Symmetry Projection in Density Functional Theory

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Basic Elements of the Mean-Field Theory

- Many-body Hamiltonian

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c^\dagger_{n_1} c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} c^\dagger_{n_1} c^\dagger_{n_2} c_{n_4} c_{n_3},$$

$$\overline{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$$

$$c_n |-\rangle = 0$$

- Quasiparticle transformation

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

Transformation matrix is required to be unitary as the quasiparticle operators need to satisfy the same commutation relations as that of original fermions

$$\mathcal{W}^\dagger \mathcal{W} = \mathcal{W} \mathcal{W}^\dagger = I$$

$$\begin{aligned} U^\dagger U + V^\dagger V &= I, & \qquad UU^\dagger + V^* V^T &= I \\ U^T V + V^T U &= 0, & \qquad UV^\dagger + V^* U^T &= 0 \end{aligned}$$

Basic Elements of the Mean-Field Theory

- HFB densities

$$\rho_{nn'} = \langle\Phi|c^\dagger_{n'} c_n|\Phi\rangle, \qquad \kappa_{nn'} = \langle\Phi|c_{n'} c_n|\Phi\rangle$$

$$\boxed{\alpha_k|\Phi\rangle = 0}$$

$$\rho = V^* V^T, \qquad \kappa = V^* U^T = -UV^\dagger$$

- HFB conditions

$$\boxed{\rho - \rho^2 = -\kappa\kappa^*, \qquad \rho\kappa = \kappa\rho^*}$$

- Generalized density matrix

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & -\sigma^* \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = \mathcal{W}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\mathcal{W}^\dagger$$

$$\boxed{\mathcal{R}^2 = \mathcal{R}}$$

- HFB Energy

$$E_{\mathrm{HFB}} = \mathrm{Tr}(e\rho) + \frac{1}{2}\mathrm{Tr}(\Gamma\rho) - \frac{1}{2}\mathrm{Tr}(\Delta\kappa^*)$$

where

$$\Gamma_{n_1 n_3} = \sum_{n_2 n_4} \overline{v}_{n_1 n_2 n_3 n_4}\rho_{n_4 n_2} \qquad , \qquad \Delta_{n_1 n_2} = \frac{1}{2}\sum_{n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4}\kappa_{n_3 n_4}$$

Energy Functional $E(\rho, \kappa) \rightarrow$ HFB Like Equations JAS and P. Ring, Nucl. Phys. A **665**, 71 (2000)

- Any arbitrary energy functional, which is completely expressible in terms of ρ and κ results into HFB like Equations

$$\delta \left\{ E(\rho, \kappa) - \mathrm{Tr}\left(\Lambda(\mathcal{R}^2 - \mathcal{R}) \right) \right\} = 0$$

$$\delta E = \sum_{n<n'} \left(\frac{\partial E}{\partial \rho_{n'n}} \delta\rho_{n'n} + \frac{\partial E}{\partial \rho^*_{n'n}} \delta\rho^*_{n'n} + \frac{\partial E}{\partial \kappa_{n'n}} \delta\kappa_{n'n} + \frac{\partial E}{\partial \kappa^*_{n'n}} \delta\kappa^*_{n'n} \right) + \sum_n \frac{\partial E}{\partial \rho_{nn}} \delta\rho_{nn}$$

- Introducing the quantities

$$h_{nn'} = \frac{\partial E}{\partial \rho_{n'n}} \quad \text{for} \quad n \le n', \qquad \Delta_{nn'} = -\frac{\partial E}{\partial \kappa^*_{n'n}} \quad \text{for} \quad n < n'$$

- Assuming the functional E is real, we find

$$h^*_{nn'} = \frac{\partial E}{\partial \rho^*_{n'n}}, \qquad \Delta^*_{nn'} = -\frac{\partial E}{\partial \kappa_{n'n}}$$

$$\delta E = \frac{1}{2} \left\{ \mathrm{Tr}\left(h\delta\rho\right) + \mathrm{Tr}\left(h^*\delta\rho^*\right) - \mathrm{Tr}\left(\Delta^*\delta\kappa\right) - \mathrm{Tr}\left(\Delta\delta\kappa^*\right) \right\}$$

Energy Functional $E(\rho, \kappa) \rightarrow$ HFB Like Equations

- Introducing the matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

We have

$$\delta E = \frac{1}{2}\mathrm{Tr}\left(\mathcal{H}\delta\mathcal{R}\right)$$

- Including the constraint leads to the variational ansatz

$$\delta\left\{E(\rho,\kappa) - \mathrm{Tr}\left(\Lambda(\mathcal{R}^2 - \mathcal{R})\right)\right\} = \frac{1}{2}\mathrm{Tr}\left\{(\mathcal{H} - \Lambda\mathcal{R} - \mathcal{R}\Lambda + \Lambda)\delta\mathcal{R}\right\} = 0$$

