Combining symmetry breaking and restoration with configuration interaction: application to the pairing problem

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Outline:

- Combining Many-Body perturbation theory and symmetry-breaking
- New development: CI based on projected quasi-particle states + variation
- Outlooks: projected QRPA theory + CI, deformation

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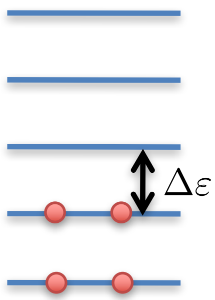
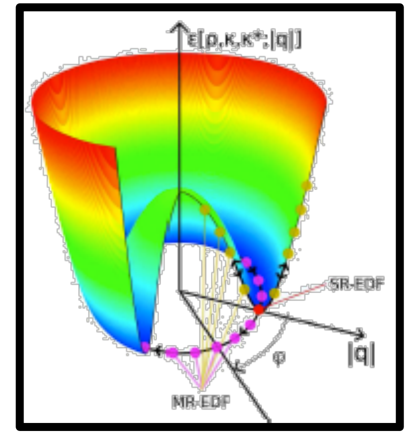
Testing ideas with the pairing model



$$H = \sum_{i=1}^{\Omega} \varepsilon_i a_i^\dagger a_i + \sum_{i \neq j}^{\Omega} v_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

Step 1: introduce symmetry breaking
Quasi-particle vacuum

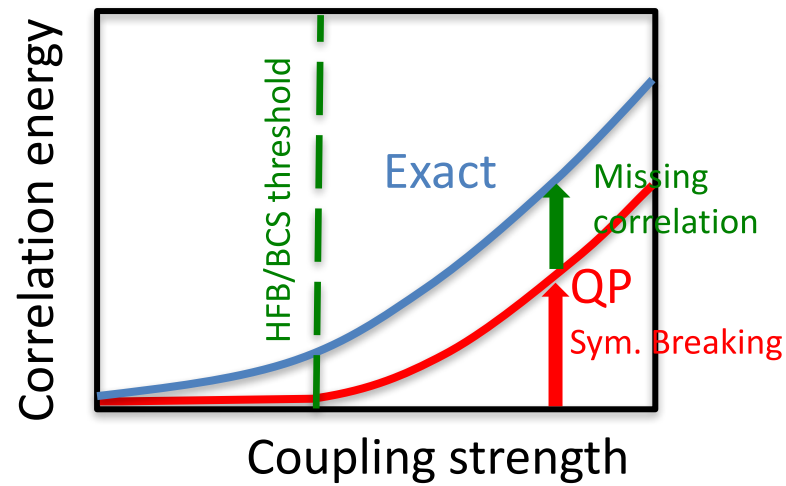
$$|QP\rangle = \Pi \beta_i |-\rangle$$



Step 2: Use projection technique

$$P^N = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \; e^{i\varphi(\hat{N} - N)} \qquad |N\rangle = P_N |QP\rangle$$

$$E_{\rm cor} = E - E_{HF}$$



Mean-Field

$$\delta \langle QP | H | QP \rangle = 0$$

Projection
After Variation
Does not solve the threshold problem

Variation After Projection

$$\delta \langle QP | P_N H P_N | QP \rangle = 0$$

Solve the problem but is rather involved.
(full VAP, Restricted VAP…)

Testing ideas with the pairing model

$$H = \sum_{i=1}^{\Omega} \varepsilon_i a_i^\dagger a_i + \sum_{i\neq j}^{\Omega} v_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

$\Delta\varepsilon$

Direct diagonalization

- Introduce a many-body basis $\{|\Psi_i\rangle\}$
- Perform direct diagonalization in a restricted or full space

$$|\Phi\rangle = \sum_i c_i |\Psi_i\rangle \qquad H|\Phi\rangle = E|\Phi\rangle$$

→ Gives eventually the exact solution (with help of symmetries, ex: seniority)

→ Gives access to excited states

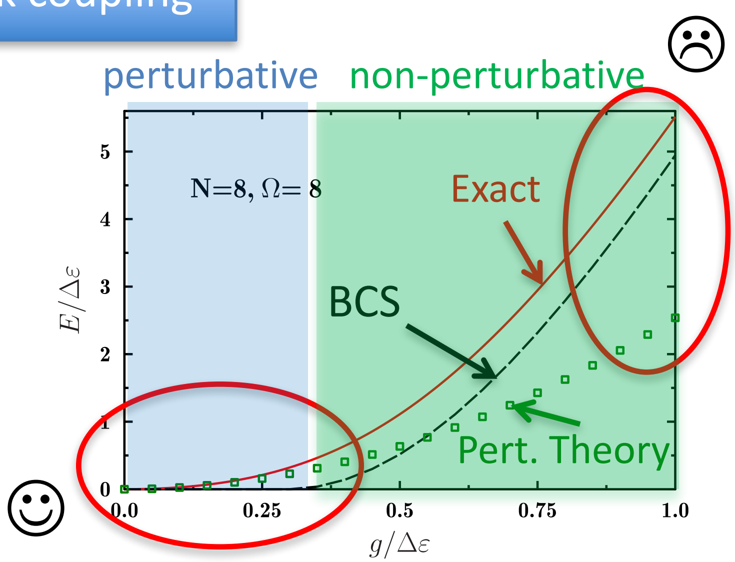
Simplification: perturbative approach to pairing at weak coupling

Normal phase: standard perturbation theory

$$H = \underbrace{\sum_{i=1}^{\Omega} \varepsilon_i a_i^\dagger a_i}_{H_0} + \underbrace{g \sum_{i\neq j}^{\Omega} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j}_{V_{\text{res}}}$$

Treated as a perturbation

→ $|\Phi_0'\rangle = |\Phi_0\rangle + \sum c_{2p2h} |\Phi_{2p2h}\rangle$



From particles to quasi-particles

$$|0, N\rangle \Rightarrow |QP\rangle$$
$$a_i^\dagger \Rightarrow \beta_i^\dagger$$

$$H \Rightarrow H_0 = E_0 + \sum E_i \beta_i^\dagger \beta_i$$

$$H|QP\rangle = \left(H_0 - \underbrace{\sum_{i \neq j} v_{ij} U_i^2 V_j^2 \beta_i^\dagger \beta_{\bar{i}}^\dagger \beta_j^\dagger \beta_{\bar{j}}^\dagger}_{V_{\mathrm{res}}} \right) |QP\rangle$$

