals in density functional theory (DFT2022)

Contents

- Introduction to nuclear EDF
- DFT and symmetry breaking
  - pairing
  - time reversal symmetry
  - proton-neutron symmetry
- References:
  - Bender et al., Rev. Mod. Phys. **75**, 121(2003)
  - Perlinska et al., Phys. Rev. C **69**, 014316 (2004)

DFT approach to nuclear structure physics

atomic nucleus

- two kinds of constituent particles: neutrons and protons
- Coulomb interaction and strong interaction
- self-bound system (no external field)

Coulomb EDF

- Direct and exchange terms

$$E_{\text{dir}} = \frac{e^2}{2}\int d\boldsymbol{r}d\boldsymbol{r}'\frac{\rho_{\text{ch}}(\boldsymbol{r})\rho_{\text{ch}}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

- Slater approximation to exchange term (homogenous Fermi gas)

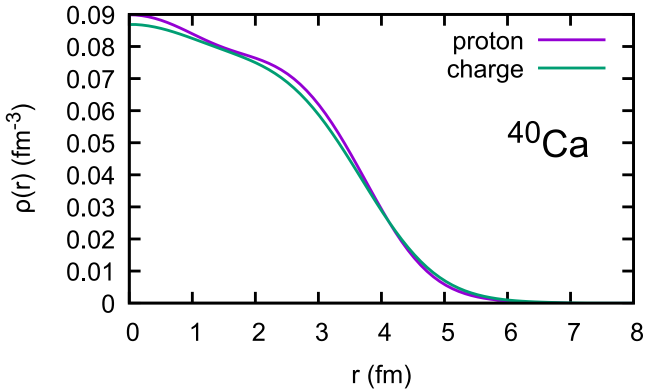
$$E_{\text{ex}} = -\frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\int d\boldsymbol{r}\rho_{\text{ch}}^{\frac{4}{3}}(\boldsymbol{r})$$

Generalized gradient approx. Naito et al., Phys. Rev. C **99**, 024309 (2019)

- Coulomb is basically considered for point proton density

$$\rho_{\text{ch}}(\boldsymbol{r}) \approx \rho_p(\boldsymbol{r})$$

neutron charge distribution/spin-orbit contribution
Friar and Negele, Adv. Nucl. Phys. **8**, 219 (1975)



SLy4, Coulomb calculated with proton density

Strong interaction

- origin: interaction between quarks in QCD

- realistic NN interaction:
  - spin and isospin dependence
  - large repulsive core
  - central/tensor/spin-orbit forces

- three-body force: necessary to obtain saturation

nuclear effective interaction

- spin and isospin dependence
- effective theory for low-energy/in-medium nuclear physics
- three-body force included as density-dependent two-body force
- local (delta function) type and non-local (gaussian) type

Skyrme effective interaction

zero-range (delta function), up to second order in relative momenta

Skyrme, Nucl. Phys. **9**, 615 (1959)
Vautherin and Brink Phys. Rev. C **5**, 626 (1972)

s: spin $\pm 1/2$
t: isospin $\pm 1/2$

$$\hat{V}(\boldsymbol{r}_1' s_1' t_1' \boldsymbol{r}_2' s_2' t_2', \boldsymbol{r}_1 s_1 t_1 \boldsymbol{r}_2 s_2 t_2)$$
$$= \Big\{ t_0(\hat{\delta}^\sigma + x_0 \hat{P}^\sigma) + \frac{1}{6} t_3 (\hat{\delta}^\sigma + x_3 \hat{P}^\sigma) \rho_0^\alpha \left[\frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2) \right]$$

density-dependent term

$$+ \frac{1}{2} t_1 (\hat{\delta}^\sigma + x_1 \hat{P}^\sigma)[\hat{\boldsymbol{k}}'^2 + \hat{\boldsymbol{k}}^2]$$
$$+ \frac{1}{2} t_e [\hat{\boldsymbol{k}}'^* \cdot \hat{\mathrm{S}} \cdot \hat{\boldsymbol{k}}'^* + \hat{\boldsymbol{k}} \cdot \hat{\mathrm{S}} \cdot \hat{\boldsymbol{k}}]$$
$$+ t_2 (\hat{\delta}^\sigma + x_2 \hat{P}^\sigma) \hat{\boldsymbol{k}}'^* \cdot \hat{\boldsymbol{k}} + t_o \hat{\boldsymbol{k}}'^* \cdot \hat{\mathrm{S}} \cdot \hat{\boldsymbol{k}}$$

tensor term

$$+ i W_0 \hat{\boldsymbol{S}} \cdot [\hat{\boldsymbol{k}}'^* \times \hat{\boldsymbol{k}}] \Big\} (\hat{\delta}^\sigma \hat{\delta}^\tau - \hat{P}^\sigma \hat{P}^\tau P^M) \hat{\delta}_{12},$$

spin-orbit term

$$\hat{\boldsymbol{k}} = \frac{1}{2i}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)$$
$$\hat{\boldsymbol{k}}' = \frac{1}{2i}(\boldsymbol{\nabla}_1' - \boldsymbol{\nabla}_2')$$

$$\hat{\mathrm{S}}^{ab}_{s_1' s_2' s_1 s_2} = \frac{3}{2}(\hat{\boldsymbol{\sigma}}^a_{s_1' s_1} \hat{\boldsymbol{\sigma}}^b_{s_2' s_2} + \hat{\boldsymbol{\sigma}}^b_{s_1' s_1} \hat{\boldsymbol{\sigma}}^a_{s_2' s_2}) - \delta_{ab} \hat{\boldsymbol{\sigma}}_{s_1' s_1} \cdot \hat{\boldsymbol{\sigma}}_{s_2' s_2}$$
$$\hat{P}^\sigma_{s_1' s_2' s_1 s_2} = \frac{1}{2}(\hat{\delta}^\sigma_{s_1' s_2' s_1 s_2} + \hat{\boldsymbol{\sigma}}_{s_1' s_1} \cdot \hat{\boldsymbol{\sigma}}_{s_2' s_2}) = \delta_{s_1' s_2} \delta_{s_2' s_1}$$
$$\hat{\delta}_{12}(\boldsymbol{r}_1' \boldsymbol{r}_2', \boldsymbol{r}_1 \boldsymbol{r}_2) = \delta(\boldsymbol{r}_1' - \boldsymbol{r}_1) \delta(\boldsymbol{r}_2' - \boldsymbol{r}_2) \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$$

Gogny effective interaction

Decharge and Gogny, Phys. Rev. C **21**, 1568 (1980)

finite-range force + density-dependent term and spin-orbit

$$\hat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{i=1,2} e^{-(\boldsymbol{r}_1-\boldsymbol{r}_2)^2/\mu_i^2} \left(W_i + B_i\hat{P}_\sigma - H_i\hat{P}_\tau - M_i\hat{P}_\sigma\hat{P}_\tau\right)$$
$$+ t_0\left(1 + x_0\hat{P}_\sigma\right)\rho^\alpha\left(\tfrac{\boldsymbol{r}_1+\boldsymbol{r}_2}{2}\right)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$+ iW_{LS}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\overleftarrow{\nabla}_1-\overleftarrow{\nabla}_2)\times\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\overrightarrow{\nabla}_1-\overrightarrow{\nabla}_2),$$

density-dependent term

spin-orbit term

$$\hat{P}^\sigma_{s_1's_2's_1s_2} = \frac{1}{2}(\hat{\delta}^\sigma_{s_1's_2's_1s_2} + \hat{\boldsymbol{\sigma}}_{s_1's_1}\cdot\hat{\boldsymbol{\sigma}}_{s_2's_2}) = \delta_{s_1's_2}\delta_{s_2's_1}$$

Nuclear DFT

- non-relativistic ones: local (Skyrme-type) and non-local (Gogny-type)
- relativistic ones

expressions based on Perlinska et al., Phys. Rev. C **69**, 014316 (2004)

density matrix $$\hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'s't') = \langle\Psi|a^{+}_{\boldsymbol{r}'s't'}a_{\boldsymbol{r}st}|\Psi\rangle$$

non-local density $$\rho_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{stt'}\hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'st')\hat{\tau}^{k}_{t't}$$ $$\hat{\tau}^{0}_{t't} = \delta_{t't}$$

k=1-3 Pauli matrix

local density $$\rho_k(\boldsymbol{r}) = \rho_k(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$

isoscalar $$\rho_0(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) + \rho_p(\boldsymbol{r})$$ $$\rho_n(\boldsymbol{r}) = \langle\Psi|a^{+}_{n}(\boldsymbol{r})a_n(\boldsymbol{r})|\Psi\rangle$$

isovector $$\rho_3(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) - \rho_p(\boldsymbol{r})$$ $$\rho_p(\boldsymbol{r}) = \langle\Psi|a^{+}_{p}(\boldsymbol{r})a_p(\boldsymbol{r})|\Psi\rangle$$