- Since $\delta\mathcal{R}$ is an arbitrary variation, we find

$$\mathcal{H} - \Lambda\mathcal{R} - \mathcal{R}\Lambda + \Lambda = 0$$

- Using $(\mathcal{R}^2 = \mathcal{R})$, the above equation can be written as

$$[\mathcal{H}, \mathcal{R}] = 0$$

- Solved by the HFB-equation

$$\boxed{\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} E}$$

Symmetry Projected Energy $\rightarrow E^I(\rho, \kappa)$

- Projection Operator

$$P^I = \int dg\, d^I(g) \hat{R}(g)$$

where the integral runs over all elements g of the symmetry group.

- Particle Number Projection

$$\hat{R}(\phi) = e^{i\phi\hat{N}}, \qquad d^N(\phi) = \frac{1}{2\pi} e^{-i\phi N}$$

- One-Dimensional angular-momentum projection

$$\hat{R}(\beta) = e^{i\beta\hat{J}_y}, \qquad d^I(\beta) = \frac{2I+1}{8\pi^2} d^I_{00}(\beta)$$

- Projected Energy

$$E^I = \frac{\langle\Phi|HP^I|\Phi\rangle}{\langle\Phi|P^I|\Phi\rangle} = \frac{\int dg\, d^I(g)\langle\Phi|H\hat{R}(g)|\Phi\rangle}{\int dg\, d^I(g)\langle\Phi|\hat{R}(g)|\Phi\rangle}$$

Projected Energy $\rightarrow E^I(\rho, \kappa)$

- Defining

$$|g\rangle = \frac{\hat{R}(g)|\Phi\rangle}{\left\langle \Phi|\hat{R}(g)|\Phi \right\rangle}, \quad \text{with} \quad |0\rangle = |\Phi\rangle$$

and

$$x(g) = d^I(g) \left\langle \Phi|\hat{R}(g)|\Phi \right\rangle$$

$$y(g) = \frac{x(g)}{\int dg\, x(g)}, \qquad \text{with} \quad \int dg\, y(g) = 1$$

- Projected Energy

$$E^I = \frac{\langle \Phi|HP^I|\Phi\rangle}{\langle \Phi|P^I|\Phi\rangle} = \frac{\int dg\, x(g)\, \langle 0|H|g\rangle}{\int dg\, x(g)} = \int dg\, y(g)\, \langle 0|H|g\rangle$$

- Norm Overlap

$$\begin{aligned}
\langle \Phi|\hat{R}(g)|\Phi\rangle &= \pm\sqrt{\det D_g}\sqrt{\det(U^T D_g^* U^* + V^T D_g^* V^*)} \\
&= \pm\sqrt{\det D_g (\det \rho)^{-1/2}}\sqrt{\det\left(\rho D_g \rho - \kappa D_g^* \kappa^*\right)} \\
&= \pm\sqrt{\det R_g (\det \rho)^{-1/2}}\sqrt{\det\left(A_g\right)} \\
&= \pm \det R_g (\det \rho)^{-1/2}\sqrt{\det\left(B_g\right)}
\end{aligned}$$

$$\rho_g = R_g \rho R_g^\dagger, \quad \rho_{-g} = R_g^\dagger \rho R_g \;, \;\; \kappa_g = R_g \kappa R_g^T, \quad \kappa_{-g} = R_g^\dagger \kappa R_g^* \;,$$
$$A_g = \rho R_g \rho - \kappa R_g^* \kappa^*, \quad B_g = \rho \rho_g - \kappa \kappa_g^*$$

Projected Energy $\rightarrow E^I(\rho, \kappa)$

- Hamiltonian Overlap (Using Generalized Wick Theorem)

$$
\begin{aligned}
\langle 0|H|g\rangle &= H(g) = H_{sp}(g) + H_{ph}(g) + H_{pp}(g) \\
&= \sum_{n_1 n_2} e_{n_1 n_2} \left\langle 0|c^\dagger_{n_1} c_{n_2}|g\right\rangle \\
&\quad + \frac{1}{2} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \left\langle 0|c^\dagger_{n_1} c_{n_3}|g\right\rangle \left\langle 0|c^\dagger_{n_2} c_{n_4}|g\right\rangle \\
&\quad + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \left\langle 0|c^\dagger_{n_1} c^\dagger_{n_2}|g\right\rangle \langle 0|c_{n_4} c_{n_3}|g\rangle
\end{aligned}
$$

