Pairing in nuclei with functional theory with particle number conservation

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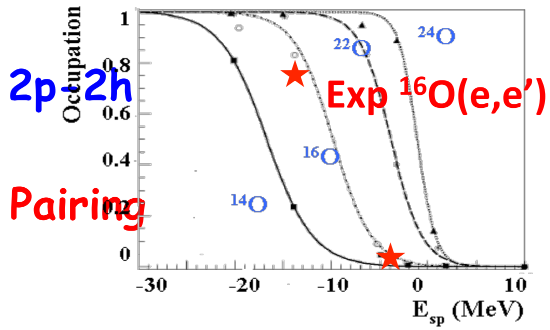
TDDM, Extended TDHF…

Correlation evolution

$$i\hbar\dot{\mathbf{C}}_{\alpha\beta} = \mathbf{V}_{\alpha\beta}((1-n_\alpha)^2 n_\beta^2 - (1-n_\beta)^2 n_\alpha^2) + \sum_\gamma \mathbf{V}_{\alpha\gamma}(1-2n_\alpha)\mathbf{C}_{\gamma\beta} - \sum_\gamma \mathbf{V}_{\gamma\beta}(1-2n_\beta)\mathbf{C}_{\alpha\gamma}$$



If pairing is neglected

$$i\hbar\frac{\partial}{\partial t}\rho_1 = [h_1[\rho],\rho_1] + \frac{1}{2}\mathrm{Tr}_2[\bar{v}_{12}, C_{12}]$$

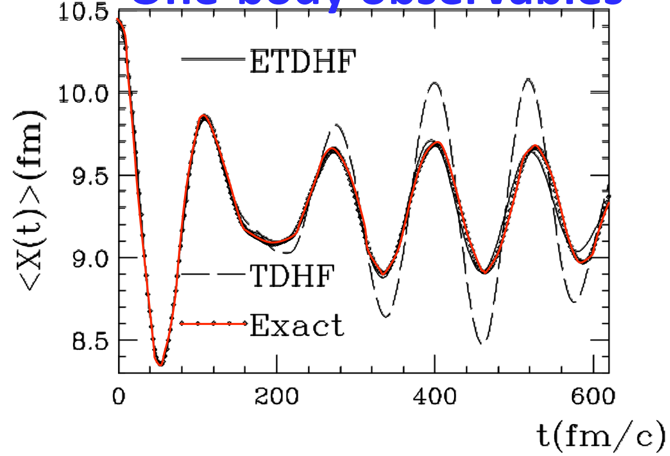
with

$$C_{12}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} U_{12}(t,s)\, F_{12}(s)\, U_{12}^\dagger(t,s)\, ds + \delta C_{12}(t)$$

$$F_{12}:\ (1-\rho_1)(1-\rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2 v_{12}(1-\rho_1)(1-\rho_2)$$

$$\frac{d}{dt}n_\lambda(t) = \int_{t_0}^{t} dt' \left\{ \bar{n}_\lambda(t')\, \mathcal{W}_\lambda^+(t,t') - n_\lambda(t')\, \mathcal{W}_\lambda^-(t,t') \right\}$$

One-body observables



Lacroix et al, NPA651 (1999) 369.

Correlation is a functional of occupation numbers (non local in time)

➡ **Let's try to find directly functionals of n_i**

EDF from a different perspective: introducing natural orbital and occupation

Starting point

$$H = \sum_{ij} \langle i|T|j\rangle a_i^+ a_j + \frac{1}{2}\sum_{ijkl} \langle ij|v_{12}|lk\rangle a_i^+ a_j^+ a_l a_k$$

Exact solution

Variational parameters

$$E_{\rm Exact} = \langle \Psi|H|\Psi\rangle = E_{\rm MF}[\rho] + E_{\rm Corr}[C_{12}]$$

$$\rho = \sum |\varphi_i\rangle n_i \langle\varphi_i| \qquad \{\varphi_i, n_i, C_{ij;kl}\}$$

$$C_{12} = \rho_{12} - \rho_1\rho_2(1-P_{12})$$

Mean-Field (EDF)

$$E_{\rm Exact} \simeq \mathcal{E}_{\rm MF}[\rho] \qquad \rho = \sum |\varphi_i\rangle\langle\varphi_i| \qquad \{\varphi_i\}_{i=1,A}$$

