Fortran Module for Density Dependent Parts of EDF

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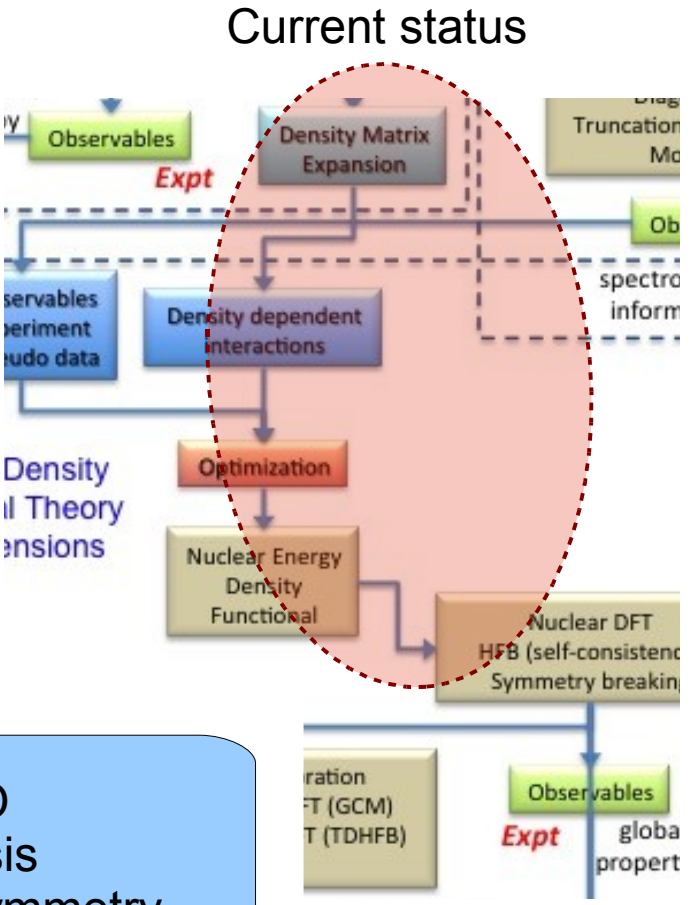
General philosophy

- Main idea is to separate details of EDF and HFB solver
- All functional details coded in fortran module UNEDF: The same module for different HFB solvers
- At the moment HFBRAD and HFBTHO works with the module



UNEDF DME module (f90)
- contains DME and Skyrme functionals
- calculates numerical values of CCs and their derivatives
- inm. properties included
- i/o for functional parameters

HFBTHO
- HO basis
- axial-symmetry

HFBRAD
- coordinate space
- spherical symmetry

Used energy density

- Skyrme EDF is constructed from bilinear terms of density matrices and their derivatives to the 2nd order
- Each term multiplied by a constant coupling constant (except density dependent C^{ρ})

$$H_t^{even}(r) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla J_t + C_t^{J}J_t^2$$

$$C_t^{\rho} = C_{t0}^{\rho} + \rho_0^{\gamma}C_{tD}^{\rho} \quad , \quad t = 0,1$$

- Generalize time-even H(r) to density dependent coupling constants

$$H_{tt'}^{even}(r) = U_{tt'}^{\rho\rho}\rho_t\rho_{t'} + U_{tt'}^{\rho\tau}\rho_t\tau_{t'} + U_{tt'}^{\rho\Delta\rho}\rho_t\Delta\rho_{t'} + U_{tt'}^{\nabla\rho\nabla\rho}\nabla\rho_t\cdot\nabla\rho_{t'}$$
$$+ U_{tt'}^{\rho\nabla J}\rho_t\nabla J_{t'} + U_{tt'}^{J\nabla\rho}J_t\cdot\nabla\rho_{t'} + U_t^{JJ}J_tJ_{t'}$$