$$
\begin{aligned}
H_{sp}(g) &= \sum_{n_1 n_2} e_{n_1 n_2} \rho_{n_2 n_1}(g) = \mathrm{Tr}\,(e\rho(g)) \\
H_{ph}(g) &= \frac{1}{2} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \rho_{n_3 n_1}(g) \rho_{n_4 n_2}(g) = \frac{1}{2} \mathrm{Tr}\,(\Gamma(g)\rho(g)) \\
H_{pp}(g) &= \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \overline{\kappa}^*_{n_1 n_2}(g) \kappa_{n_3 n_4}(g) \\
&= -\frac{1}{2} \mathrm{Tr}\,(\Delta(g)\overline{\kappa}^*(g)) = -\frac{1}{2} \mathrm{Tr}\left(\overline{\Delta}^*(g)\kappa(g)\right)
\end{aligned}
$$

Projected Energy $\rightarrow E^{I}(\rho, \kappa)$

- Projected Fields

$$
\begin{aligned}
\Gamma_{n_1 n_3}(g) &= \sum_{n_2 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2}(g) \\
\Delta_{n_1 n_2}(g) &= \frac{1}{2} \sum_{n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}(g) \\
\overline{\Delta}^{*}_{n_1 n_2}(g) &= \frac{1}{2} \sum_{n_3 n_4} \overline{\kappa}^{*}_{n_3 n_4}(g) \overline{v}_{n_3 n_4 n_1 n_2} \\
\overline{\Delta}_{n_1 n_2}(g) &= \frac{1}{2} \sum_{n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \overline{\kappa}_{n_3 n_4}(g)
\end{aligned}
$$

- Transition Densities

$$
\begin{aligned}
\rho(g) &= R_g \rho A_g^{-1} \rho = \rho_g B_g^{-1} \rho \\
\kappa(g) &= R_g \rho A_g^{-1} \kappa = \rho_g B_g^{-1} \kappa \ , \\
\overline{\kappa}^{*}(g) &= R_g^{*} \kappa^{*} A_g^{-1} \rho = \kappa_g^{*} B_g^{-1} \rho
\end{aligned}
$$

Projected HFB Formalism

- Projected Equations

$$\begin{pmatrix} h^I & \Delta^I \\ -\Delta^{I\,*} & -h^{I\,*} \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} E$$

- Projected Fields

$$\begin{aligned} h^I_{nn'} &= \frac{\partial E^I}{\partial \rho_{n'n}} \\ \Delta^I_{nn'} &= -\frac{\partial E^I}{\partial \kappa^*_{n'n}} \end{aligned}$$

Particle Number Projection
JAS, P. Ring, E. Lopez and R. Rossignoli, Phys. Rev. C **66**, 044318 (2002)

- Number Projection Operator

$$P^N = \frac{1}{2\pi}\int d\phi \; e^{i\phi(\hat{N}-N)}$$

- Number Projected HFB Equation

$$\mathcal{H}^N \begin{pmatrix} U \\ V \end{pmatrix} = \mathcal{E}_\rangle \begin{pmatrix} U \\ V \end{pmatrix}$$

where

$$\mathcal{H}^N = \begin{pmatrix} \varepsilon^N + \Gamma^N + \Lambda^N & \Delta^N \\ -(\Delta^N)^* & -(\varepsilon^N)^* - (\Gamma^N)^* - (\Lambda^N)^* \end{pmatrix}$$

- Expressions for the fields are

$$\begin{aligned}
\varepsilon^N &= \frac{1}{2}\int d\phi \; y(\phi)\left\{Y(\phi)\mathrm{Tr}[e\,\rho(\phi)] + [1 - 2ie^{-i\phi}\sin\phi\rho(\phi)]e\;C(\phi)\right\} \\
&\quad + h.c. \\
\Gamma^N &= \frac{1}{2}\int d\phi \; y(\phi)\left(Y(\phi)\frac{1}{2}\mathrm{Tr}[\Gamma(\phi)\rho(\phi)] + \frac{1}{2}[1 - 2ie^{-i\phi}\sin\phi\rho(\phi)]\Gamma(\phi)C(\phi)\right) \\
&\quad + h.c. \\
\Lambda^N &= -\frac{1}{2}\int d\phi \; y(\phi)\left(Y(\phi)\frac{1}{2}\mathrm{Tr}[\Delta(\phi)\overline{\kappa}^*(\phi)] - 2ie^{-i\phi}\sin\phi\; C(\phi)\Delta(\phi)\overline{\kappa}^*\right) \\
&\quad + h.c \\
\Delta^N &= \frac{1}{2}\int d\phi \; y(\phi)e^{-2i\phi}C\,(\phi)\,\Delta(\phi) - (..)^T
\end{aligned}$$