Nuclear EDF

- EDF derived from the effective interaction (Skyrme, Gogny)
  - Skyrme: SLy4, SkM*, SkO', SAMi, ...
  - Gogny: D1S, D1M, ...
  - note: effective interaction is fitted to reproduce experimental data

- EDF whose coupling constants are adjusted to reproduce experimental data
  - no direct connection with effective interaction
    but EDF form is often taken from effective interaction
  - more degrees of freedom within the framework of DFT
  - Several local EDFs available
  - non-local EDF: Raimondi et al., J. Phys. G **41**, 055112 (2014)

Skyrme-type EDF

- Skyrme force: zero range, depends up to second order in relative momenta
- corresponding EDF: functional of local densities, with up to two derivatives

Under time-reversal symmetry we have three local densities

particle density

$$\rho_k(\boldsymbol{r}) = \rho_k(\boldsymbol{r}, \boldsymbol{r}')_{\boldsymbol{r}=\boldsymbol{r}'}$$

kinetic density

$$\tau_k(\boldsymbol{r}) = [(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}')\rho_k(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$$

spin-current density

$$\mathsf{J}_k(\boldsymbol{r}) = \frac{1}{2i}[(\boldsymbol{\nabla} - \boldsymbol{\nabla}') \otimes \boldsymbol{s}_k(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$\boldsymbol{s}_k(\boldsymbol{r}, \boldsymbol{r}') = \sum_{ss'tt'} \hat{\rho}(\boldsymbol{r}st, \boldsymbol{r}'s't')\hat{\boldsymbol{\sigma}}_{s's}\hat{\tau}^k_{t't}$$

isoscalar EDF

density-dependent term

$$\chi_0(\boldsymbol{r}) = C_0^{\rho}[\rho_0]\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^{\tau}\rho_0\tau_0 + C_0^{J0}J_0^2 + C_0^{J1}\boldsymbol{J}_0^2 + C_0^{J2}\underline{\mathsf{J}}_0^2 + C_0^{\nabla J}\rho_0\boldsymbol{\nabla}\cdot\boldsymbol{J}_0$$

isovector EDF

tensor term

spin-orbit term

$$\chi_1(\boldsymbol{r}) = C_1^{\rho}\rho_3^2 + C_1^{\Delta\rho}\rho_3\Delta\rho_3 + C_1^{\tau}\rho_3\tau_3 + C_1^{J0}J_3^2 + C_1^{J1}\boldsymbol{J}_3^2 + C_1^{J2}\underline{\mathsf{J}}_3^2 + C_1^{\nabla J}\rho_3\boldsymbol{\nabla}\cdot\boldsymbol{J}_3$$

Local and non-local EDF

Bender et al. Rev. Mod. Phys. **75**, 121 (2003)

Non-local EDF

$$E_{\mathrm{dir}}=\frac{1}{2}\int\int d^3r d^3r' \rho(\mathbf{r},\mathbf{r})v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\mathbf{r}'),$$

$$E_{\mathrm{ex}}=\frac{1}{2}\int\int d^3r d^3r' \rho(\mathbf{r},\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}',\mathbf{r}).$$

exchange term

$$\rho\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\right)\approx\rho(\boldsymbol{R})+i\boldsymbol{r}_{\mathrm{rel}}\cdot\boldsymbol{j}(\boldsymbol{R})+\frac{1}{2}\boldsymbol{r}_{\mathrm{rel}}^2\left[\tau(\boldsymbol{R})-\frac{1}{4}\Delta\rho(\boldsymbol{R})\right]$$

local exchange functional

$$\left|\rho\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\right)\right|^2\approx\rho^2(\boldsymbol{R})-\boldsymbol{r}_{\mathrm{rel}}^2\left[\rho(\boldsymbol{R})\tau(\boldsymbol{R})-\boldsymbol{j}^2(\boldsymbol{R})-\frac{1}{4}\rho(\boldsymbol{R})\Delta\rho(\boldsymbol{R})\right]$$

direct term

$$\rho\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2},\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\right)\approx\rho(\boldsymbol{R})+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\cdot\boldsymbol{\nabla}\rho(\boldsymbol{R})+\frac{\boldsymbol{r}_{\mathrm{rel}}^2}{8}\Delta\rho(\boldsymbol{R})$$

$$\left|\rho\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2},\boldsymbol{R}+\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\right)\rho\left(\boldsymbol{R}-\frac{\boldsymbol{r}_{\mathrm{rel}}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\mathrm{rel}}}{2}\right)\right|\approx\rho^2(\boldsymbol{R})+\frac{1}{4}[\boldsymbol{r}_{\mathrm{rel}}\cdot\boldsymbol{\nabla}\rho(\boldsymbol{R})]^2+\frac{1}{4}\boldsymbol{r}_{\mathrm{rel}}^2\rho(\boldsymbol{R})\Delta\rho(\boldsymbol{R})$$

DFT and symmetry breaking

- spontaneous symmetry breaking (in the absence of the external field)
  - efficient way to include correlations within mean-field framework
  - consistency with DFT ?
- symmetry breaking introduces new densities in DFT

- often broken symmetries:
  - (isospin symmetry): explicitly broken by Coulomb
  - rotational symmetry (deformation of the local density)
    - within axial symmetry(most of the ground states) / triaxial
  - gauge symmetry (particle number violation due to pairing) (new densities and terms in EDF)
  - parity symmetry
  - time-reversal symmetry (new densities and terms in EDF)
  - proton-neutron symmetry(pn-mixing) (new densities and terms in EDF)

Pairing

like-particle pairing: correlation between two fermions

two-particle wave function: (space) * (spin) * (isospin)

symmetric | antisymmetric (singlet) | symmetric (triplet)

pair density matrix

$$\hat{\tilde{\rho}}(\boldsymbol{r}st, \boldsymbol{r}'s't') = -2s'\langle\Psi|a_{\boldsymbol{r}'-s't'}a_{\boldsymbol{r}st}|\Psi\rangle$$

non-local pair density

$$\tilde{\rho}_t(\boldsymbol{r}, \boldsymbol{r}') = \sum_s \hat{\tilde{\rho}}(\boldsymbol{r}st, \boldsymbol{r}'st)$$

local pair density

$$\tilde{\rho}_t(\boldsymbol{r}) = \tilde{\rho}_t(\boldsymbol{r}, \boldsymbol{r})$$

pair EDF

$$\tilde{\chi}_t(\boldsymbol{r}) = \tilde{C}_t^{\rho}[\rho_0]|\tilde{\rho}_t(\boldsymbol{r})|^2 = \frac{V_t}{4}\left[1 - \eta\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right]|\tilde{\rho}_t(\boldsymbol{r})|^2$$

EDF optimization

SVmin $$E = \int d^3r \, \{\mathcal{E}_{\rm kin} + \mathcal{E}_{\rm Skyrme}\} + E_{\rm Coulomb} + E_{\rm pair} + E_{\rm cm}$$

Klupfel et al., Phys. Rev. C **79**, 034310 (2007)

$$\mathcal{E}_{\rm kin} = \frac{\hbar^2}{2m_{\rm p}}\tau_{\rm p} + \frac{\hbar^2}{2m_{\rm n}}\tau_{\rm n}$$

$$\begin{aligned}\mathcal{E}_{\rm Skyrme} = &\frac{B_0 + B_3\rho^\alpha}{2}\rho^2 - \frac{B_0' + B_3'\rho^\alpha}{2}\tilde{\rho}^2 + B_1(\rho\tau - \mathbf{j}^2)\\ &- B_1'(\tilde{\rho}\tilde{\tau} - \tilde{\mathbf{j}}^2) - \frac{B_2}{2}\rho\Delta\rho + \frac{B_2'}{2}\tilde{\rho}\Delta\tilde{\rho}\\ &-\frac{1}{2}B_4\,[\rho\nabla\cdot\mathbf{J} + \boldsymbol{\sigma}\cdot(\nabla\times\mathbf{j})]\\ &-\frac{1}{2}(B_4 + b_4')\,[\tilde{\rho}\nabla\cdot\tilde{\mathbf{J}} + \tilde{\boldsymbol{\sigma}}\cdot(\nabla\times\tilde{\mathbf{j}})]\\ &+\frac{C_1}{2}(\mathbf{J}^2 - \boldsymbol{\sigma}\cdot\boldsymbol{\tau}) - \frac{C_1'}{2}(\tilde{\mathbf{J}}^2 - \tilde{\boldsymbol{\sigma}}\cdot\tilde{\boldsymbol{\tau}}), \qquad (3c)\end{aligned}$$

