Pairing with number conservation:

S. Krewald et al, nucl-th/0412018

- Based on extended density matrix (EDM)

- EDM from doubling degrees of freedom
  - $R^2 = R$
  - usual HFB EDM for quasi-particle ground state
  - new κ pairing field differs from HFB pairing field for correlated ground states with fixed N.

- Formulate Kohn-Sham for EDM
  - nonlocal
  - particle number conserving

Pairing within DFT

Exact approach for Richardson model (constant pairing):

$$H = \sum_{j=1}^{\Omega} \sum_{s=\downarrow,\uparrow} \varepsilon_j \hat{a}^\dagger_{js} \hat{a}_{js} - g \sum_{i,j=1}^{\Omega} \hat{a}^\dagger_{i\downarrow} \hat{a}^\dagger_{i\uparrow} \hat{a}_{j\uparrow} \hat{a}_{j\downarrow}$$

Density functional is the Legendre transform:

$$F(\{n_k\}) = E - \sum_{k=1}^{\Omega} n_k \varepsilon_k \qquad n_k \equiv \frac{\partial E}{\partial \varepsilon_k}$$

Relation between occupation numbers and the density:

$$\begin{aligned} \frac{\delta F(\{n_k\})}{\delta \phi^*_\alpha(x)} &= \sum_k \frac{\partial F}{\partial n_k} \frac{\delta n_k}{\delta \phi^*_\alpha(x)} \\ &= n_\alpha \sum_k \frac{\partial F}{\partial n_k} \langle k|\alpha\rangle u_k(x) \end{aligned}$$

$$\langle \alpha | k \rangle = \int d^3x \phi^*_\alpha(x) u_k(x)$$

KS occupation number (0 or 2)

KS orbital

Orbital of pairing Hamiltonian

Exact density functionals in two limits (nucl-th/0609084)

BCS limit (large number of pairs):

$$\begin{aligned} F_{BCS} &\equiv E_{BCS} - \sum_{j=1}^{\Omega} \varepsilon_j n_j \\ &= -\frac{\Delta^2}{g} \\ &= -\frac{g}{4}\left(\sum_{j=1}^{\Omega}\sqrt{n_j(2-n_j)}\right)^2 \end{aligned}$$

Sources of nonlocalities:

1. Square of local functional
2. Relation between density and occupation numbers

Strong-coupling limit:

$$E(\{\varepsilon_j\}) = E^{(1)} + 2N\overline{\varepsilon} + g\sum_{j\geq 2}\sum_{\lambda}\frac{c_\lambda}{g^j}\prod_{i=1}^{k}\overline{(\varepsilon-\overline{\varepsilon})^{\lambda_i}}$$

$$\overline{\varepsilon} \equiv \frac{1}{\Omega}\sum_{k=1}^{\Omega}\varepsilon_k$$

Expansion in central moments of single-particle energies

$$F(\{n_j\}) = E^{(1)} + g\sum_{j\geq 2}\sum_{\lambda} d_\lambda \Omega^j \prod_{i=1}^{k}\overline{(n-\overline{n})^{\lambda_i}}$$

Expansion in central moments of occupation numbers