- Amplitudes $U_{tt'}$ are functions of densities

Used energy density

- For cross terms ($t \neq t'$) the fulfillment of the isospin invariance of the whole energy density term must be set to U function
- Due to density dependence $\rho\Delta\rho$ and $(\nabla\rho)^2$ no longer connected by partial integration (also $J\nabla\rho$ and $\rho\nabla J$)
- Time-odd terms not yet considered
- U amplitudes in module are public variables for hfb solver to use

```
!
! === PUBLIC VARIABLES ===
!
! Use pointers to prevent conflicts with UNEDF public variabes
! Example: Use UNEDF, pr=>my_pr, ipr=>my_ipr, Crho=>my_Crho ...
!
Integer, Parameter, Public :: pr=Kind(1.0D0), ipr=Kind(1)                ! to set the precision of the DFT solv
Logical, Public :: use_charge_density, use_cm_cor
Real(pr), Public, Dimension(0:3,0:7) :: Urhorho,Urhotau,UrhoDrho,Unablarho  ! ph DME amplitudes
Real(pr), Public, Dimension(0:3,0:7) :: UJnablarho,UrhonablaJ,UJJ
Real(pr), Public, Dimension(0:3,0:7) :: Urhorhopr                        ! pp amplitudes
Real(pr), Public, Dimension(0:1) :: UEnonstdr,UFnonstdr,URnonstdr        ! Other amplitudes
Real(pr), Public :: hbzero,sigma,e2charg                                 ! hbr^2/2m, DD sigma, e^2 charge
Real(pr), Public, Dimension(0:1) :: Crho,Cdrho,Ctau,CrDr,CrdJ,CJ,CpV0,CpV1  ! basic coupling constants
Real(pr), Public :: E_NM,K_NM,SMASS_NM,RHO_NM,ASS_NM,LASS_NM,VMASS_NM,P_NM,KA_NM
Real(pr), Public :: CHrho                                                ! Crho(0) from the Hartree term in NM
Logical, Public :: use_DME3N_terms,use_j2terms
Integer(ipr), Public :: DMEorder,DMElda
!
! === PRIVATE VARIABLES ===
!
Real(pr), Private, Dimension(0:1) :: nuCrho,nuCdrho,nuCtau,nuCrDr        ! basic coupling constants in natural
Real(pr), Private, Dimension(0:1) :: nuCrdJ,nuCJ,nuCpV0,nuCpV1           !
Real(pr), Private :: t0,t1,t2,t3,x0,x1,x2,x3,b4,b4p,te,to
Real(pr), Private :: nuLambda,nufpi                                      ! parameters associated to natural uni
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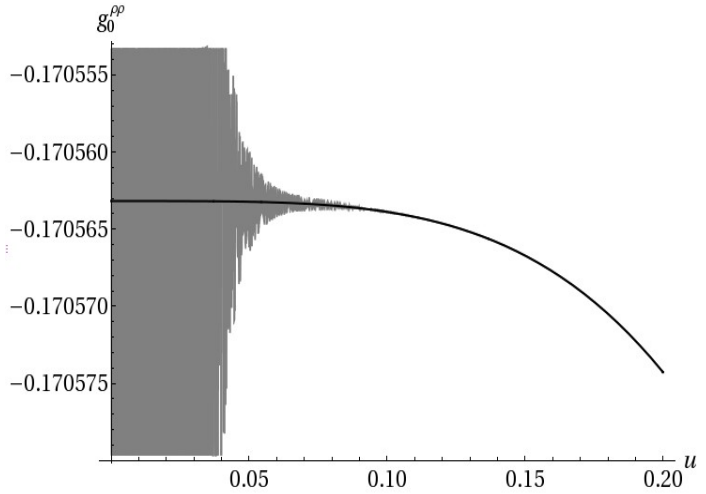
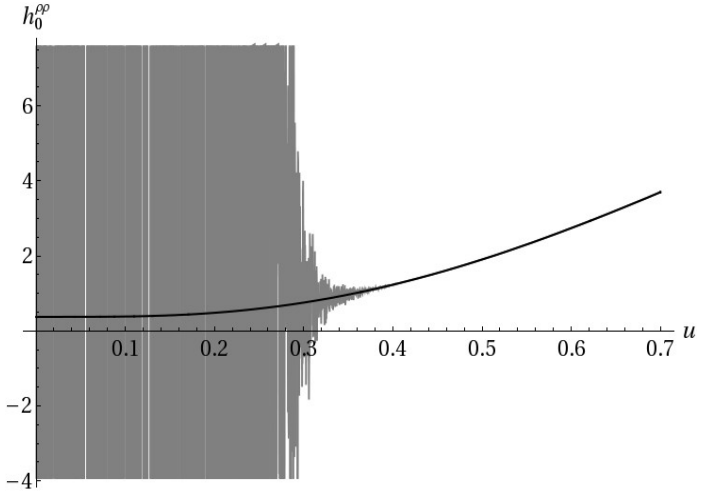
Module for DME functional

- Based on EDF of B. Gebremariam, S. K. Bogner, and T. Duguet, Comput. Phys. Comm. 181 (2010) 1167
- Contains all expressions for U-amplitudes (and their derivatives) coming from the DME of chiral perturbation potential up to N2LO (2N & 3N terms) $\Rightarrow$ U is a function of ρ_0
- For very small ρ_0 Taylor expansion used to handle numerical noise





$u=k_F/m_\pi$

Conclusions & Outlook

- A fortran module for EDF coming from the DME of chiral perturbation potential has been developed
- The structure of module allows flexible way to code EDF for different HFB solvers
- Similar module also coded for Fayans functional, DME of Minnesota potential and NV DME of Gogny
- DME module to be published in CPC