$$\begin{aligned}E_{\rm Coulomb} = &\, e^2\frac{1}{2}\int d^3r\,d^3r'\frac{\rho_{\rm p}(\mathbf{r})\rho_{\rm p}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\\ &-\frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\int d^3r[\rho_{\rm p}]^{4/3},\end{aligned}$$

$$E_{\rm pair} = \frac{1}{4}\sum_q v_{0,q}\int d^3r\,\xi_q^2\left[1 - \frac{\rho}{\rho_{\rm pair}}\right],$$

$$E_{\rm cm} = -\frac{1}{2mA}\langle(\hat{P}_{\rm cm})^2\rangle, \quad \hat{P}_{\rm cm} = \sum_i \hat{p}_i.$$

experimental data set to fit

- 64 binding energies
- 28 diffraction radius
- 26 surface thickness
- 50 rms radius
- 19 proton odd-even staggering values
- 16 neutron odd-even staggering values
- 7 single-particle level splittings

fitted parameters: t and x

EDF optimization

UNEDF project

Kortelainen et al., Phys. Rev. C **89**, 054314 (2014)

$$E[\rho,\tilde{\rho}] = \int d^3\boldsymbol{r}[\mathcal{E}_{\rm Kin}(\boldsymbol{r}) + \chi_0(\boldsymbol{r}) + \chi_1(\boldsymbol{r}) + \tilde{\chi}(\boldsymbol{r}) + \mathcal{E}_{\rm Coul}(\boldsymbol{r})]$$

$$\chi_t(\boldsymbol{r}) = C_t^{\rho\rho}\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{JJ}\sum_{\mu\nu} J_{\mu\nu,t}J_{\mu\nu,t} + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t$$

$$C_t^{\rho\rho} = C_{t0}^{\rho\rho} + C_{t\rm D}^{\rho\rho}\rho_0^\gamma$$

$$\tilde{\chi}(\boldsymbol{r}) = \frac{1}{4}\sum_{q=n,p} V_0^q\left[1 - \frac{1}{2}\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right]\tilde{\rho}^2(\boldsymbol{r})$$

experimental data set to fit

- 47 deformed binding energies
- 29 spherical binding energies
- 28 proton point radii
- 13 odd-even staggering values
- 4 fission isomer excitation energies
- 9 single-particle level splittings

RMS deviation in energy ~ 2 MeV

TABLE IV. Comparison of parameter values for SLy4 and all three functionals UNEDF0, UNEDF1, and UNEDF2.

x	SLy4	UNEDF0	UNEDF1	UNEDF2
ρ_c	0.16000	0.16053	0.15871	0.15631
E/A	−15.972	−16.056	−15.8	−15.8
K	229.901	230.0	220.0	239.930
$a_{\rm sym}$	32.004	30.543	28.987	29.131
L	45.962	45.080	40.005	40.0
$1/M_s^*$	1.439	0.9	0.992	1.074
$C_0^{\rho\Delta\rho}$	−76.996	−55.261	−45.135	−46.831
$C_1^{\rho\Delta\rho}$	+15.657	−55.623	−145.382	−113.164
V_0^n	−258.200	−170.374	−186.065	−208.889
V_0^p	−258.200	−199.202	−206.580	−230.330
$C_0^{\rho\nabla J}$	−92.250	−79.531	−74.026	−64.309
$C_1^{\rho\nabla J}$	−30.750	45.630	−35.658	−38.650
C_0^{JJ}	0.000	0.000	0.000	−54.433
C_1^{JJ}	0.000	0.000	0.000	−65.903

Momentum-dependence in pairing EDF

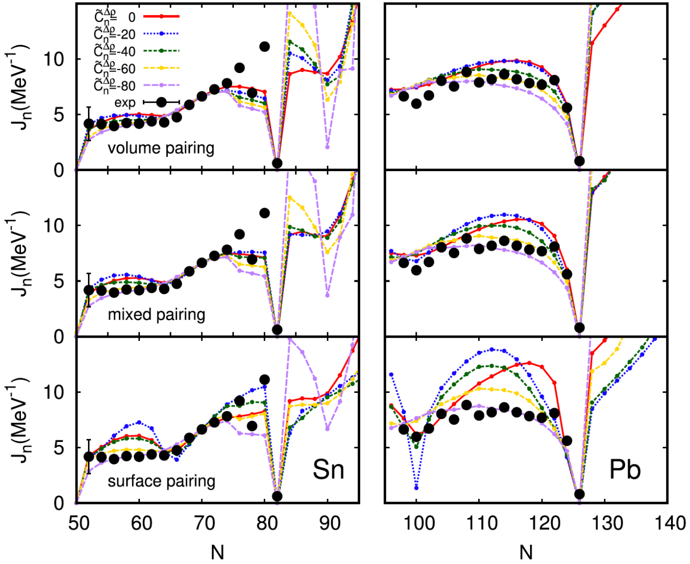
- Pairing EDF based on delta interaction: energy cutoff required
- Coupling constant is usually readjusted to the experimental data (OES/pairing gap)
- standard pairing EDF includes only the first term with density dependent coupling constant

$$\tilde{\chi}_t(\boldsymbol{r}) = \boxed{\tilde{C}_t^{\rho}[\rho_0]|\tilde{\rho}_t|^2} + \tilde{C}_t^{\Delta\rho}\mathrm{Re}(\tilde{\rho}_t^*\Delta\tilde{\rho}_t) + \tilde{C}_t^{\tau}\mathrm{Re}(\tilde{\rho}_t^*\tilde{\tau}_t) \qquad \tilde{C}_t^{\rho}[\rho_0] = \frac{V_t}{4}\left[1-\eta_t\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right]$$

kinetic pair density $\tilde{\tau}_t(\boldsymbol{r}) = [(\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}')\tilde{\rho}_t(\boldsymbol{r},\boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$

momentum dependent terms are usually not included (except SkP)

effect of momentum dependent term
on pairing rotational moment of inertia
(double binding energy difference of even-even systems)



NH, J. Phys. G **45**, 024004 (2018)

Spin-triplet pairing

NH, Oishi, Yoshida in preparation

Spin-triplet (S=1) pairing between like-particles (T=1)

two-particle wave function: (space) * (spin) * (isospin)

antisymmetric | symmetric (triplet) | symmetric (triplet)

non-local spin pair density
$$\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') = \sum_{ss'} \tilde{\rho}(\boldsymbol{r}st,\boldsymbol{r}'s't)\hat{\boldsymbol{\sigma}}_{s's}$$

$$\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') = -\tilde{\boldsymbol{s}}_t(\boldsymbol{r}',\boldsymbol{r})$$ antisymmetric in transposition of the coordinates

non-local spin-triplet pairing EDF: S1P (Oishi et al., Eur. Phys. J. A **57**, 180 (2021))

local (isovector) pair densities generated from non-local spin pair density

tensor pair density
$$\tilde{\mathsf{J}}_t(\boldsymbol{r}) = \frac{1}{2i}\left[(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\otimes\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$\begin{aligned}
\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') &= \tilde{\boldsymbol{s}}_t\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\rm rel}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\rm rel}}{2}\right)\\
&= \tilde{\boldsymbol{s}}_t(\boldsymbol{R},\boldsymbol{R}) + \boldsymbol{r}_{\rm rel}\cdot\left[\frac{\partial}{\partial\boldsymbol{r}_{\rm rel}}\otimes\boldsymbol{s}_t\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\rm rel}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\rm rel}}{2}\right)\Big|_{\boldsymbol{r}_{\rm rel}=0}\right] + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)\\
&= \frac{1}{2}\boldsymbol{r}_{\rm rel}\cdot(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\otimes\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'=\boldsymbol{R}} + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)\\
&= i\boldsymbol{r}_{\rm rel}\cdot\tilde{\mathsf{J}}_t(\boldsymbol{R}) + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)
\end{aligned}$$