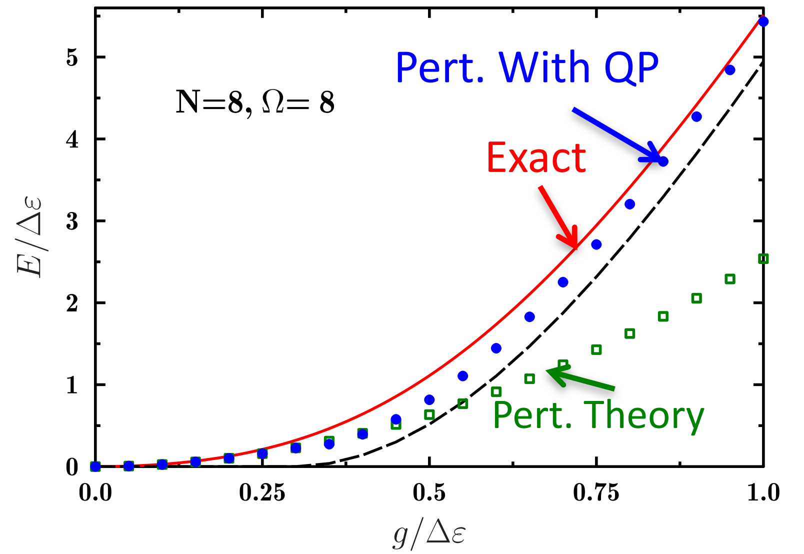
Step 1: Perturbation theory

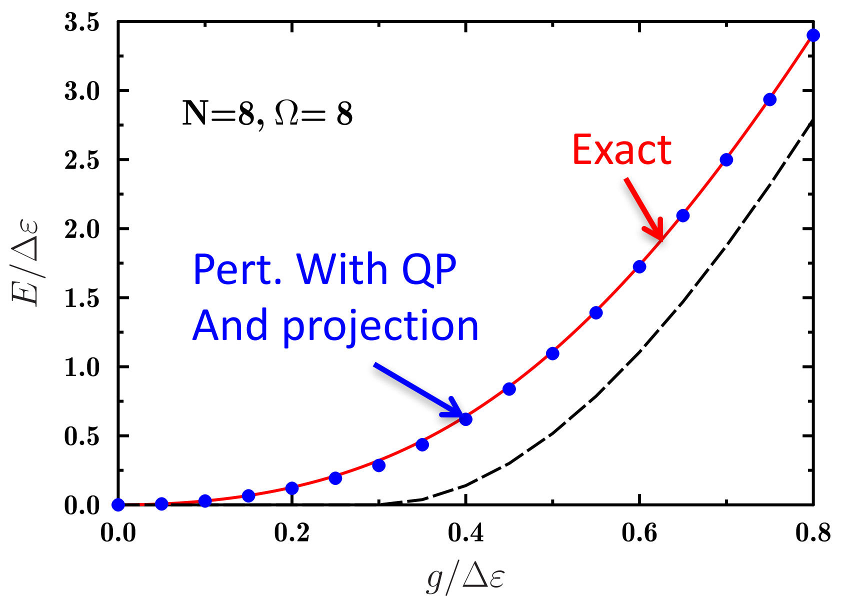
$$|\Phi_0'\rangle = |QP\rangle + \sum c_{4\mathrm{QP}} |\Phi_{4\mathrm{QP}}\rangle$$

Step 2: Projection on particle number

$$E_0 = \frac{\langle \Phi_0' | P_N H P_N | \Phi_0' \rangle}{\langle \Phi_0' | P_N | \Phi_0' \rangle}$$ (PAV like method)

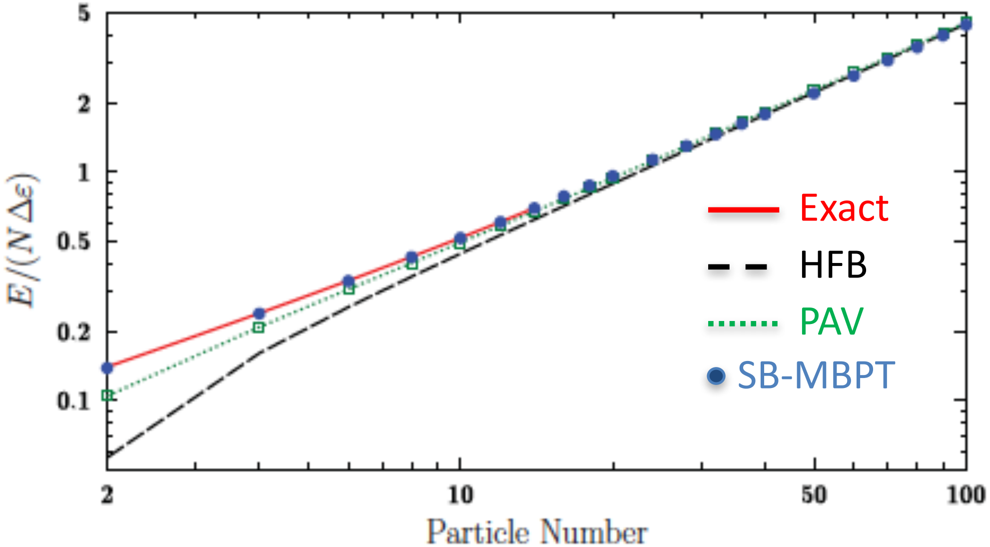
Very nice surprise





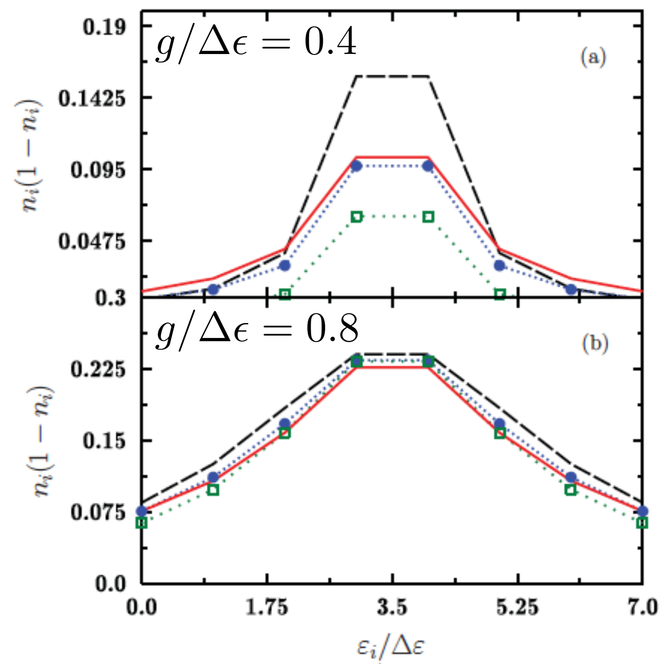
Lacroix and Gambacurta PRC86, (2012).

Scales nicely with particle number



Single-particle occupancy

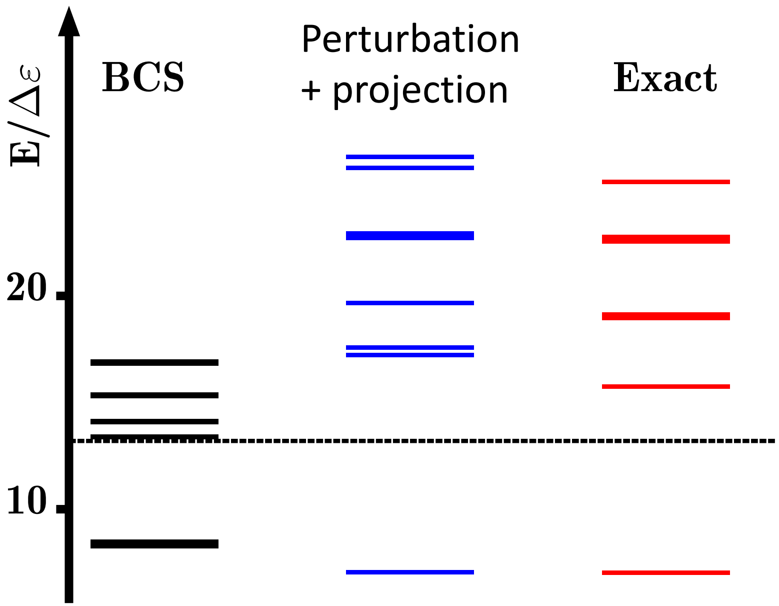
$N = \Omega = 8$



Lacroix and Gambacurta PRC86, (2012).