Mean-Field + Pairing

$$E_{\rm Exact} \simeq \mathcal{E}_{\rm MF}[\rho] + \mathcal{E}_{\rm Pair}[\kappa]$$

$$\rho = \sum |\varphi_i\rangle n_i \langle\varphi_i| \qquad \{\varphi_i, n_i\}_{i=1,\infty}$$

$$C_{i\bar{i},j\bar{j}} \simeq \sqrt{n_i(1-n_i)}\sqrt{n_j(1-n_j)}$$

MF + Pairing +Conf. Mixing

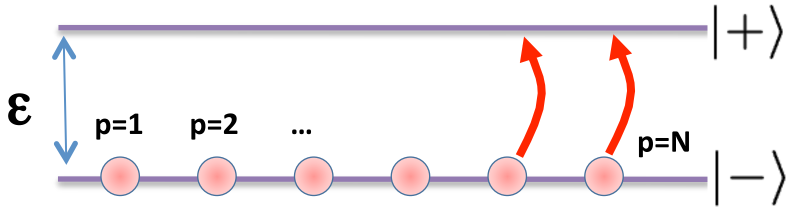
or

$$E_{\rm Exact} \simeq \mathcal{E}_{\rm MF}[\varphi_i, n_i] + \mathcal{E}_{\rm Corr}[\varphi_i, n_i]$$

Improve the functional of occupation numbers and natural orbitals

DMFT - Gilbert (1975).
Lieb (1983), Papenbrock, Bhattacharyya, PRC75 (2007)

Lipkin Model



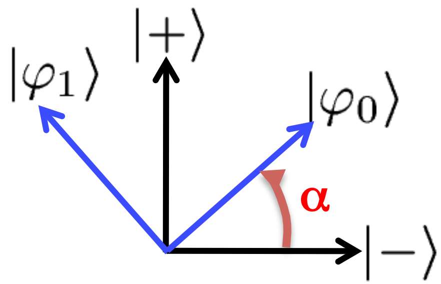
See for instance : Ring and Schuck book
Severyukhin, Bender, Heenen, PRC74 (2006)

$$H = \varepsilon J_0 - \frac{V}{2}(J_+J_+ + J_-J_-)$$

$$J_0 = \frac{1}{2}\sum_{p=1}^{N}\left(c^\dagger_{+,p}c_{+,p} - c^\dagger_{-,p}c_{-,p}\right)$$