Spin-triplet pair condensation

NH, Oishi, Yoshida in preparation

SLy4 + spin-singlet pairing only

spin-singlet

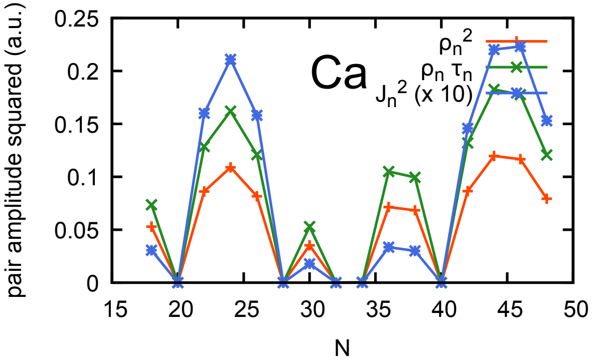
$$\int d\boldsymbol{r}|\tilde{\rho}_t(\boldsymbol{r})|^2 \qquad \int d\boldsymbol{r}\mathrm{Re}[\tilde{\rho}_t^*(\boldsymbol{r})\tilde{\tau}_t(\boldsymbol{r})]$$

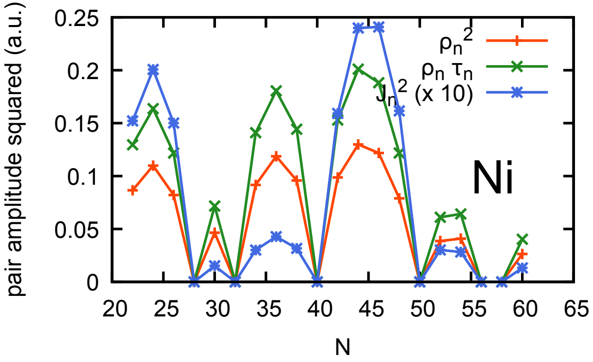
spin-triplet

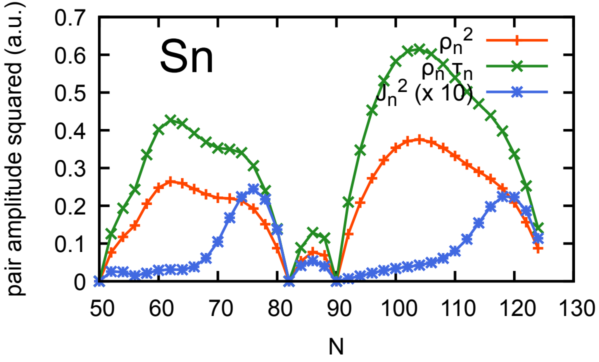
$$\int d\boldsymbol{r}|\tilde{\boldsymbol{J}}_t(\boldsymbol{r})|^2$$

non-zero component of tensor pairing under spherical symmetry

$$\tilde{\boldsymbol{J}}_{ta}(\boldsymbol{r}) = \sum_{bc} \varepsilon_{abc}\tilde{\mathrm{J}}_{tbc}(\boldsymbol{r})$$







- Spin-singlet pair EDF produces spin-triplet condensation
- Spin-triplet condensation has orbital dependence
- Relatively large at intruder orbits (20<N<28, 40<N<50, 70<N<82, 112<N<126)
- future plan: three terms in pair EDF from spin-triplet pairing $\tilde{C}_t^{J0}|\tilde{J}_t|^2 + \tilde{C}_t^{J1}|\tilde{\boldsymbol{J}}_t|^2 + \tilde{C}_t^{J2}|\underline{\tilde{\mathrm{J}}}_t|^2$

Time-odd densities

New local densities are present when time-reversal symmetry is broken

spin density $\boldsymbol{s}_k(\boldsymbol{r}) = \boldsymbol{s}_k(\boldsymbol{r}, \boldsymbol{r}')_{\boldsymbol{r}=\boldsymbol{r}'}$

current density $\boldsymbol{j}_k(\boldsymbol{r}) = \frac{1}{2i}[(\boldsymbol{\nabla} - \boldsymbol{\nabla}')\rho_k(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$

spin-kinetic density $\boldsymbol{T}_k(\boldsymbol{r}) = [(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}')\boldsymbol{s}_k(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$

tensor-kinetic density $\boldsymbol{F}_k(\boldsymbol{r}) = \frac{1}{2}[(\boldsymbol{\nabla} \otimes \boldsymbol{\nabla}' + \boldsymbol{\nabla}' \otimes \boldsymbol{\nabla}) \cdot \boldsymbol{s}_k(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}$

isoscalar EDF

$$C_0^s \boldsymbol{s}_0^2 + C_0^{\Delta s} \boldsymbol{s}_0 \cdot \Delta \boldsymbol{s}_0 + C_0^T \boldsymbol{s}_0 \cdot \boldsymbol{T}_0 + C_0^j \boldsymbol{j}_0^2 + C_0^{\nabla j} \boldsymbol{s}_0 \cdot (\boldsymbol{\nabla} \times \boldsymbol{j}_0) + C_0^{\nabla s} (\boldsymbol{\nabla} \cdot \boldsymbol{s}_0)^2 + C_0^F \boldsymbol{s}_0 \cdot \boldsymbol{F}_0$$

isovector EDF

$$C_1^s \boldsymbol{s}_3^2 + C_1^{\Delta s} \boldsymbol{s}_3 \cdot \Delta \boldsymbol{s}_3 + C_1^T \boldsymbol{s}_3 \cdot \boldsymbol{T}_3 + C_1^j \boldsymbol{j}_3^2 + C_1^{\nabla j} \boldsymbol{s}_3 \cdot (\boldsymbol{\nabla} \times \boldsymbol{j}_3) + C_1^{\nabla s} (\boldsymbol{\nabla} \cdot \boldsymbol{s}_3)^2 + C_1^F \boldsymbol{s}_3 \cdot \boldsymbol{F}_3$$

Time-reversal symmetry

Time-reversal symmetry is broken in:

- odd-mass systems
  - widely used equal-filling approximation keeps time-reversal symmetry
  - full inclusion of time-odd fields
    - Schunck et al., Phys. Rev. C **81**, 024316 (2010)
    - Kasuya and Yoshida, PTEP **2021**, 013D01
- excited states (excitation atop time-even system) / time-dependent dynamics
  - rotational bands
    - Dobaczewski and Dudek, Phys. Rev. C **52**, 1827 (1995)
    - Yoshida, Phys. Rev. C **105**, 024313 (2022)
  - vibrations: QRPA

coupling constants

- local gauge symmetry connects some time-odd couplings to the time-even couplings

$$|\Psi'\rangle = \exp\left\{ i\sum_{j=1}^{A} \phi(\boldsymbol{r}_j) \right\} |\Psi\rangle \qquad C_t^{j} = -C_t^{\tau} \qquad C_t^{J0} = -\frac{1}{3}C_t^{T} - \frac{2}{3}C_t^{F} \qquad C_t^{J1} = -\frac{1}{2}C_t^{T} + \frac{1}{4}C_t^{F} \qquad C_t^{J2} = -C_t^{T} - \frac{1}{2}C_t^{F} \qquad C_t^{\nabla j} = +C_t^{\nabla J}$$

- local spin terms (C^{s}, $C^{\Delta s}$, $C^{\nabla s}$) are not constrained by the local gauge symmetry
- time-odd part of the EDF is not yet systematically readjusted

Proton-neutron symmetry

transition to neighboring nuclei

- β decay ((N,Z) to (N-1,Z+1)), electron capture ((N,Z) to (N+1,Z-1))
- excitation to isobaric analogues states (IASs)

EDF with pn densities

$$\rho_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{stt'} \hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'st')\hat{\tau}^k_{t't} \qquad \rho_k(\boldsymbol{r}) = \rho_k(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$\rho_1(\boldsymbol{r}) = \rho_{np}(\boldsymbol{r}) + \rho_{pn}(\boldsymbol{r}) \qquad \rho_{pn}(\boldsymbol{r}) = \langle\Psi|a_n^+(\boldsymbol{r})a_p(\boldsymbol{r})|\Psi\rangle$$

$$\rho_2(\boldsymbol{r}) = -i\{\rho_{np}(\boldsymbol{r}) - \rho_{pn}(\boldsymbol{r})\} \qquad \rho_{np}(\boldsymbol{r}) = \langle\Psi|a_p^+(\boldsymbol{r})a_n(\boldsymbol{r})|\Psi\rangle$$

(time reversal symmetry cancels ρ_2)

All other ph densities (kinetic,current,spin,spin-orbit,tensor,tensor-kinetic,spin-kinetic) has same isospin structure (k=0 isoscalar, k=1-3 isovector)