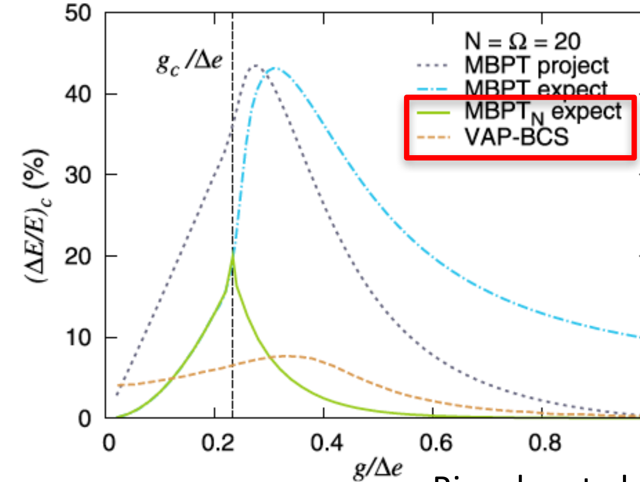
Second order MBPT with symmetry-breaking for pairing: some success

Result of perturbation + projection technique



More precise comparisons

$$(\Delta E/E)_c = \left(1 - \frac{E_c^{\text{approx}}}{E_c^{\text{exact}}}\right) \times 100\%$$

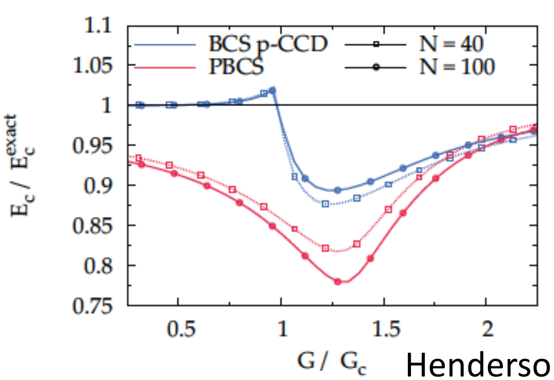


$$\frac{\langle N|H|N\rangle}{\langle N|N\rangle}$$

Ripoche et al, PRC (2017)

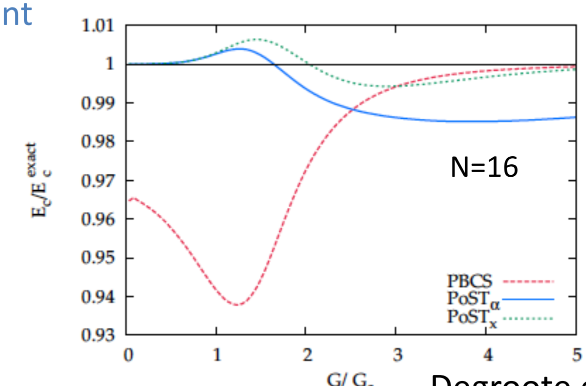
Alternative Many-body technique with symmetry breaking

Coupled-Cluster



Henderson et al, PRC (2014)

Recent improvement



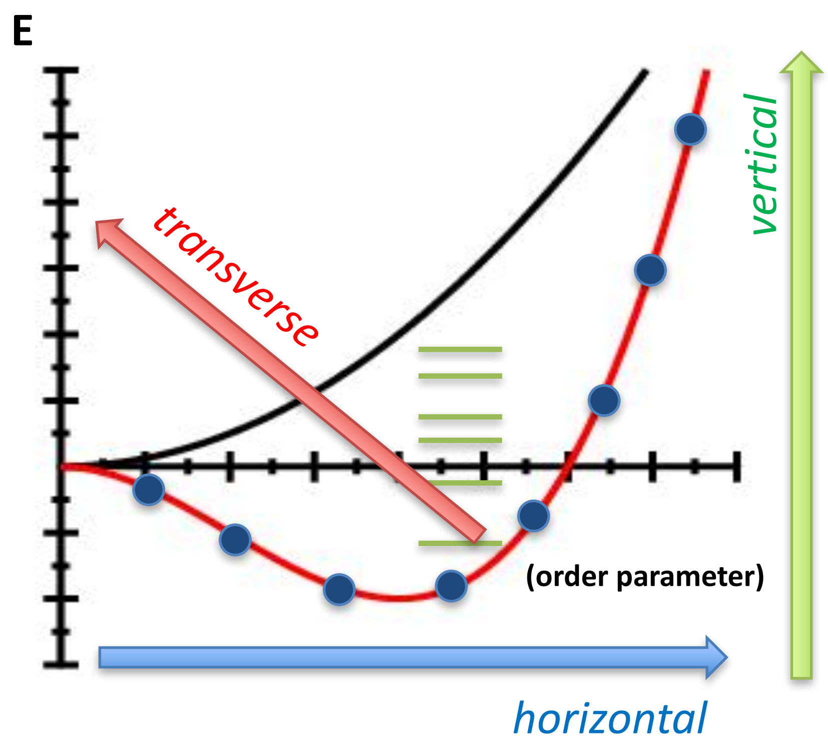
~1-2% error !

Degroote et al, PRB (2016)

Current Goals: Explore the possibility to combine many-body technique and symmetry breaking

- Provide competitive and versatile many-body techniques
- Provide new accurate tools for ab-initio approaches

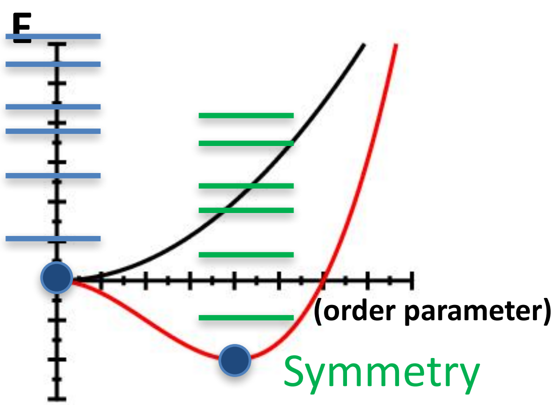
Strategy Use *vertical* or *horizontal* approach or a *transverse* approach



- From MBPT to CI approach
- Perform diagonalization in a very restricted space
- How far can we push? Competiveness?
- Redundancy and non-orthogonality Of many-body states?
- Application to other symmetries?

Up to now…

Symmetry preserving case



Symmetry Breaking case

- Apply MBPT with Slater or QP states
- $$|\Phi_\alpha\rangle = c^0_\alpha |0\rangle + \sum_{4QP} c^{4QP}_\alpha |4QP\rangle$$
- $$E_\alpha = \frac{\langle \Phi_\alpha | P_N H P_N | \Phi_\alpha \rangle}{\langle \Phi_\alpha | P_N | \Phi_\alpha \rangle}$$

Now

- Use the projected QP states as a basis for diagonalization

Similar idea was used in Gambacurta, Lacroix PRC(2014)

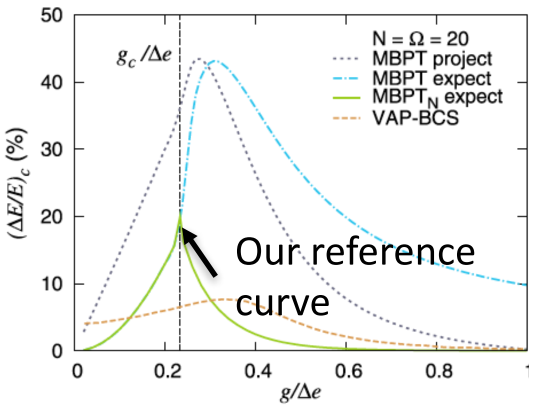
Solve BCS, HFB Generate GS, 2QP,4QP, … → Project → Projected (non-orthogonal) GS, 2QP,4QP, … → Ortho-normalize → New N-body Basis (strongly entangled state) → Diag H