$$J_+ = \sum_{p=1}^{N} c^\dagger_{+,p}c_{-,p}, \quad J_- = J_+^\dagger,$$

Natural orbitals and Hartree-Fock solution

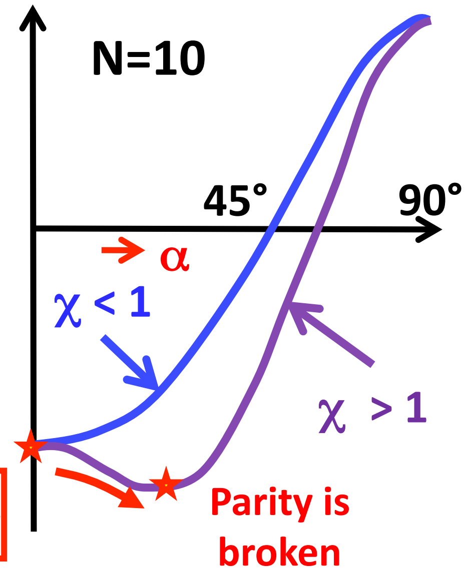


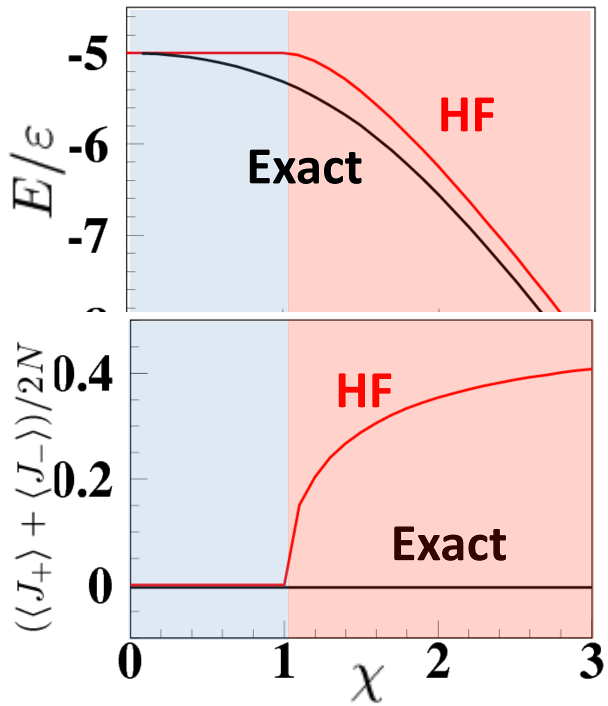
HF functional : $n_{0,1}$ = 1 or 0

$$|\Phi\rangle = \Pi_{p=1}^{N} a^\dagger_{0,p}|-\rangle$$

$$\mathcal{E}_{MF}[\alpha,\varphi] = -\frac{\varepsilon N}{2}\left\{\cos(2\alpha) + \frac{\chi}{2}\sin^2(2\alpha)\cos(2\varphi)\right\}$$

with $\chi = \dfrac{V(N-1)}{\varepsilon}$





Conf. Mixing is exact in the Lipkin model

Lacroix, PRC79 (2009)

Goal : $E_{\text{Exact}} \simeq \mathcal{E}_{\text{MF}}[\varphi_i, n_i] + \mathcal{E}_{\text{Corr}}[\varphi_i, n_i]$

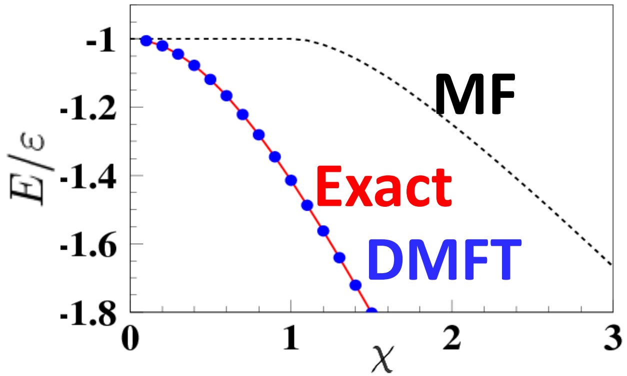
$$\rho = \sum_{p=1}^{N} \left\{ |\varphi_{0,p}\rangle n_0 \langle \varphi_{0,p}| + |\varphi_{1,p}\rangle n_1 \langle \varphi_{1,p}| \right\}$$

?

$$\mathcal{E}_{\text{MF}} = -\frac{\varepsilon}{2} N \left\{ \cos(2\alpha)(2n_0 - 1) + \frac{\chi}{2} \sin^2(2\alpha)(2n_0 - 1)^2 \right\}$$

The N=2 case

$$\mathcal{E}^{N=2}_{\text{Corr}} = -2V \left\{ \sin^2(2\alpha) n_0 (1 - n_0) + \left(\sin^4(\alpha) + \cos^4(\alpha)\right) \sqrt{n_0(1-n_0)} \right\}$$



Large N limit

Dusuel and Vidal, PRL93 (2004).

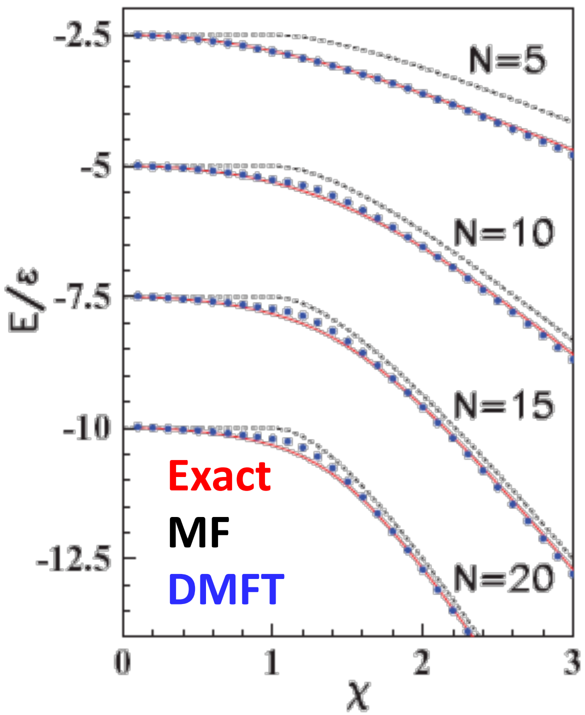
$$\langle J_x^2 \rangle \propto N^{4/3}$$