Isospin-invariant EDF

isoscalar functional

$$\chi_0(\boldsymbol{r}) = C_0^\rho \rho_0^2(\boldsymbol{r})$$

isoscalar density

$$\rho_0(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) + \rho_p(\boldsymbol{r})$$

isovector functional
(conventional)

$$\chi_1(\boldsymbol{r}) = C_1^\rho \rho_3^2(\boldsymbol{r})$$

$$\rho_3(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) - \rho_p(\boldsymbol{r})$$

isovector functional
(isospin-rotation invariant)

$$\chi_1(\boldsymbol{r}) = C_1^\rho \{\rho_1^2(\boldsymbol{r}) + \rho_2^2(\boldsymbol{r}) + \rho_3^2(\boldsymbol{r})\}$$

$$= C_1^\rho \vec{\rho}(\boldsymbol{r}) \circ \vec{\rho}(\boldsymbol{r})$$

isoscalar in total

k=1,2 neutron-proton mixing terms
time-reversal symmetry cancels k=2 term

neutron-proton term shares the coupling constants with isovector (k=3) term
no new coupling constants in ph channel within the isospin symmetry

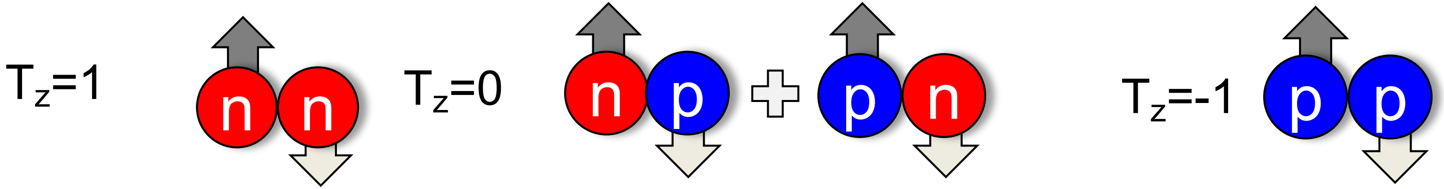
Sato-san's talk on Dec. 13

Neutron-proton pairing

Spin-singlet (S=0) isospin-triplet (T=1) pairing (isovector pairing)

two-particle wave function: (space) * (spin) * (isospin)

symmetric antisymmetric (singlet) symmetric (triplet)

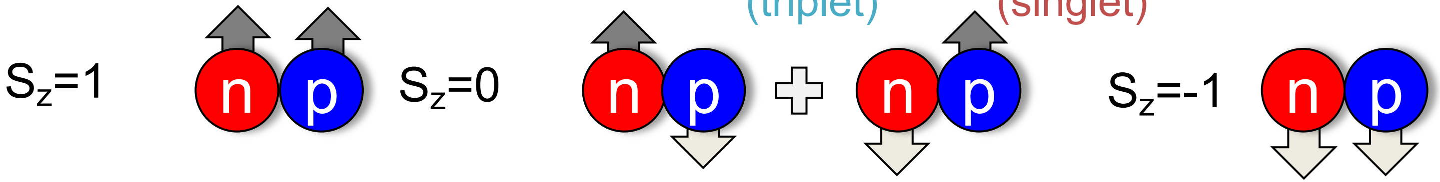


np coupling constant ~ nn and pp coupling constants

Spin-triplet (S=1) isospin-singlet (T=0) pairing (isoscalar pairing)

two-particle wave function: (space) * (spin) * (isospin)

symmetric symmetric (triplet) antisymmetric (singlet)



isoscalar pairing coupling constant: independent from others

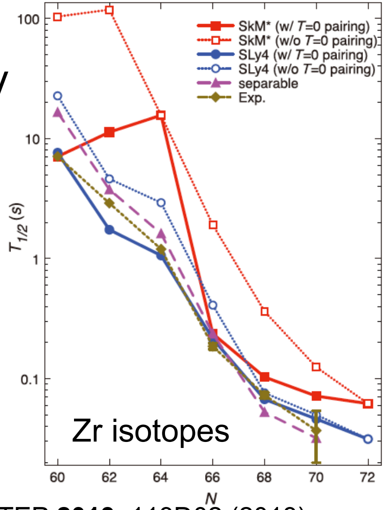
Constraining proton-neutron EDF

neutron-proton pairing condensation?

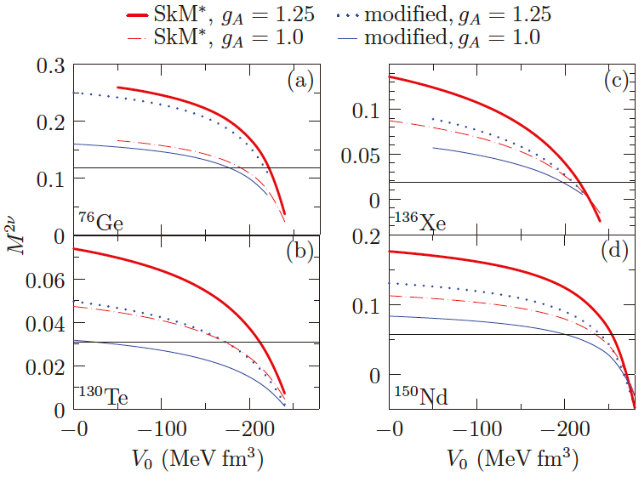
- around N=Z nuclei (protons and neutrons occupy the same level)
- isovector or isoscalar pair condensation?
- experimental observables that indicate np pair condensation?
  Wigner energy? odd-odd N=Z nuclei? rotational MOI?
- reviews: Afanasjev, Fifty years of Nuclear BCS, p.138, arXiv:1205.2134
  Frauendorf and Macchiavelli, Prog. Part. Nucl. Phys. **78**, 24 (2014)

neutron-proton pairing correlation

- beta-decay and double-beta decay
- Gamow-Teller resonances



Yoshida, PTEP **2013**, 113D02 (2013)



Mustonen and Engel, Phys. Rev. C **87**, 064302 (2013)

Constraining proton-neutron EDF

Mustonen and Engel, Phys. Rev. C **93**, 014304 (2016)

isovector (k=1) time-odd EDF

$$\chi_1^{\mathrm{odd}}(\boldsymbol{r}) = C_1^s[\rho_0]\boldsymbol{s}_1^2 + C_1^{\Delta s}\boldsymbol{s}_1 \cdot \Delta\boldsymbol{s}_1 + C_1^j\boldsymbol{j}_1^2 + C_1^T\boldsymbol{s}_1 \cdot \boldsymbol{T}_1 + C_1^{s\nabla j}\boldsymbol{s}_1 \cdot \boldsymbol{\nabla} \times \boldsymbol{j}_1 + C_1^F\boldsymbol{s}_1 \cdot \boldsymbol{F}_1 + C_1^{\nabla s}(\boldsymbol{\nabla} \cdot \boldsymbol{s}_1)^2$$

isoscalar pairing

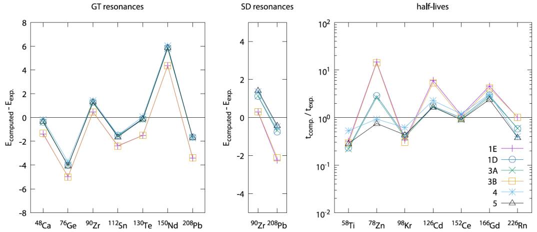
$$\tilde{\chi}_0(\boldsymbol{r}) = \frac{V_0}{4}\left[1 - \eta\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right]|\tilde{\boldsymbol{s}}_0(\boldsymbol{r})|^2$$

V_1(isovector)~ -250 MeV fm^3

experimental data set

Set	GT resonances	SD resonances	β-decay half-lives
A	^{208}Pb, ^{112}Sn, ^{76}Ge, ^{130}Te, ^{90}Zr, ^{48}Ca	None	^{48}Ar, ^{60}Cr, ^{72}Ni, ^{82}Zn, ^{92}Kr, ^{102}Sr, ^{114}Ru, ^{126}Cd, ^{134}Sn, ^{148}Ba
B	Same as A	None	^{52}Ti, ^{74}Zn, ^{92}Sr, ^{114}Pd, ^{134}Te, ^{156}Sm, ^{180}Yb, ^{200}Pt, ^{226}Rn, ^{242}U
C	Same as A	None	^{52}Ti, ^{72}Ni, ^{92}Sr, ^{114}Ru, ^{134}Te, ^{156}Nd, ^{180}Yb, ^{204}Pt, ^{226}Rn, ^{242}U
D	Those of A and ^{150}Nd	None	^{58}Ti, ^{78}Zn, ^{98}Kr, ^{126}Cd, ^{152}Ce, ^{166}Gd, ^{204}Pt
E	Same as D	^{90}Zr, ^{208}Pb	^{58}Ti, ^{78}Zn, ^{98}Kr, ^{126}Cd, ^{152}Ce, ^{166}Gd, ^{226}Rn