Particle Number Projection

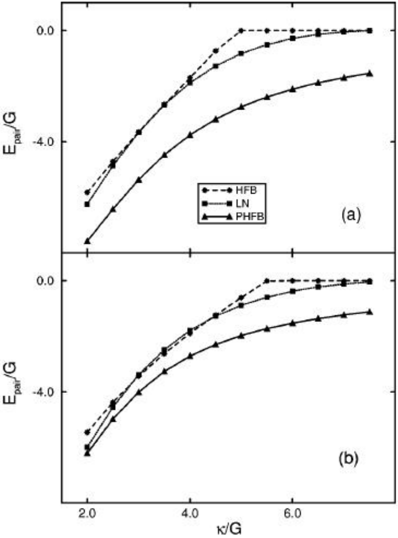
$$\begin{aligned}\Gamma_{n_1 n_3}(\phi) &= \sum_{n_2 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2}(\phi) \\ \Delta_{n_1 n_2}(\phi) &= \frac{1}{2} \sum_{n_3 n_4} \overline{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}(\phi) \\ \overline{\Delta}^*_{n_3 n_4}(\phi) &= \frac{1}{2} \sum_{n_1 n_2} \overline{\kappa}^*_{n_1 n_2}(\phi) \overline{v}_{n_1 n_2 n_3 n_4},\end{aligned}$$

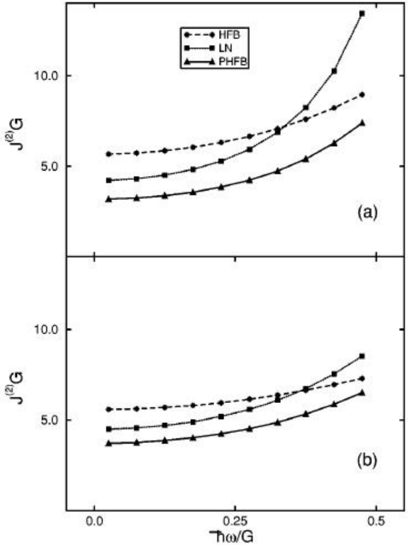
$$\begin{aligned}\rho(\phi) &= C(\phi)\rho \\ \kappa(\phi) &= C(\phi)\kappa = \kappa C^{T}(\phi) \\ \overline{\kappa}(\phi) &= e^{2i\phi}\kappa C^*(\phi) = e^{2i\phi} C^\dagger(\phi)\kappa \\ C(\phi) &= e^{2i\phi}\left(1 + \rho(e^{2i\phi} - 1)\right)^{-1} \\ x(\phi) &= \frac{1}{2\pi} \frac{e^{i\phi(N)} \det(e^{i\phi})}{\sqrt{\det C(\phi)}}, \\ y(\phi) &= \frac{x(\phi)}{\int dg\, x(\phi)}, \quad \int dg\, y(\phi) = 1,\end{aligned}$$

and

$$Y(\phi) = ie^{-i\phi} \sin\phi\; C(\phi) - i \int d\phi' y(\phi') e^{-i\phi'} \sin\phi'\; C(\phi')$$

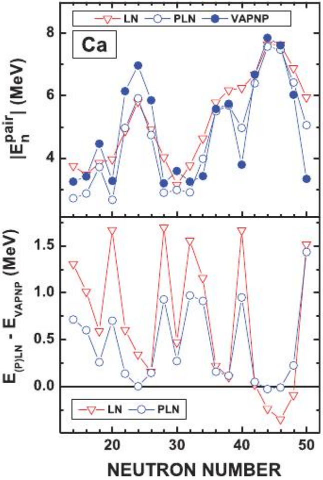
Particle Number Projection in a Schematic Model

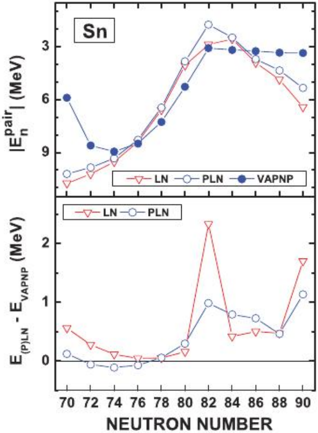




JAS, P. Ring, E. Lopez and R. Rossignoli, Phys. Rev. C **66**, 044318 (2002)

Particle Number Projection with Skyrme Force





M.V. Stoitsov et al., Phys. Rev. C **76**, 014308 (2007)