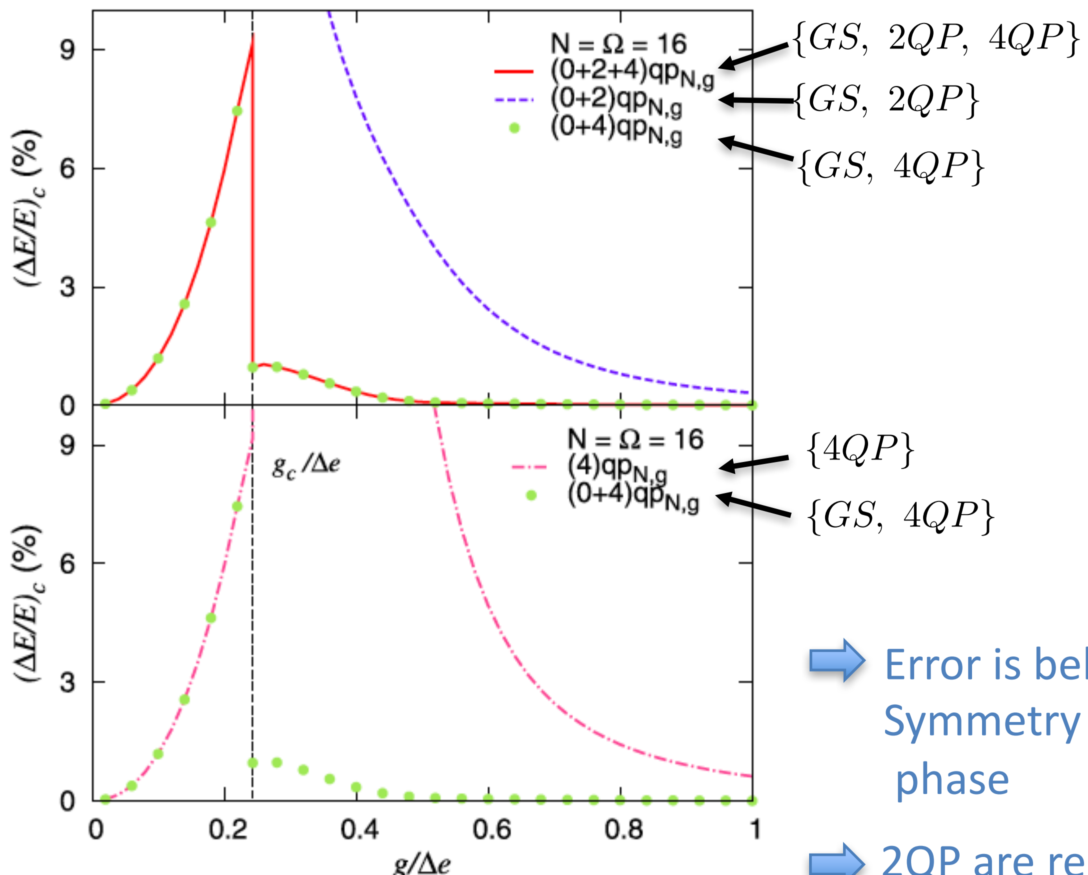
Generate states

Diag. the Norm matrix. Reject redundant states

Compute matrix elements Diagonalization

$$H = \sum_{i=1}^{\Omega} \varepsilon_i a_i^\dagger a_i + \sum_{i \neq j}^{\Omega} v_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

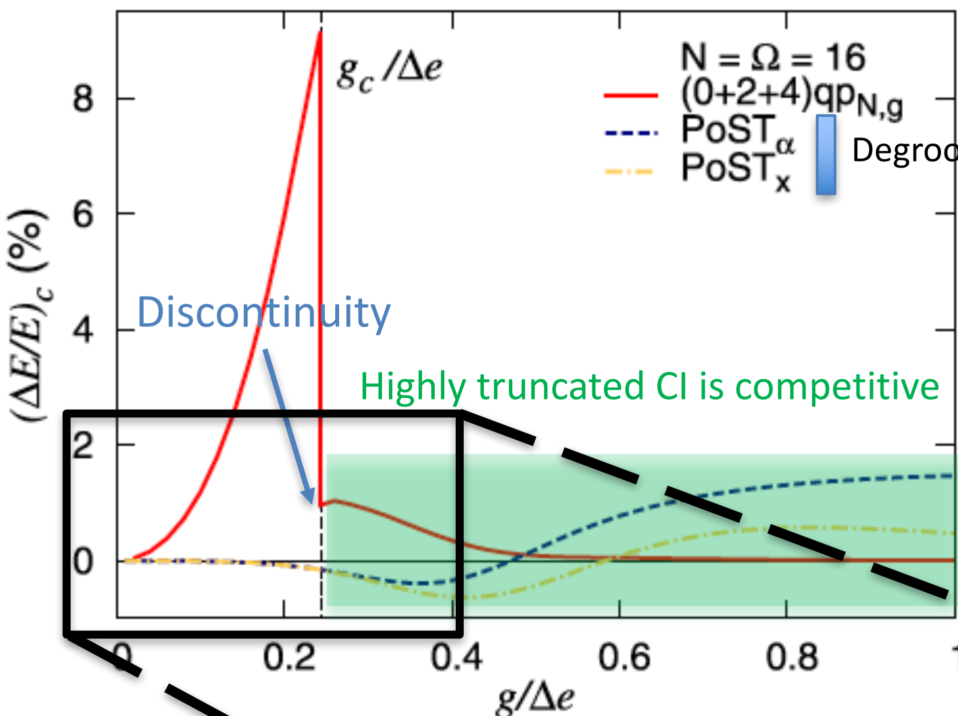




Ripoche, Lacroix, Gambacurta, Ebran, Duguet PRC (2017)

- Error is below 2% in Symmetry Breaking phase
- 2QP are redundant
- GS is essential

Comparison with *state of the art* coupled cluster



Ripoche, Lacroix, Gambacurta, Ebran, Duguet PRC (2017)