Fit	Starting point	Target set	Q values	fitted parameters
1A	SkO′	A	Comp.	$V_0 = -173.176$, $C_1^s = 128.279$
1B	SkO′	B	Comp.	$V_0 = -176.614$, $C_1^s = 133.038$
1C	SkO′	C	Comp.	$V_0 = -176.097$, $C_1^s = 126.966$
1D	SkO′	E	Comp.	$V_0 = -209.384$, $C_1^s = 129.297$
1E	SkO′	E	Exp.	$V_0 = -159.397$, $C_1^s = 99.8479$
2	SV-min	D	Comp.	$V_0 = -165.567$, $C_1^s = 132.271$
3A	SkO′	E	Comp.	$V_0 = -195.174$, $C_1^s = 144.833$, $C_1^T = -20.1618$, $C_1^F = -10.3125$
3B	SkO′	E	Exp.	$V_0 = -165.158$, $C_1^s = 120.27$, $C_1^T = -17.7435$, $C_1^F = -17.9902$
4	Fit 3A	E	Comp.	$C_1^j = 54.5$, $C_1^{\nabla j} = -78.7965$, $C_1^{\nabla s} = -87.5$
5	SkO′	E	Comp.	$V_0 = -191.875$, $C_1^s = 146.182$, $C_1^j = -86.4276$



Correlation between the data and coupling constants

Mustonen and Engel, Phys. Rev. C **93**, 014304 (2016)

$\mathcal{O}$	$d\mathcal{O}/dC_1^s$	$d\mathcal{O}/dV_0$	$d\mathcal{O}/dC_1^F$	$d\mathcal{O}/dC_1^T$	$d\mathcal{O}/dC_1^{\nabla s}$	$d\mathcal{O}/dC_1^{\Delta s}$	$d\mathcal{O}/dC_1^j$	$d\mathcal{O}/dC_1^{\nabla j}$
^{208}Pb E_{GTR}	57.261	−0.000	2.434	5.869	0.429	−1.002	0.000	0.143
^{112}Sn E_{GTR}	29.498	−1.032	1.432	2.863	0.286	−0.573	0.000	0.000
^{76}Ge E_{GTR}	45.115	−7.225	2.004	4.295	0.429	−1.145	0.000	0.000
^{130}Te E_{GTR}	53.790	−3.096	2.434	5.297	0.429	−1.002	0.143	0.000
^{90}Zr E_{GTR}	29.498	−1.032	1.288	2.720	0.429	−1.002	−0.143	0.143
^{48}Ca E_{GTR}	32.968	−0.000	1.432	3.149	0.573	−1.288	0.000	0.000
^{208}Pb E_{SDR}	52.055	−0.000	2.291	4.008	0.286	−1.575	−0.143	−0.143
^{90}Zr E_{SDR}	29.498	−0.000	1.575	2.004	0.286	−1.432	−0.286	−0.143
^{58}Ti $\log_{10}t$	4.749	−4.318	0.203	0.445	0.045	−0.109	−0.011	−0.002
^{78}Zn $\log_{10}t$	6.889	−2.922	0.256	0.589	0.164	−0.382	0.253	−0.025
^{98}Kr $\log_{10}t$	5.410	−3.252	0.265	0.559	0.050	−0.116	−0.012	−0.003
^{126}Cd $\log_{10}t$	5.583	−4.641	0.252	0.496	0.017	−0.050	0.001	0.007
^{152}Ce $\log_{10}t$	5.409	−2.474	0.293	0.540	0.051	−0.120	0.003	−0.009
^{166}Gd $\log_{10}t$	5.081	−2.924	0.250	0.497	0.035	−0.132	−0.007	−0.010
^{204}Pt $\log_{10}t$	3.755	−3.340	−0.015	0.160	−0.018	−0.316	−0.076	0.026

Only C_1^s(isovector spin coupling) and V_0(isoscalar pairing coupling) can be determined using this data set

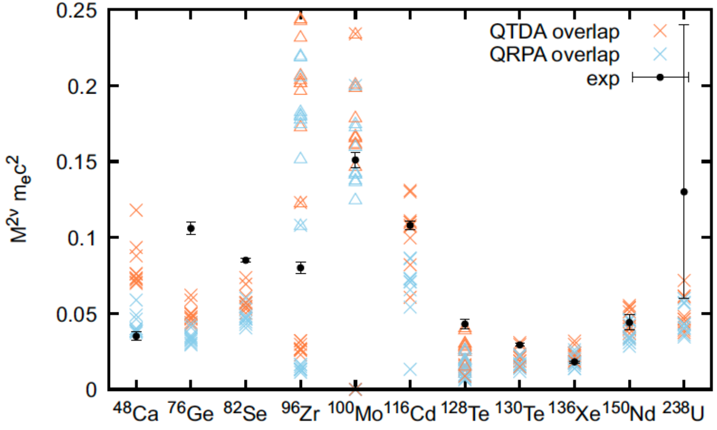
2νββ decay nuclear matrix element

NH and Engel, Phys. Rev. C **105**, 044314 (2022)

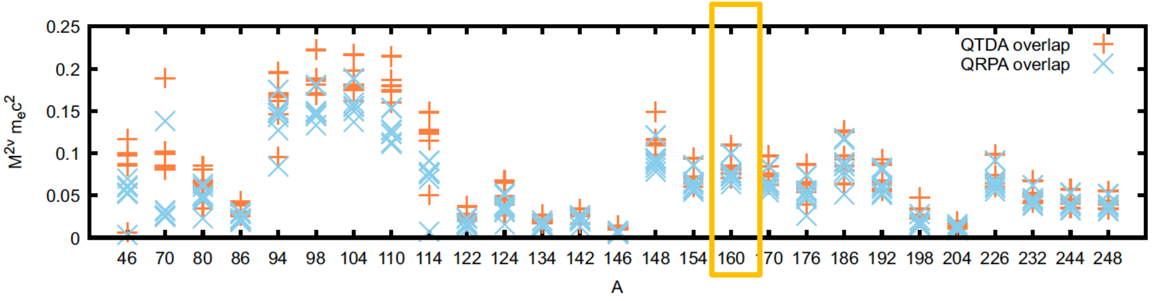
- EDF fitted to β decay half-life (10 parameter sets)
- pnFAM calculation

prediction for NME values of unmeasured 2νββ decay

2νββ NME
comparison with experiments



^{160}Gd NME



^{160}Gd NME: 0.0455 MeV^{-1} (Hirsch et al., PRC**66**(2002))

QRPA(EDF): 0.12 – 0.21 MeV^{-1} → PIKACHU experiment

Future plan: constraints on pnEDF coupling constants using 2νββ half-life

Pair densities in isospin representation

pair density matrix $\hat{\kappa}(\boldsymbol{r}st,\boldsymbol{r}'s't') = \langle\Psi|a_{\boldsymbol{r}'s't'}a_{\boldsymbol{r}st}|\Psi\rangle$

Perlinska et al., Phys. Rev. C **69**, 014316 (2014)

$\hat{\tilde{\rho}}(\boldsymbol{r}st,\boldsymbol{r}'s't') = -2s'\langle\Psi|a_{\boldsymbol{r}'-s't'}a_{\boldsymbol{r}st}|\Psi\rangle$ (time reversal)

$\hat{\breve{\rho}}(\boldsymbol{r}st,\boldsymbol{r}'s't') = 4s't'\langle\Psi|a_{\boldsymbol{r}'-s'-t'}a_{\boldsymbol{r}st}|\Psi\rangle$ (isospin symm.)

non-local pp density $\breve{\rho}_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{stt'}\hat{\breve{\rho}}(\boldsymbol{r}st,\boldsymbol{r}'st')\hat{\tau}^k_{t't}$

local pp density $\breve{\rho}_k(\boldsymbol{r}) = \breve{\rho}_k(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$

$\breve{\rho}_{\rm n}(\boldsymbol{r}) = \langle\Psi|a_{\rm n}(\boldsymbol{r})a_{\rm n}(\boldsymbol{r})|\Psi\rangle$ $\breve{\rho}_1(\boldsymbol{r}) = \breve{\rho}_{\rm n}(\boldsymbol{r}) + \breve{\rho}_{\rm p}(\boldsymbol{r})$