Particle Number Projection with Gogny Force

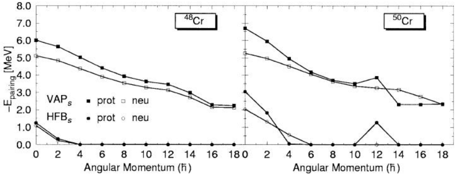
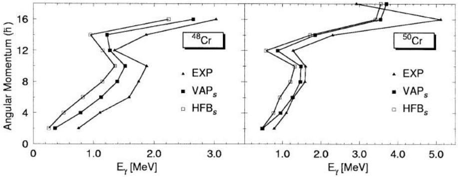


Fig. 5. Pairing correlation energies in the HFB_s and VAP_s approaches or the nucleus ^{48}Cr and ^{50}Cr, respectively.



M. Anguiano, J.L. Egido and L.M. Robledo, Nucl. Phys. A **696**, 467 (2001)

Generalized Projected Operator

- Three Dimensional Angular Momentum Projection

$$P^I = \int dg\, D^I(g)\hat{R}(g)$$

$$\hat{R}(g) = e^{i\alpha \hat{J}_z}\ e^{i\beta \hat{J}_y}\ e^{i\gamma \hat{J}_z}, \qquad D^I(g) = \frac{2I+1}{8\pi^2} D^I_{MK}(\alpha,\beta,\gamma)$$

- Norm and Hamiltonian overlap integrals depend on both ρ and κ and cannot be simplified. For instance, the norm overlap

$$\langle\Phi|\hat{R}(g)|\Phi\rangle = \pm\sqrt{\det R_g}(\det\rho)^{-1/2}\sqrt{\det\left(A_g\right)}$$

where

$$A_g = \rho R_g \rho - \kappa R_g^* \kappa^*$$

Generalized Projected Fields

- Hartree Fock Field

$$
\begin{aligned}
h^{l}_{n'n} &= \frac{\partial E^{l}}{\partial \rho_{nn'}} \\
&= \int dg \left\{ \frac{\partial y(g)}{\partial \rho_{nn'}} H(g) + y(g) \frac{\partial H(g)}{\partial \rho_{nn'}} \right\} \\
&= \int dg \left\{ \frac{\partial y(g)}{\partial \rho_{nn'}} H(g) + y(g) \left(\frac{\partial H_{sp}(g)}{\partial \rho_{nn'}} + \frac{\partial H_{ph}(g)}{\partial \rho_{nn'}} + \frac{\partial H_{pp}(g)}{\partial \rho_{nn'}} \right) \right\}
\end{aligned}
$$

$$
\frac{\partial y(g)}{\partial \rho_{nn'}} = y(g) Y_{n'n}(g)
$$

$$
\begin{aligned}
Y(g) &= X(g) - \int dg' y(g') X(g') \\
X(g) &= \frac{1}{2} \left(-\rho^{-1} + R_g \rho A_g^{-1} + A_g^{-1} \rho R_g \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial H_{sp}(g)}{\partial \rho_{nn'}} &= \Big(e R_g \rho A_g^{-1} + A_g^{-1} \rho e R_g \\
&\quad - A_g^{-1} \rho e \rho(g) R_g - \rho(g) e R_g \rho A_g^{-1} \Big)_{n'n} , \\
\frac{\partial H_{ph}(g)}{\partial \rho_{nn'}} &= \Big(\Gamma(g) R_g \rho A_g^{-1} + A_g^{-1} \rho \Gamma(g) R_g \\
&\quad - A_g^{-1} \rho \Gamma(g) \rho(g) R_g - \rho(g) \Gamma(g) R_g \rho A_g^{-1} \Big)_{n'n} , \\
\frac{\partial H_{pp}(g)}{\partial \rho_{nn'}} &= \Big(\Delta(g) R_g^{*} \kappa^{*} A_g^{-1} - A_g^{-1} \rho \Delta(g) \bar{\kappa}^{*}(g) R_g \\
&\quad - \rho(g) \Delta(g) R_g^{*} \kappa^{*} A_g^{-1} + A_g^{-1} \kappa \bar{\Delta}^{*}(g) R_g \\
&\quad - A_g^{-1} \kappa \bar{\Delta}^{*}(g) \rho(g) R_g - \kappa(g) \bar{\Delta}^{*}(g) R_g \rho A_g^{-1} \Big)_{n'n}
\end{aligned}
$$