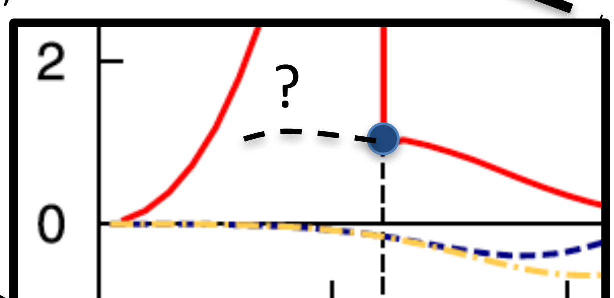
Discussion on the discontinuity

$g < g_c$ $\quad n_{\mathrm{st}} = 1 + n_{2p2h} = 1 + \Omega^2/4$

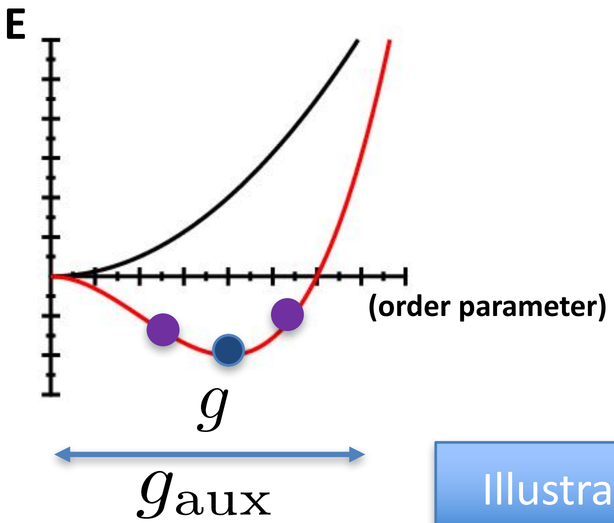
$\Omega = 16 \Rightarrow$ 65 states

$g > g_c$ $\quad n_{\mathrm{st}} = 1 + n_{4QP} = 1 + \Omega(\Omega - 1)/2$

$\Omega = 16 \Rightarrow$ 121 states



QP(g_0) states with g_0 different from g can be used

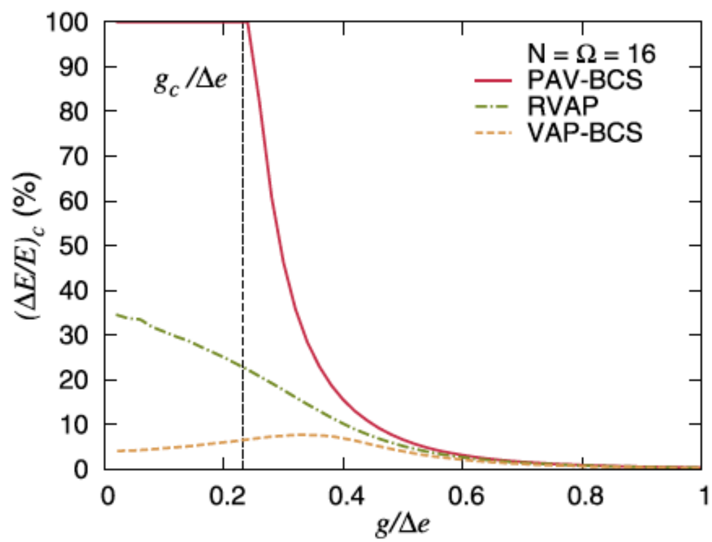


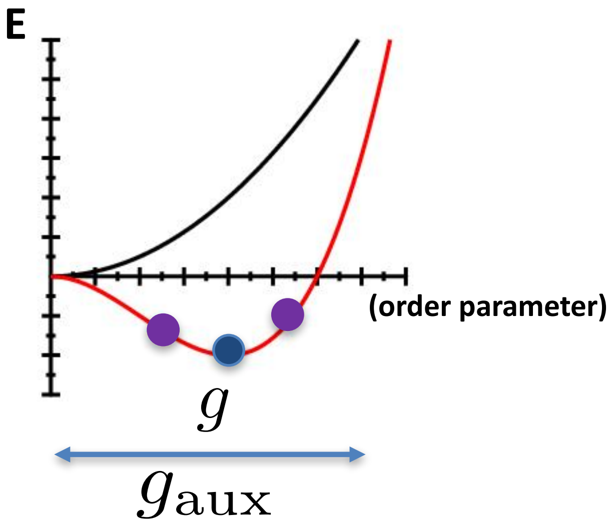
The idea is to use some parameters to vary the Hilbert space of states (ex. the interaction strength)

Similar spirit as the Restricted VAP

Rodriguez, Egido, Robledo, PRC (2005)

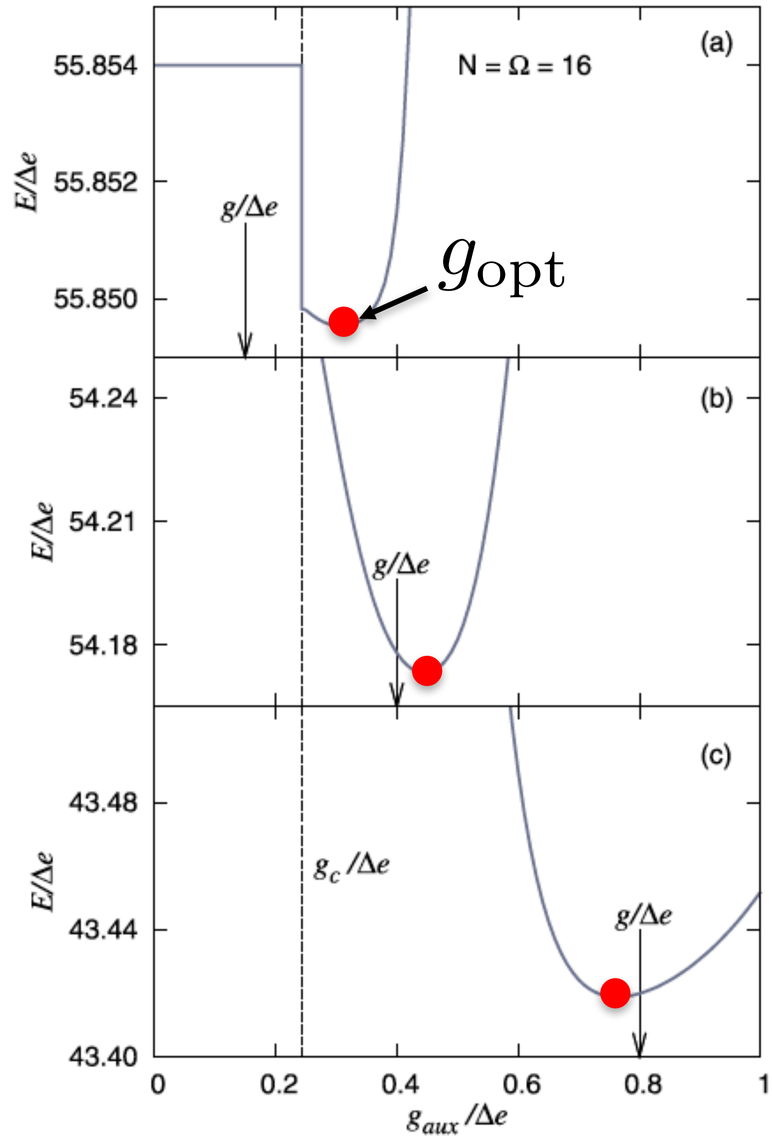
Illustration of the standard Restricted VAP



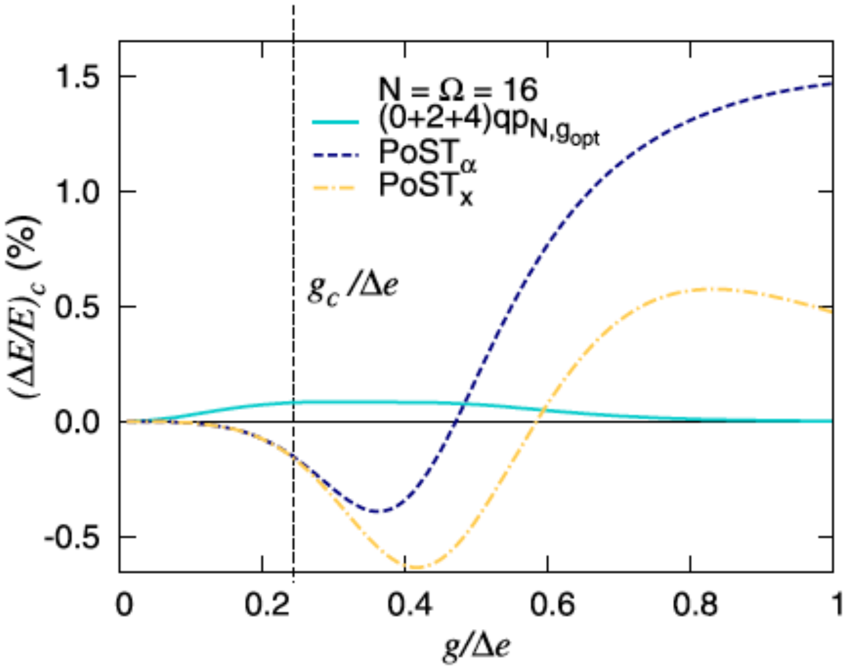


$$\{GS,\ 2QP,\ 4QP\}(g_{\text{aux}})$$

$$E_\alpha(g_{\text{aux}})$$



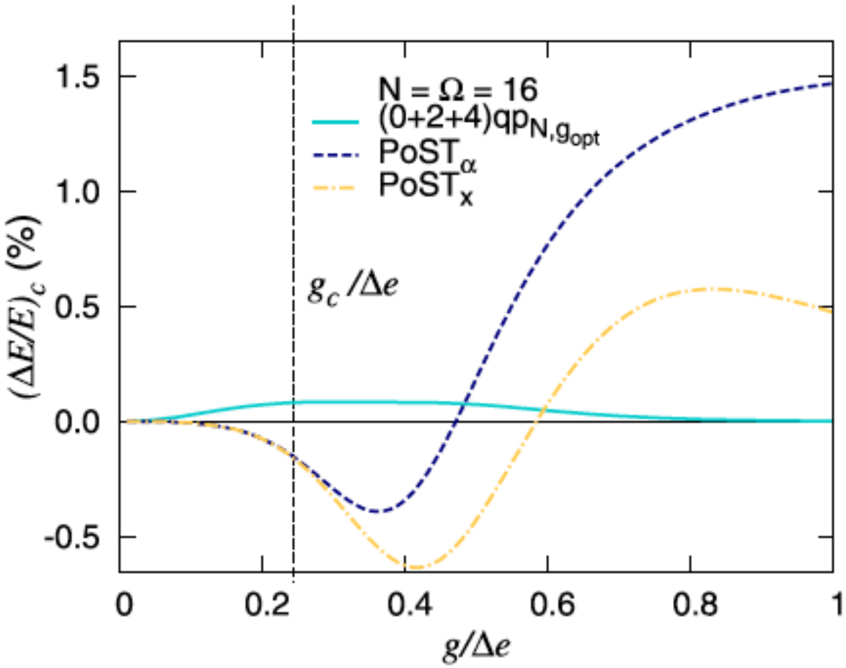
Number of states: comparison with symmetry-conserving CI