$\breve{\rho}_{\rm p}(\boldsymbol{r}) = \langle\Psi|a_{\rm p}(\boldsymbol{r})a_{\rm p}(\boldsymbol{r})|\Psi\rangle$ $\breve{\rho}_2(\boldsymbol{r}) = i[\breve{\rho}_{\rm n}(\boldsymbol{r}) - \breve{\rho}_{\rm p}(\boldsymbol{r})]$

isovector np pairing

$\breve{\rho}_{np}(\boldsymbol{r}) = \langle\Psi|a_{\rm n}(\boldsymbol{r})a_{\rm p}(\boldsymbol{r}) - a_{\rm p}(\boldsymbol{r})a_{\rm n}(\boldsymbol{r})|\Psi\rangle$ $\breve{\rho}_3(\boldsymbol{r}) = 2\breve{\rho}_{\rm np}(\boldsymbol{r})$ $\breve{\rho}_0(\boldsymbol{r}) = 0$ (Pauli principle)

non-local spin pp density $\breve{\boldsymbol{s}}_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{ss'tt'}\hat{\breve{\rho}}(\boldsymbol{r}st,\boldsymbol{r}'s't')\boldsymbol{\sigma}_{s's}\hat{\tau}^k_{t't}$

local pp spin density (isoscalar pairing) $\breve{\boldsymbol{s}}_0(\boldsymbol{r}) = \breve{\boldsymbol{s}}_0(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'} = \breve{\boldsymbol{s}}_{\rm np}(\boldsymbol{r})$

k=1-3 zero due to Pauli principle

Ground state np pair condensation

pair density matrix (isospin formalism) $\breve{\rho}(\boldsymbol{r}st, \boldsymbol{r}'s't') = 4s't'\langle\Psi|\hat{a}_{\boldsymbol{r}'-s'-t'}\hat{a}_{\boldsymbol{r}st}|\Psi\rangle$

non-local pair density $\breve{\rho}_k(\boldsymbol{r}, \boldsymbol{r}') = \sum_{stt'} \breve{\rho}(\boldsymbol{r}st, \boldsymbol{r}'st')\hat{\tau}^k_{t't}$

local pair density $\breve{\rho}_k(\boldsymbol{r}) = \breve{\rho}_k(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}=\boldsymbol{r}'}$

isovector pairing functional (conventional)

$$\breve{\chi}_{\mathrm{n}}(\boldsymbol{r}) = \breve{C}^{\rho}_{\mathrm{n}}[\rho_0]|\breve{\rho}_{\mathrm{n}}(\boldsymbol{r})|^2$$
$$\breve{\chi}_{\mathrm{p}}(\boldsymbol{r}) = \breve{C}^{\rho}_{\mathrm{p}}[\rho_0]|\breve{\rho}_{\mathrm{p}}(\boldsymbol{r})|^2$$

→

isovector pairing functional (isospin-rotation invariant)

$$\breve{\chi}_1(\boldsymbol{r}) = \breve{C}^{\rho}_1[\rho_0]\{|\breve{\rho}_1(\boldsymbol{r})|^2 + |\breve{\rho}_2(\boldsymbol{r})|^2 + |\breve{\rho}_3(\boldsymbol{r})|^2\}$$
$$= \breve{C}^{\rho}_1[\rho_0]\vec{\breve{\rho}}^{*}(\boldsymbol{r}) \circ \vec{\breve{\rho}}(\boldsymbol{r})$$

k= 3 neutron-proton pairing terms

$$\breve{\rho}_1(\boldsymbol{r}) = \breve{\rho}_{\mathrm{n}}(\boldsymbol{r}) + \breve{\rho}_{\mathrm{p}}(\boldsymbol{r})$$
$$\breve{\rho}_2(\boldsymbol{r}) = i[\breve{\rho}_{\mathrm{n}}(\boldsymbol{r}) - \breve{\rho}_{\mathrm{p}}(\boldsymbol{r})]$$
$$\breve{\rho}_3(\boldsymbol{r}) = 2\breve{\rho}_{\mathrm{np}}(\boldsymbol{r})$$

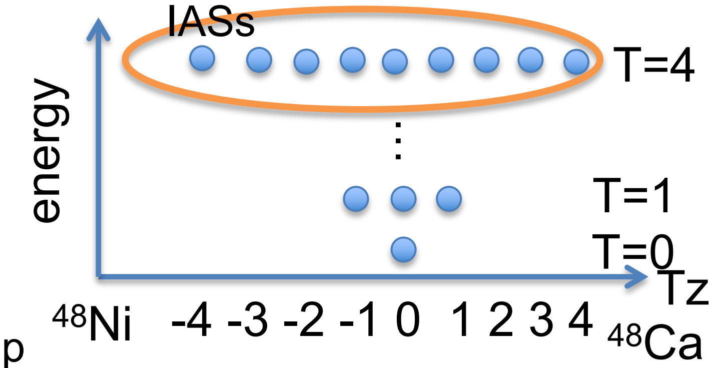
isoscalar pairing functional (np)

$$\breve{\chi}_0(\boldsymbol{r}) = \breve{C}^{s}_0[\rho_0]|\breve{\boldsymbol{s}}_0(\boldsymbol{r})|^2$$

Pairing in isobaric analogue states

Isobaric analogue states: |T Tz> states : cranking in isospace

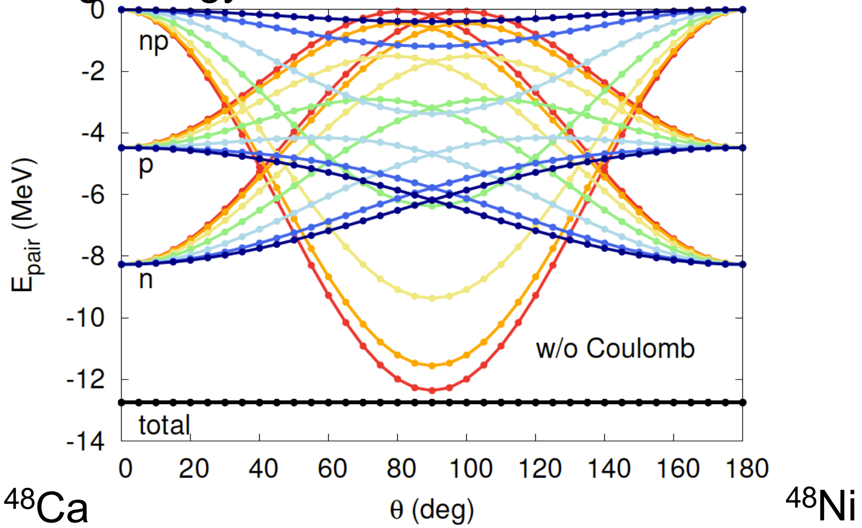
NH, Sheikh, Dobaczewski, Nazarewicz, in prep.



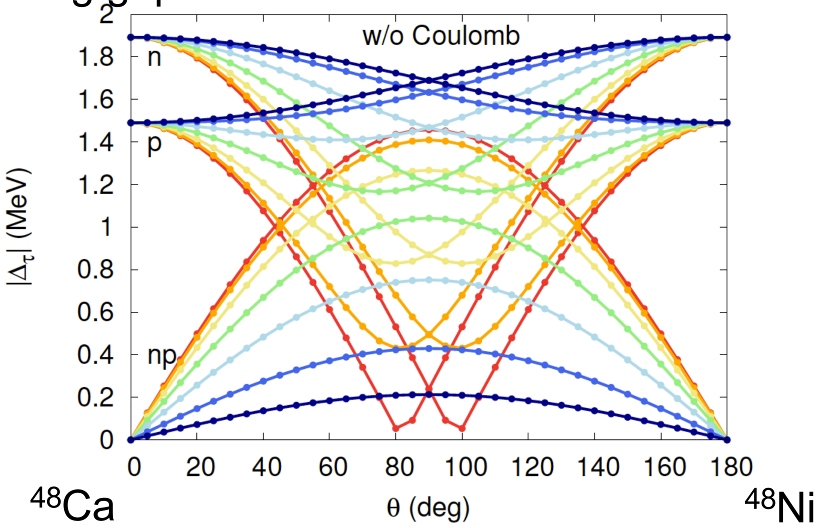
A=48 T=4 states, from ^{48}Ca (Tz=4) to ^{48}Ni (Tz=-4)
w/o Coulomb: with artificially strong pairing

calculation starting from ^{48}Ca,
with proton gauge angle at ^{48}Ca
φ=0,30,60,…,150,180 ($\Delta_p \sim |\Delta_p| e^{i\varphi}$)

pairing energy



pairing gap



Isospin rotation about 2nd axis

ph density

$$\begin{pmatrix}\rho_0(\theta')\\ \rho_1(\theta')\\ \rho_2(\theta')\\ \rho_3(\theta')\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \cos\theta' & 0 & \sin\theta'\\ 0 & 0 & 1 & 0\\ 0 & -\sin\theta' & 0 & \cos\theta'\end{pmatrix}\begin{pmatrix}\rho_0(0^\circ)\\ \rho_1(0^\circ)\\ \rho_2(0^\circ)\\ \rho_3(0^\circ)\end{pmatrix}$$

isoscalar (n+p)
np-mixed

isovector (n-p)

pp density

$$\begin{pmatrix}\breve\rho_0(\theta')\\ \breve\rho_1(\theta')\\ \breve\rho_2(\theta')\\ \breve\rho_3(\theta')\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \cos\theta' & 0 & \sin\theta'\\ 0 & 0 & 1 & 0\\ 0 & -\sin\theta' & 0 & \cos\theta'\end{pmatrix}\begin{pmatrix}\breve\rho_0(0)\\ \breve\rho_1(0)\\ \breve\rho_2(0)\\ \breve\rho_3(0)\end{pmatrix}$$