Generalized Projected Fields

- Pairing Field

$$\begin{aligned}\Delta^{I}_{n'n} &= -\frac{\partial E^{I}}{\partial \kappa^{*}_{nn'}} \\ &= -\int dg \left\{ \frac{\partial y(g)}{\partial \kappa^{*}_{nn'}} H(g) + y(g) \frac{\partial H(g)}{\partial \kappa^{*}_{nn'}} \right\} \\ &= -\int dg \left\{ \frac{\partial y(g)}{\partial \kappa^{*}_{nn'}} H(g) + y(g) \left(\frac{\partial H_{sp}(g)}{\partial \kappa^{*}_{nn'}} + \frac{\partial H_{ph}(g)}{\partial \kappa^{*}_{nn'}} + \frac{\partial H_{pp}(g)}{\partial \kappa^{*}_{nn'}} \right) \right\}\end{aligned}$$

$$\frac{\partial y(g)}{\partial \kappa^{*}_{nn'}} = y(g) T_{n'n}(g),$$

$$\begin{aligned}T(g) &= Z(g) - \int dg' y(g') Z(g') \\ Z(g) &= -\frac{1}{2} \left(A_g^{-1} \kappa R_g^{*} - (\cdots)^{T} \right)\end{aligned}$$

$$\begin{aligned}\frac{\partial H_{sp}(g)}{\partial \kappa^{*}_{nn'}} &= \left(A_g^{-1} \rho e \kappa(g) R_g^{*} - (\cdots)^{T} \right)_{n'n} \\ \frac{\partial H_{ph}(g)}{\partial \kappa^{*}_{nn'}} &= \left(A_g^{-1} \rho \Gamma(g) \kappa(g) R_g^{*} - (\cdots)^{T} \right)_{n'n} \\ \frac{\partial H_{pp}(g)}{\partial \kappa^{*}_{nn'}} &= -\frac{1}{2} \Bigg[\left(A_g^{-1} \rho \Delta(g) R_g^{*} - (\cdots)^{T} \right)_{n'n} \\ &\quad + \left(A_g^{-1} \rho \Delta(g) \bar{\kappa}^{*}(g) \rho^{-1} \kappa R_g^{*} - (\cdots)^{T} \right)_{n'n} \\ &\quad + \left(A_g^{-1} \kappa \bar{\Delta}^{*}(g) \kappa(g) R_g^{*} - (\cdots)^{T} \right)_{n'n} \Bigg]\end{aligned}$$

Generalized Projected Fields - HFB Limit

- Limiting Expressions for Projected Matrices

$$
\begin{aligned}
R_g &= 1;\ y(g) = 1;\ Y(g) = 0;\ T(g) = 0;\ A(g) = \rho \\
\rho(g) &= \rho;\ \kappa(g) = \kappa;\ \bar{\kappa}^*(g) = \kappa^* \ , \\
\Gamma(g) &= \Gamma;\ \Delta(g) = \Delta;\ \bar{\Delta}^*(g) = \Delta^*
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial H_{sp}}{\partial \rho_{nn'}} &= e_{n'n} + e_{n'n} - (e\rho)_{n'n} - (\rho e)_{n'n} \ , \\
\frac{\partial H_{sp}}{\partial \kappa^*_{nn'}} &= (e\kappa)_{n'n} - (e\kappa)_{nn'} \ .
\end{aligned}
$$

- HFB

$$
\begin{aligned}
E_{\mathrm{HFB}} &= \mathrm{Tr}(e\rho) + \frac{1}{2}\mathrm{Tr}(\Gamma\rho) - \frac{1}{2}\mathrm{Tr}(\Delta\kappa^*) \\
&= H_{sp} + H_{ph} + H_{pp}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial H_{sp}}{\partial \rho_{nn'}} &= e_{n'n} \\
\frac{\partial H_{sp}}{\partial \kappa_{nn'}} &= 0
\end{aligned}
$$

$$
\begin{aligned}
H_{sp} &= \mathrm{Tr}(e\rho) \\
&= \mathrm{Tr}(e\rho) + \mathrm{Tr}(e\rho) - \mathrm{Tr}(e\rho) \\
&= \mathrm{Tr}(e\rho) + \mathrm{Tr}(e\rho) - \mathrm{Tr}\Big(e(\rho^2 - \kappa\kappa^*)\Big)
\end{aligned}
$$