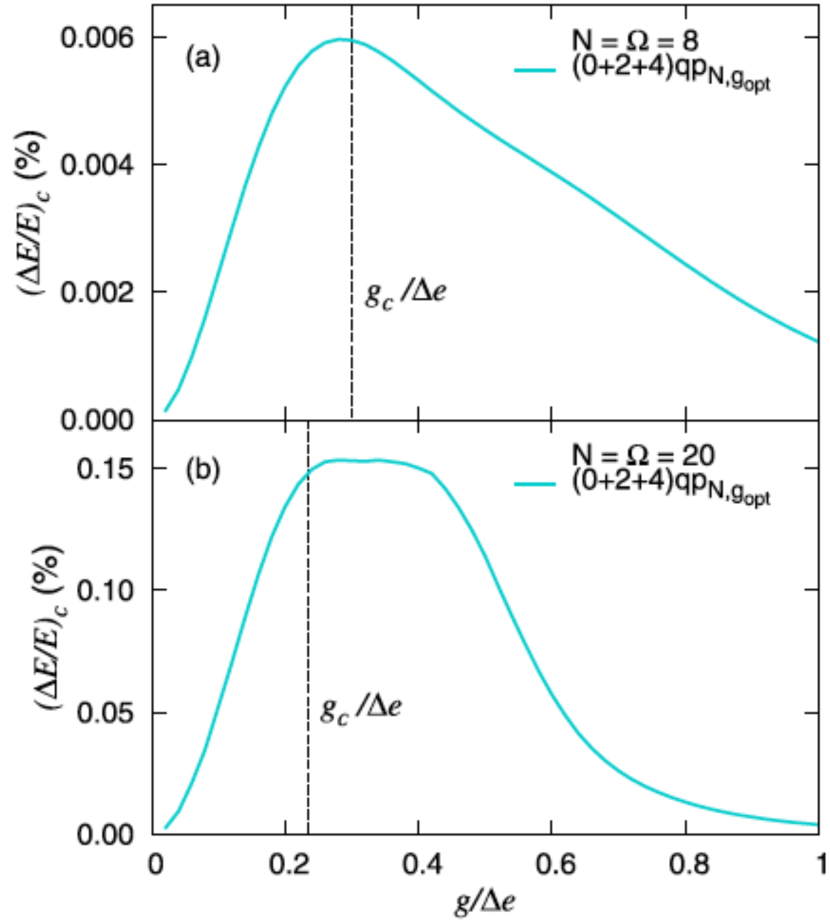


$N = 16$	n_{st}	$g = 0.18$	$g = 0.54$	$g = 0.66$
2p-2h	65	0.64%	20.92%	29.37%
4p-4h	849	0.01%	5.22%	9.59%
6p-6h	3985	0.00%	0.60%	1.66%
8p-8h	8885	0.00%	0.03%	0.12%
$(0+2)\text{qp}_{N,g}$	17	100%	3.52%	1.70%
$(0+4)\text{qp}_{N,g}$	121	0.64%	0.07%	0.04%
$(0+2+4)\text{qp}_{N,g}$	137	0.64%	0.07%	0.04%
$(0+2)\text{qp}_{N,g_{opt}}$	17	9.20%	3.34%	1.66%
$(0+4)\text{qp}_{N,g_{opt}}$	121	0.07%	0.07%	0.03%
$(0+2+4)\text{qp}_{N,g_{opt}}$	137	0.07%	0.07%	0.03%
Exact	12870	0.00%	0.00%	0.00%

mp-mh from Pillet et al, PRC (2005)

Different particle/Model space

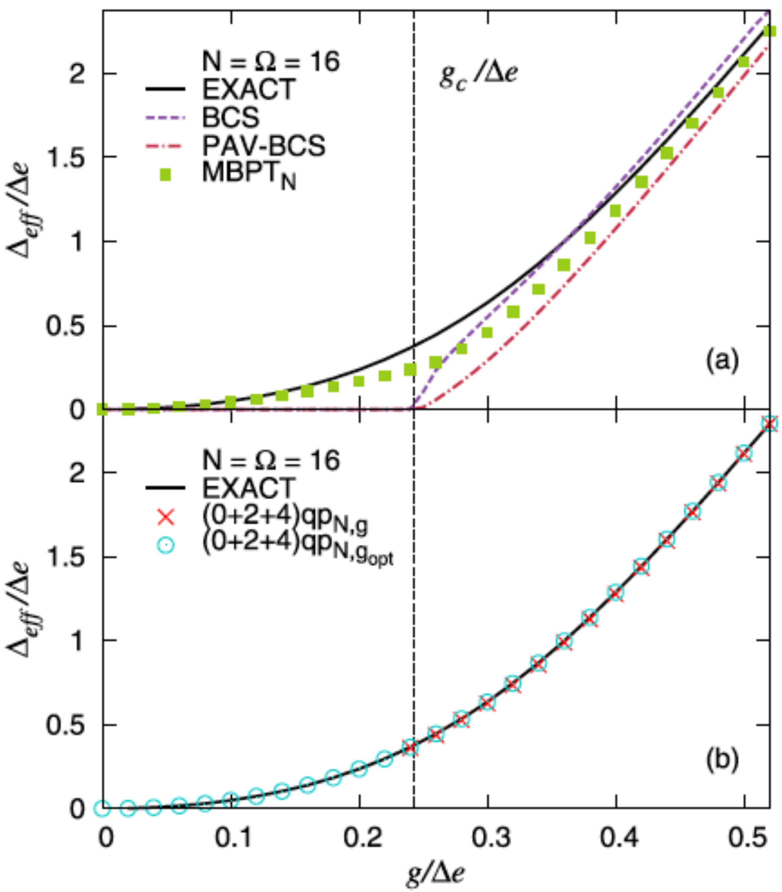




Other observables

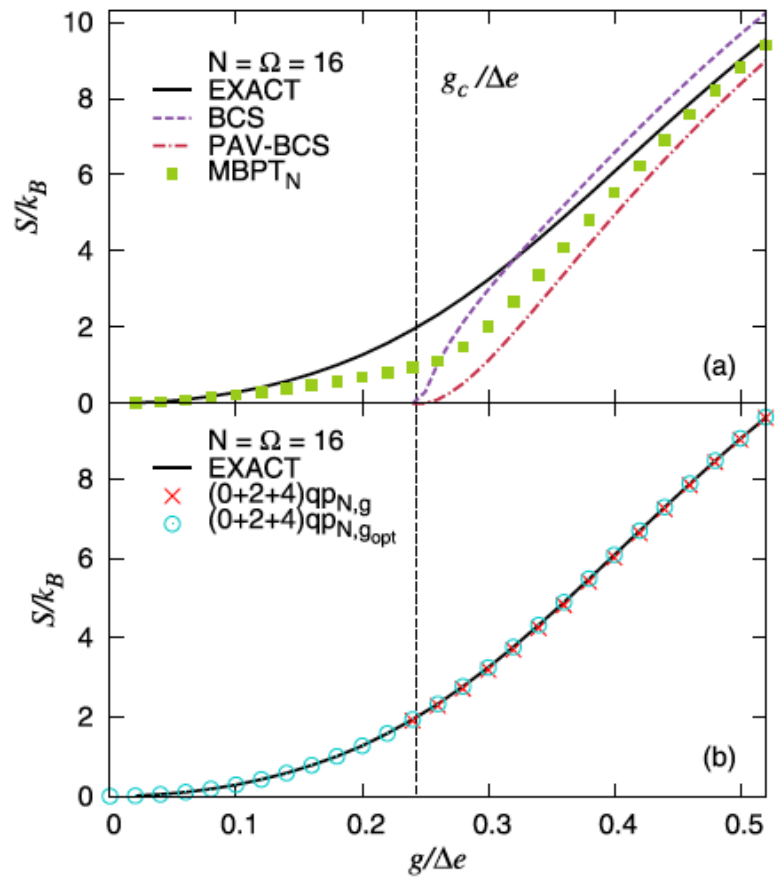
Effective Gap

$$\Delta_{\mathrm{eff}}(g) = g \sum_{k=1}^{\Omega} \sqrt{\langle a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{k}} a_k \rangle - \frac{1}{4}\langle (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) \rangle^2}$$