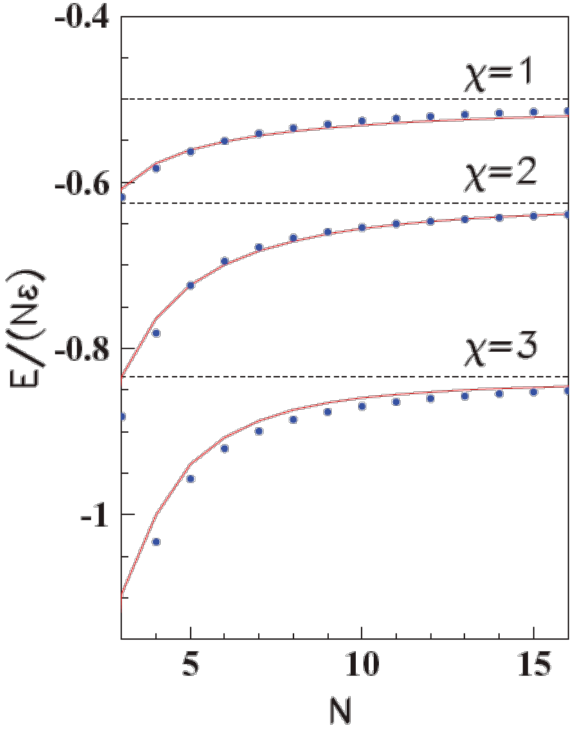
$$\mathcal{E}^{N}_{\text{Corr}} \propto N^{4/3}$$

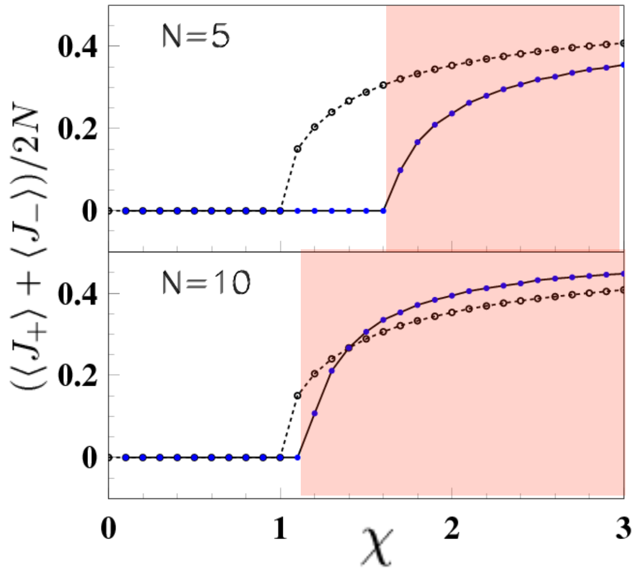
Indep Pair approx

$$\mathcal{E}^{N}_{\text{Corr}}[\varphi_i, n_i] = \eta(N) \frac{N(N-1)}{2} \mathcal{E}^{N=2}_{\text{Corr}}[\varphi_i, n_i]$$

Fitted parameter $\eta(N) = 1.5 N^{-2/3}$







Important issues

- Symmetry breaking: restoration or not ?
- Excited states ? Lowest state for each J^{π} (Yes) others (Maybe) ?
- Dynamics (Yes)- then excited state (Yes)

What about a functional for pairing with particle number conservation?

Functional Theory for Pairing with particle number conservation

BCS *vs* Projected BCS state

Illustration: Richardson Hamiltonian

$$E \rightarrow \mathcal{E}(n_i, C_{ij}) = \sum_i \varepsilon_i n_i + -\frac{g}{2}\sum_{i,j} C_{ij} \quad \text{with} \quad n_i = \frac{\langle \Phi | a_i^\dagger a_i | \Phi \rangle}{\langle \Phi | \Phi \rangle}, \quad C_{ij} = \frac{\langle \Phi | a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