Application to Density Functional Theory

- Coordinate Representation

$$\begin{aligned}\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \langle\Phi|c^\dagger_{\mathbf{r}'\sigma'}c_{\mathbf{r}\sigma}|\Phi\rangle \\ \kappa(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \langle\Phi|c_{\mathbf{r}'\sigma'}c_{\mathbf{r}\sigma}|\Phi\rangle\end{aligned}$$

$$\begin{aligned}c^\dagger_{\mathbf{r}\sigma} &= \sum_n \phi^*_n(\mathbf{r}\sigma)c^\dagger_n \ , \\ c_{\mathbf{r}\sigma} &= \sum_n \phi_n(\mathbf{r}\sigma)c_n\end{aligned}$$

$$\begin{aligned}\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \sum_{nn'} \rho_{nn'}\ \phi^*_{n'}(\mathbf{r}'\sigma')\ \phi_n(\mathbf{r}\sigma) \\ \kappa(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \sum_{nn'} \kappa_{nn'}\ \phi_{n'}(\mathbf{r}'\sigma')\ \phi_n(\mathbf{r}\sigma)\end{aligned}$$

$$\begin{aligned}\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma',g) &= \sum_{nn'} \rho_{nn'}(g)\ \phi^*_{n'}(\mathbf{r}'\sigma')\ \phi_n(\mathbf{r}\sigma) \\ \kappa(\mathbf{r}\sigma,\mathbf{r}'\sigma',g) &= \sum_{nn'} \kappa_{nn'}(g)\ \phi_{n'}(\mathbf{r}'\sigma')\ \phi_n(\mathbf{r}\sigma)\end{aligned}$$

Application to DFT

- Projected Energy

$$E^I(\rho,\kappa) = \int dg\, y(g)\, H(g)$$

where

$$H(g) = \frac{\langle\Phi|\hat{H}\hat{R}(g)|\Phi\rangle}{\langle\Phi|\hat{R}(g)|\Phi\rangle} = \int d^3\mathbf{r}\, \mathcal{H}(\mathbf{r},g)$$

- Rotated Fields

$$\begin{aligned}
h_{nn'}(g) &= \frac{\partial H(g)}{\partial \rho_{n'n}(g)} \\
&= \sum_{\sigma\sigma'} \int d^3\mathbf{r}\, \phi_n^*(\mathbf{r}\sigma)\, h(\mathbf{r},\sigma,\sigma',g)\, \phi_{n'}(\mathbf{r}\sigma') \ , \\
\Delta_{nn'}(g) &= \frac{\partial H(g)}{\partial \bar{\kappa}^*_{n'n}(g)} \\
&= \sum_{\sigma\sigma'} \int d^3\mathbf{r}\, \phi_n^*(\mathbf{r}\sigma)\, \Delta(\mathbf{r},\sigma,\sigma',g)\, \phi_{n'}(\mathbf{r}\sigma') \\
\bar{\Delta}^*_{nn'}(g) &= \frac{\partial H(g)}{\partial \kappa_{n'n}(g)} \\
&= \sum_{\sigma\sigma'} \int d^3\mathbf{r}\, \phi_n^*(\mathbf{r}\sigma)\, \bar{\Delta}^*(\mathbf{r},\sigma,\sigma',g)\, \phi_{n'}(\mathbf{r}\sigma')
\end{aligned}$$

Application to DFT

- HF Field

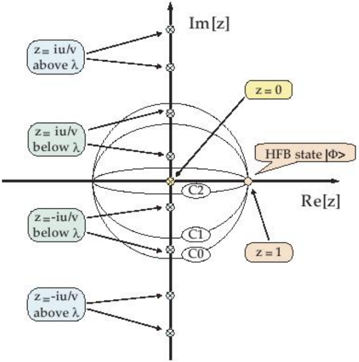
$$
\begin{aligned}
h^I_{nn'} &= \frac{\partial E^I}{\partial \rho_{n'n}} \\
&= \int y(g) \left[\frac{1}{y(g)} \frac{\partial y(g)}{\partial \rho_{n'n}} H(g) + \sum_{\alpha\beta} \frac{\partial H(g)}{\partial \rho_{\alpha\beta}(g)} \frac{\partial \rho_{\alpha\beta}(g)}{\partial \rho_{n'n}} \right. \\
&+ \left. \sum_{\alpha\beta} \frac{\partial H(g)}{\partial \kappa_{\alpha\beta}(g)} \frac{\partial \kappa_{\alpha\beta}(g)}{\partial \rho_{n'n}} + \sum_{\alpha\beta} \frac{\partial H(g)}{\partial \bar{\kappa}^*_{\alpha\beta}(g)} \frac{\partial \bar{\kappa}^*_{\alpha\beta}(g)}{\partial \rho_{n'n}} \right] \\
&= \int y(g) \left[\frac{1}{y(g)} \frac{\partial y(g)}{\partial \rho_{n'n}} H(g) + \sum_{\alpha\beta} h_{\beta\alpha}(g) \frac{\partial \rho_{\alpha\beta}(g)}{\partial \rho_{n'n}} \right. \\
&+ \left. \sum_{\alpha\beta} \bar{\Delta}^*_{\beta\alpha}(g) \frac{\partial \kappa_{\alpha\beta}(g)}{\partial \rho_{n'n}} + \sum_{\alpha\beta} \Delta_{\beta\alpha}(g) \frac{\partial \bar{\kappa}^*_{\alpha\beta}(g)}{\partial \rho_{n'n}} \right] \\
&= \int y(g) \left[\frac{1}{y(g)} Y_{nn'} H(g) + \left(h(g) R(g) \rho A_g^{-1} - A_g^{-1} \rho h(g) \rho(g) R_g + h.c. \right)_{nn'} \right. \\
&+ \left. \left(A_g^{-1} \kappa \bar{\Delta}^*(g) R_g - A_g^{-1} \kappa \bar{\Delta}^*(g) \rho(g) R_g - \kappa(g) \bar{\Delta}^*(g) R_g \rho\, A_g^{-1} + h.c. \right)_{nn'} \right]
\end{aligned}
$$