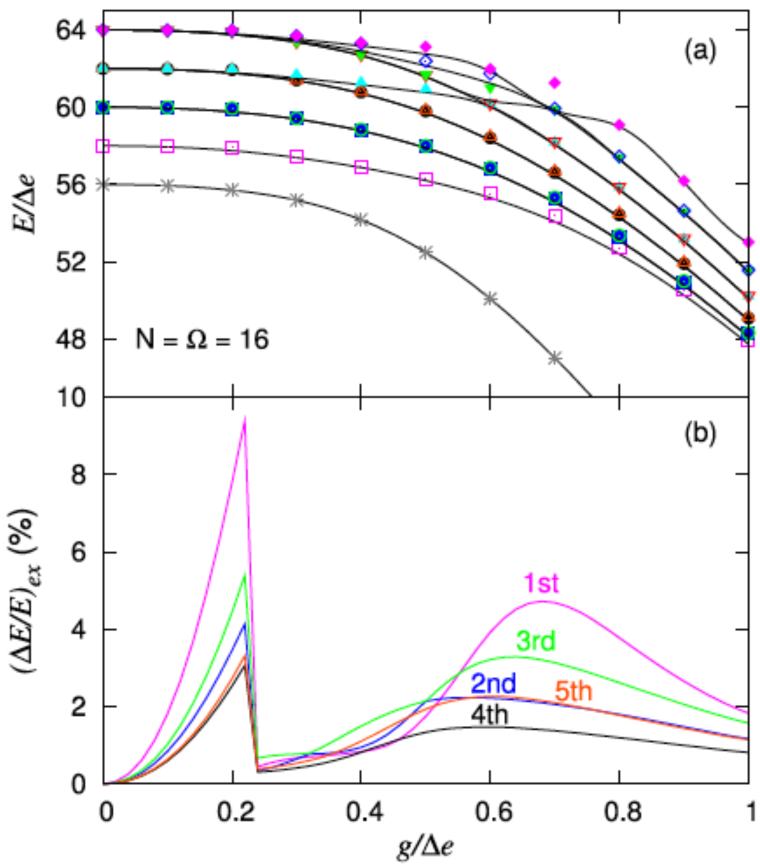
One-body entropy

$$\frac{S}{k_B} = -2 \sum_{k=1}^{\Omega} \{ \langle a_k^\dagger a_k \rangle \ln \langle a_k^\dagger a_k \rangle + (1 - \langle a_k^\dagger a_k \rangle) \ln (1 - \langle a_k^\dagger a_k \rangle) \}$$