$\breve\rho_0(\boldsymbol{r}) = 0$

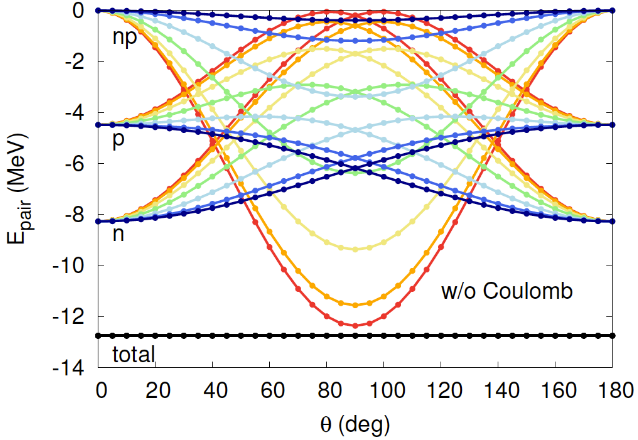
$\breve\rho_1(\boldsymbol{r}) = \breve\rho_{\rm n}(\boldsymbol{r}) + \breve\rho_{\rm p}(\boldsymbol{r})$

$\breve\rho_2(\boldsymbol{r}) = i[\breve\rho_{\rm n}(\boldsymbol{r}) - \breve\rho_{\rm p}(\boldsymbol{r})]$

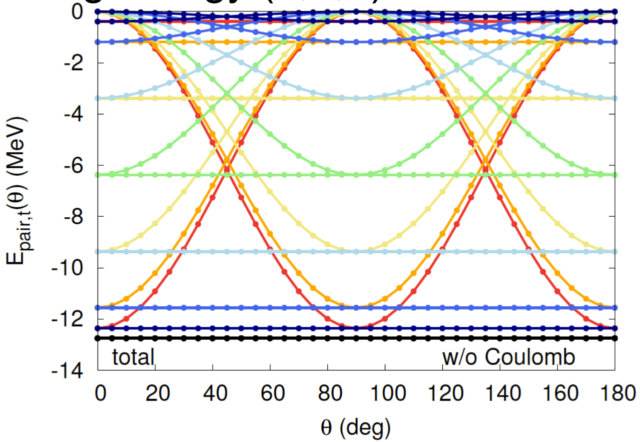
$\breve\rho_3(\boldsymbol{r}) = 2\breve\rho_{\rm np}(\boldsymbol{r})$

φ: relative gauge angle at $T=T_z$ (^{48}Ca)

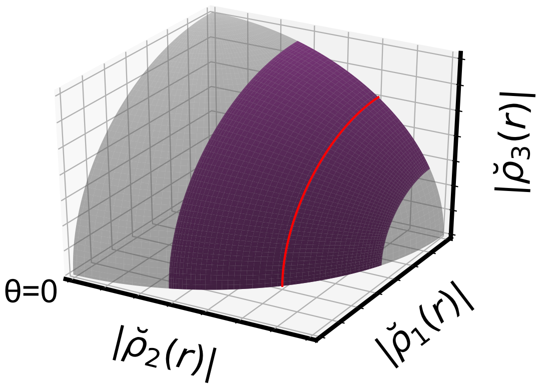
pairing energy (n, p, np)



pairing energy (1,2,3)



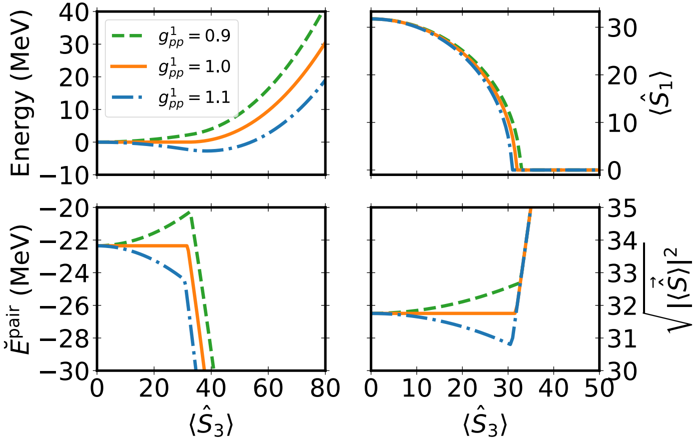
red curve: only one pairing is present at θ=0°
purple: region covered by the relative gauge angle θ=90°



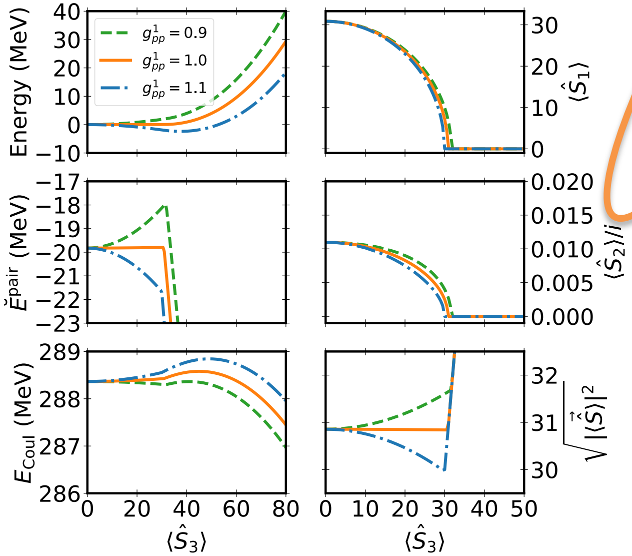
Isovector pn pairing in ground state

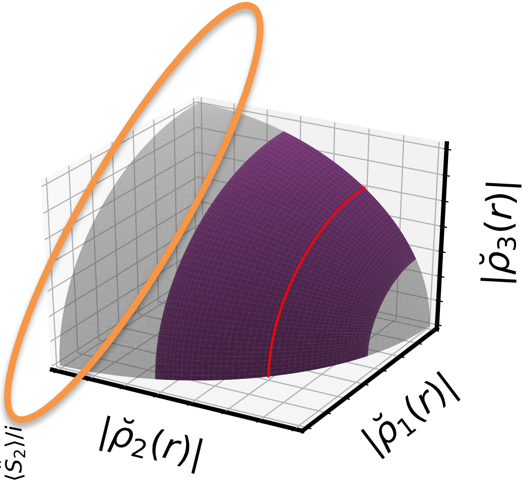
Constraint DFT on <S_3> (np pair condensate) $\langle \hat{S}_k \rangle = \int d\boldsymbol{r}\, \breve{\rho}_k(\boldsymbol{r})$

without Coulomb



with Coulomb





<S_2>=0

$$\breve{\chi}(\boldsymbol{r}) = \breve{C}_1^{\rho} \left[|\breve{\rho}_1(\boldsymbol{r})|^2 + |\breve{\rho}_2(\boldsymbol{r})|^2 + g_{pp} |\breve{\rho}_3(\boldsymbol{r})|^2 \right]$$

Future plan: include isoscalar np pairing

Summary

- Recent development of nuclear energy density functional
  - symmetry breaking introduces new densities in nuclear EDF

- Optimized EDF is available for
  - time-even densities fitted to ground-state experimental data
  - isovector pn part and isoscalar pn pairing fitted to beta decay and GT resonance
  - some couplings constants are not well constrained with g.s. data (isovector effective mass)

- Extensions to
  - momentum dependence on pairing
  - spin-triplet pairing
  - time-odd fields
  - proton-neutron mixing

- Collaborators
  - Takashi Nakatsukasa (Tsukuba), Koichi Sato (Kochi)
  - Tsunenori Inakura (Tokyo Tech), Hitoshi Nakada (Chiba)
  - Tomohiro Oishi, Kenichi Yoshida (Kyoto)
  - Witek Nazarewicz(MSU), Jacek Dobaczewski(York), Javid Sheikh(Kashmir)
  - Jon Engel(UNC)