BCS

$$|BCS\rangle \propto \prod_i (1 + x_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$$

$$x_i = (v_i / u_i)$$

$$n_i = \frac{|x_i|^2}{(|x_i|^2 + 1)}$$

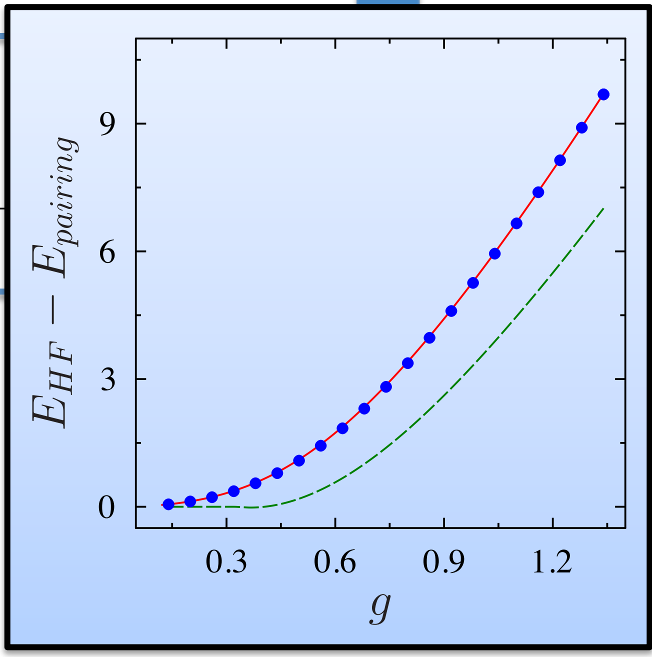
$$C_{ij} = \frac{x_i^* x_j}{(|x_i|^2 + 1)(|x_j|^2}$$

PBCS

$$|N\rangle = \left(\sum_i x_i a_i^\dagger a_{\bar{i}}^\dagger \right)^N |-\rangle$$

$$= N|x_i|^2 \frac{\sum^{\neq}_{(i_1,\cdots i_{N-1}) \neq (i)} |x_{i_1}|^2 \cdots |x_{i_{N-1}}|^2}{\sum^{\neq}_{(i_1,\cdots i_N)} |x_{i_1}|^2 \cdots |x_{i_N}|^2}$$

$$= N x_i^* x_j \frac{\sum^{\neq}_{(i_1,\cdots i_K) \neq (i,j)} |x_{i_1}|^2 \cdots |x_{i_K}|^2}{\sum^{\neq}_{(i_1,\cdots i_N)} |x_{i_1}|^2 \cdots |x_{i_N}|^2}$$



Sandulescu and Bertsch, PRC 78, (2008)

Functional Theory for Pairing with particle number conservation

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BCS

$$|BCS\rangle \propto \prod_i (1 + x_i a_i^\dagger a_{\bar{i}}^\dagger) |-\rangle$$

$$x_i = (v_i / u_i)$$

$$n_i = \frac{|x_i|^2}{(|x_i|^2 + 1)}$$

$$C_{ij} = \frac{x_i^* x_j}{(|x_i|^2 + 1)(|x_j|^2 + 1)}$$

$$|x_i|^2 = \frac{n_i}{(1 - n_i)}$$

PBCS

$$|N\rangle = \left(\sum_i x_i a_i^\dagger a_{\bar{i}}^\dagger \right)^N |-\rangle$$

$$n_i = N |x_i|^2 \frac{\sum^{\neq}_{(i_1, \cdots i_{N-1}) \neq (i)} |x_{i_1}|^2 \cdots |x_{i_{N-1}}|^2}{\sum^{\neq}_{(i_1, \cdots i_N)} |x_{i_1}|^2 \cdots |x_{i_N}|^2}$$

$$C_{ij} = N x_i^* x_j \frac{\sum^{\neq}_{(i_1, \cdots i_K) \neq (i,j)} |x_{i_1}|^2 \cdots |x_{i_K}|^2}{\sum^{\neq}_{(i_1, \cdots i_N)} |x_{i_1}|^2 \cdots |x_{i_N}|^2}$$

?