- Pairing Field

$$
\begin{aligned}
\Delta^I_{nn'} &= -\frac{\partial E^I}{\partial \kappa^*_{n'n}} \\
&= -\int y(g) \left[\frac{1}{y(g)} T_{nn'} H(g) + \left(A_g^{-1} \rho h(g) \kappa(g) R^*_g - (\cdots)^T \right)_{nn'} \right. \\
&+ \left. \left(A_g^{-1} \kappa \bar{\Delta}^*(g) \kappa(g) R^*_g + A_g^{-1} \rho \Delta(g) R^*_g + A_g^{-1} \rho \Delta(g) \bar{\kappa}^* \rho^{-1} \kappa R^*_g - (\cdots)^T \right)_{nn'} \right]
\end{aligned}
$$

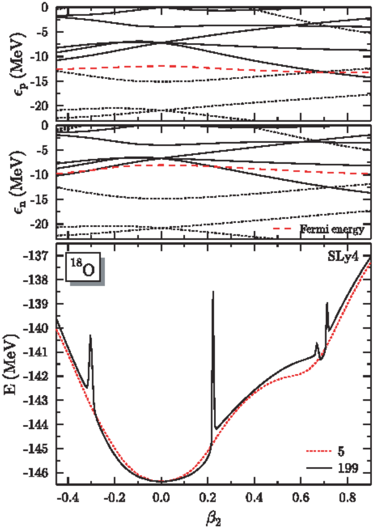
Divergence Problem in Projected DFT

$$\rho_z(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle\Phi|a^+_{\mathbf{r}'\sigma'}a_{\mathbf{r}\sigma}|\Phi(z)\rangle/\langle\Phi|\Phi(z)\rangle$$
$$= \sum_n \frac{z^2 v_n^2}{u_n^2 + z^2 v_n^2}\varphi_n(\mathbf{r}\sigma)\varphi_n^*(\mathbf{r}'\sigma'),$$
$$\chi_z(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle\Phi|a_{\mathbf{r}'\sigma'}a_{\mathbf{r}\sigma}|\Phi(z)\rangle/\langle\Phi|\Phi(z)\rangle$$
$$= \sum_n \frac{z^2 u_n v_n}{u_n^2 + z^2 v_n^2}\varphi_n(\mathbf{r}\sigma)2\sigma'\varphi_n^*(\mathbf{r}', -\sigma'),$$
$$\bar{\chi}_z(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle\Phi|a^+_{\mathbf{r}\sigma}a^+_{\mathbf{r}'\sigma'}|\Phi(z)\rangle/\langle\Phi|\Phi(z)\rangle$$
$$= \sum_n \frac{u_n v_n}{u_n^2 + z^2 v_n^2}\varphi_n^*(\mathbf{r}\sigma)2\sigma'\varphi_n(\mathbf{r}', -\sigma').$$



J. Dobaczewski et al., Phys. Rev. C **76**, 054315 (2007)

Divergence Problem in Projected DFT



M. Bender, T. Duguet and D. Lacroix, Phys. Rev. C **79**, 044319 (2009)

Summary and Outlook

Summary

1. Variation of an arbitrary energy functional depending on ρ and κ results into HFB like equations.
2. Projected energy functional can be completely expressed in terms of ρ and κ.
3. Expressions for the projected Fields have been explicitly derived for a generalized projection operator.
4. Number projected HFB equations have been applied to schematic and to the DFT models.

Outlook

1. Application of the projected HFB equations to angular momentum and isospin projection for Hamiltonian problems.
2. Study in detail the divergence problem in DFT.