$$\mathcal{E}(\{x_i\})$$

$$\mathcal{E}(\{n_i\})$$

Implicit Functional of occupation numbers for Pairing

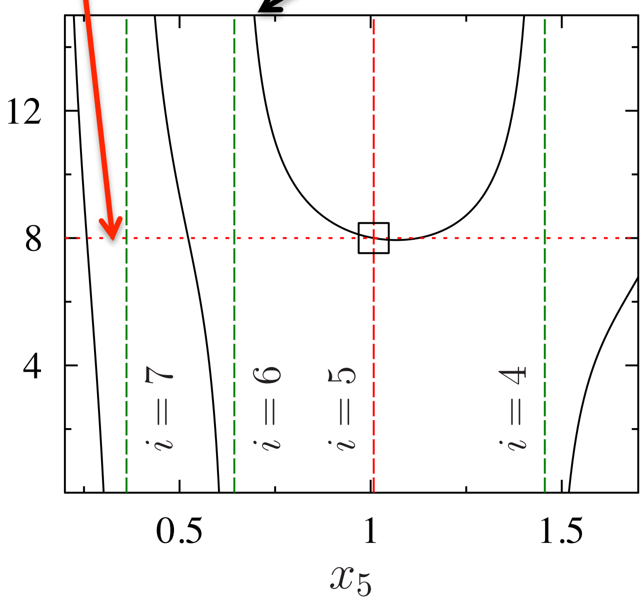
Existence of the functional

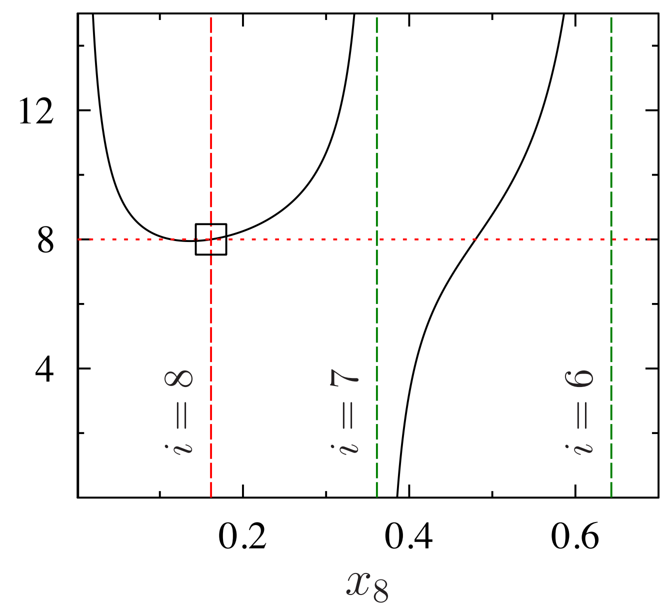
$$\mathcal{E}(\{x_i\}) \;\longrightarrow\; \mathcal{E}(\{n_i\})$$

Can we prove that the x_i are functional of the n_i? Yes

$$N(1-n_i) \quad = \quad \sum_{j\neq i}(n_j-n_i)\left\{\frac{|x_j|^2}{|x_j|^2-|x_i|^2}\right\}$$

$\Rightarrow$ The $\{x_i\}$ are implicit functional of the occupation



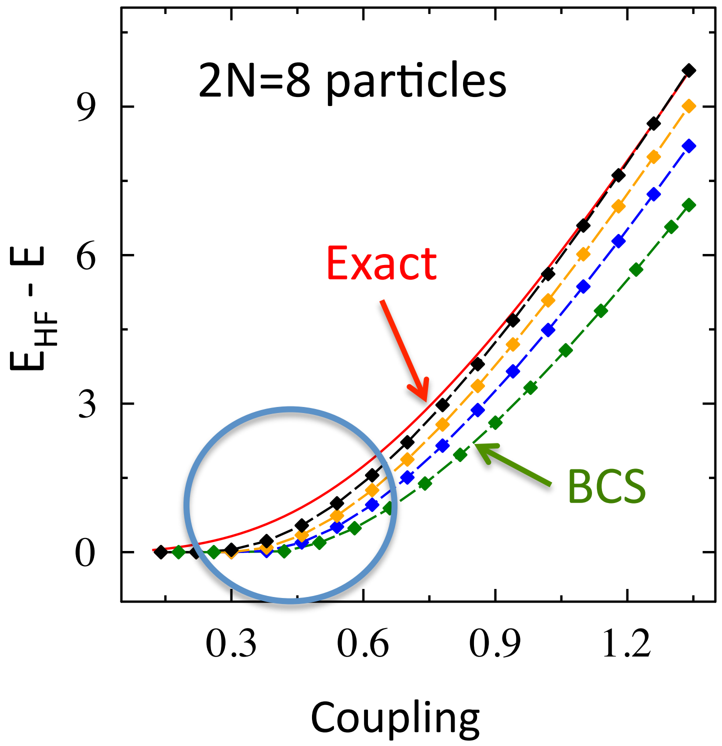


Explicit Functional of occupation numbers for Pairing

$$n_i = N|x_i|^2 \frac{\sum^{\neq}_{(i_1,\cdots i_{N-1})\neq(i)} |x_{i_1}|^2 \cdots |x_{i_{N-1}}|^2}{\sum^{\neq}_{(i_1,\cdots i_N)} |x_{i_1}|^2 \cdots |x_{i_N}|^2} \quad \Longrightarrow \quad x_i = \mathcal{F}(n_i) \ ?$$

A new systematic expansion beyond BCS:

$$\begin{aligned} |x_i|^2 \simeq & \left(\frac{n_i}{1-n_i}\right)\Big\{1 \quad \longleftarrow \text{BCS} \\ & - \frac{1}{N} n_i \\ & + \frac{1}{N(N-1)} \sum_{j\neq i} n_j^2 [1-(n_i+n_j)] \\ & + \frac{1}{N(N-1)(N-2)} \sum^{\neq}_{k,j} n_j^2 n_k^2 \,[2-(n_i+n_j+n_k)] \\ & + \quad \cdots \quad \Big\} \end{aligned}$$



Lacroix and Hupin, submitted to PRL

Explicit Functional of occupation numbers for Pairing

All contributions can be approximately summed to give:

$$|x_i|^2 = \left(\frac{n_i}{1 - n_i} \right) [a_0 + a_1 n_i + \cdots]$$

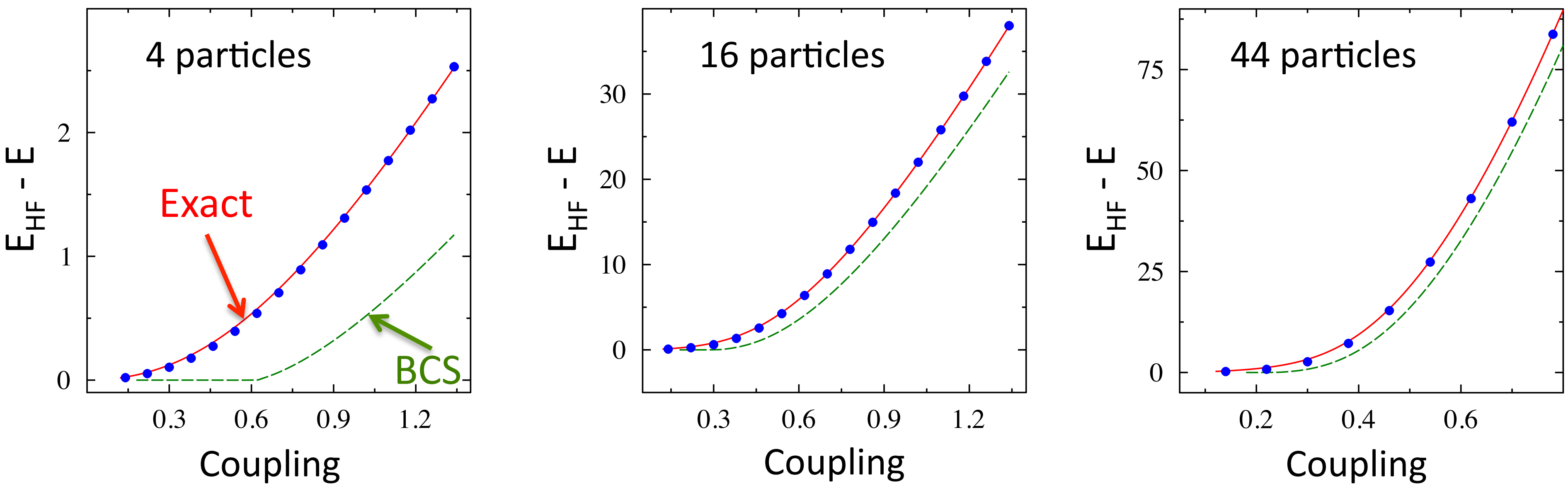
$$a_1 = -\frac{1}{N} \frac{1 - s_2^N}{1 - s_2}$$

with

$$a_0 = 1 - (s_2 - s_3) \frac{\partial a_1}{\partial s_2}$$

$$s_2 = \frac{1}{N} \sum_i n_i^2 \qquad s_3 = \frac{1}{N} \sum_i n_i^3$$

Application



Perspectives and future applications

- Generalization to other algebraic model
- Time-Dependent EDF with pairing
  1-TDHF+BCS (K. Washiyama)
  2-Beyond BCS
- Application to nuclear structure and ultrasmall metallic grain (G. Hupin)