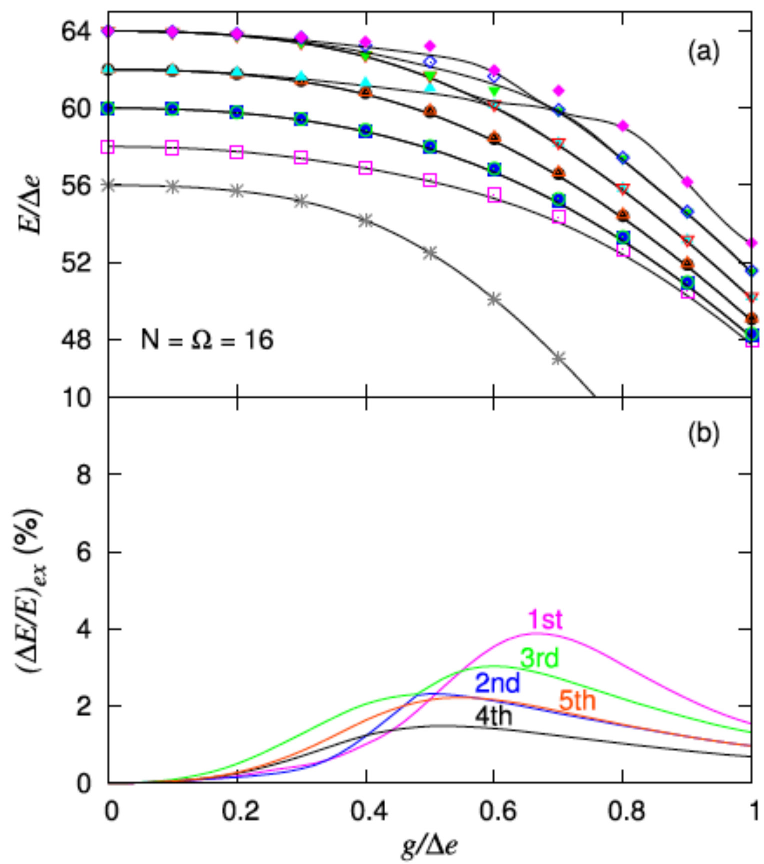


Excited states

Without restricted variation



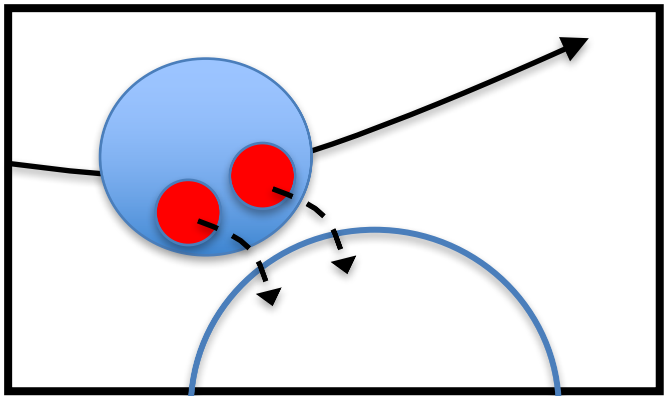
With restricted variation

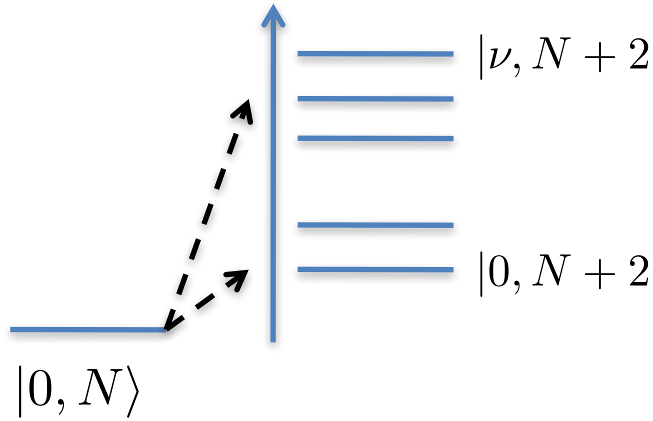


Similar method applied
to two nucleon pair transfer

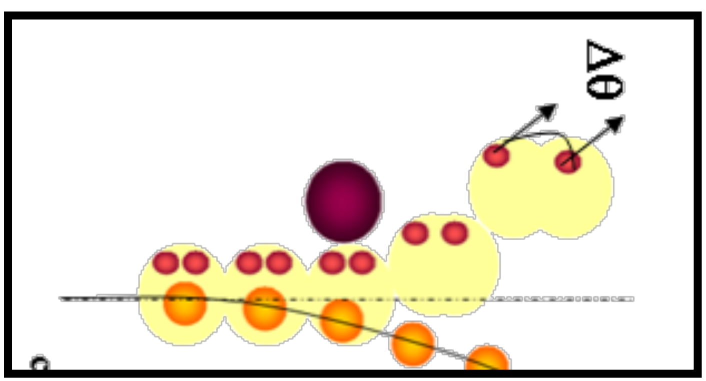
transfer and break-up reactions

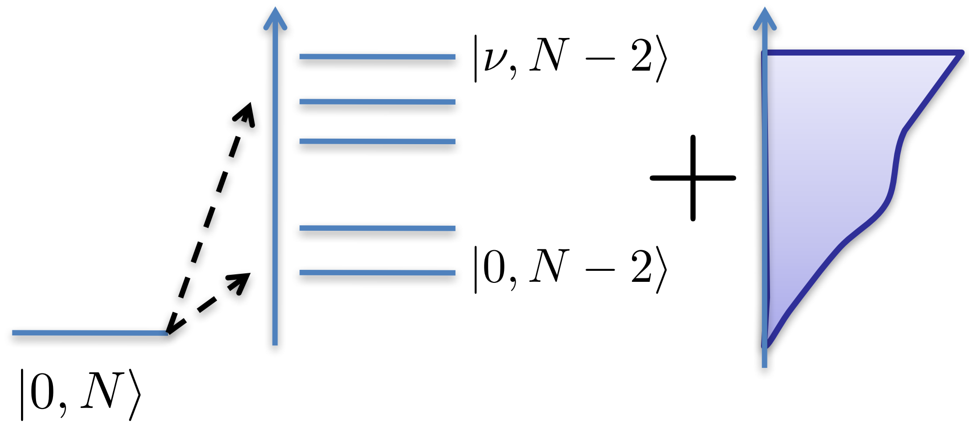
2n-transfer reactions





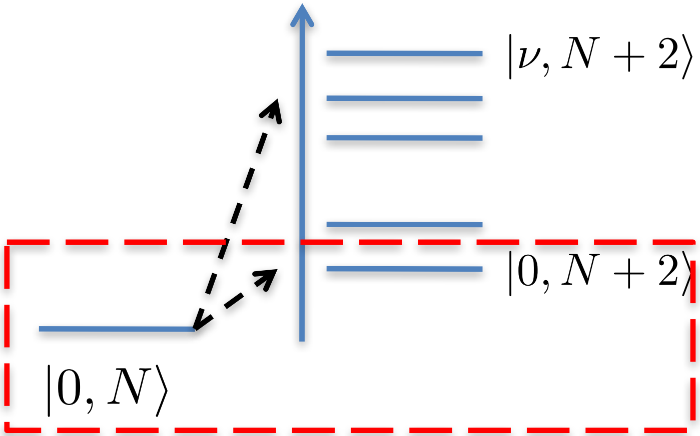
2n-break-up reactions





Description

$$
\begin{aligned}
|\Psi(t)\rangle \;=\; e^{-itE_0^N/\hbar} \Big\{ & \sum_\nu c_\nu^N e^{-it(E_\nu^N - E_0^N)/\hbar} |\nu, N\rangle \\
& + \sum_\nu c_\nu^{N-2} e^{-it(E_\nu^{N-2} - E_0^N)/\hbar} |\nu, N-2\rangle \\
& + \sum_\nu c_\nu^{N+2} e^{-it(E_\nu^{N+2} - E_0^N)/\hbar} |\nu, N+2\rangle \Big\}
\end{aligned}
$$



Assuming a pair transfer excitation operator:

Bes and Broglia, NPA 80 (1966), Ripka and R. Padjen, NPA132 (1969).

$$\hat{T} = \sum_i (T_{i\bar{i}} a_i^\dagger a_{\bar{i}}^\dagger + T_{i\bar{i}}^* a_{\bar{i}} a_i)$$

$$|\Psi(t)\rangle \Rightarrow S(E) = \sum_\nu |\langle N+2, \nu|\hat{T}|N,0\rangle|^2 \delta\left(E - \Delta E_\nu^{N+2}\right) + \sum_\nu \underline{|\langle N-2, \nu|\hat{T}}\underline{|N,0\rangle}|^2 \delta\left(E - \underline{\Delta E_\nu^{N-2}}\right)$$

Nuclear structure input

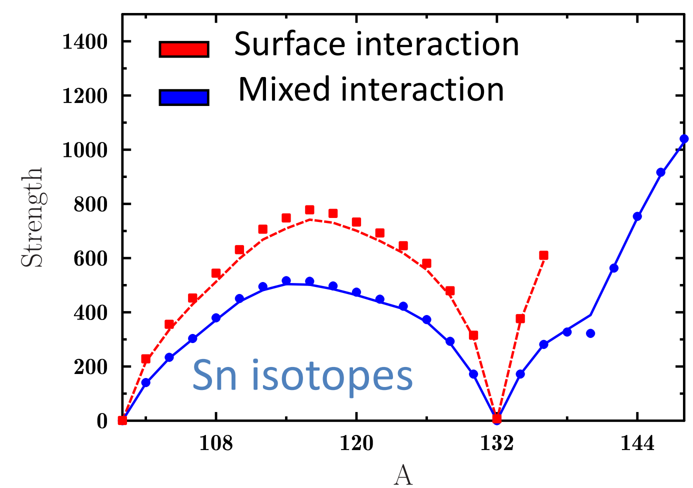
Transfer from Ground state (GS) to GS : the mean-field strategy based on quasi-particles

$$|0, N\rangle \simeq |QP\rangle = \prod_{i>0} \left(U_i + V_i a_i^\dagger a_{\bar{i}}^\dagger\right) |0\rangle$$

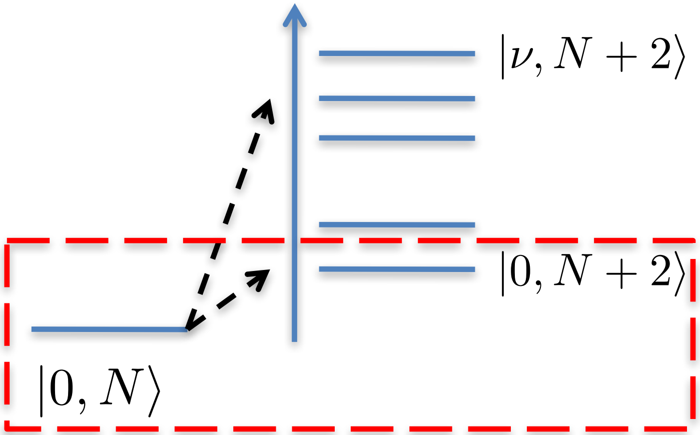
$$\Downarrow$$

$$\left.\begin{array}{l} |\langle N+2, 0|\hat{T}|N,0\rangle|^2 \\ |\langle N-2, 0|\hat{T}|N,0\rangle|^2 \end{array}\right| \simeq |\langle QP|\hat{T}|QP\rangle|^2$$

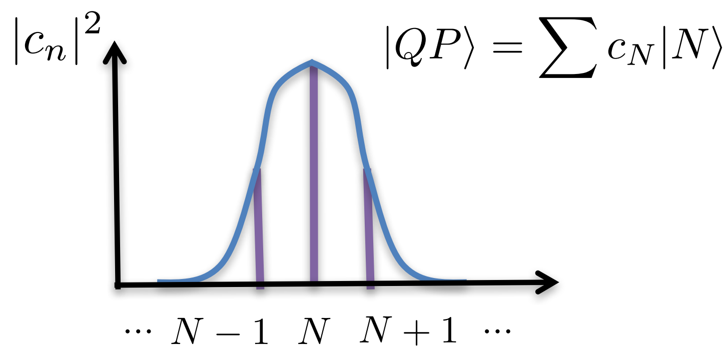
Illustration



Grasso, Lacroix, Vitturi, PRC85 (2012)

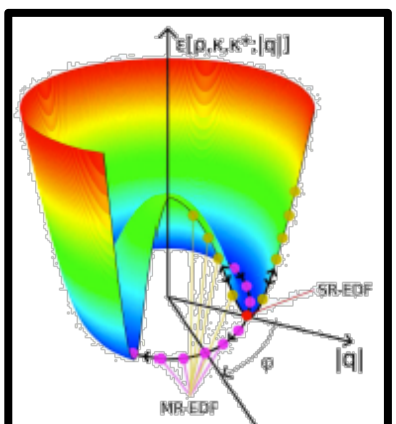


Particle number non-conservation

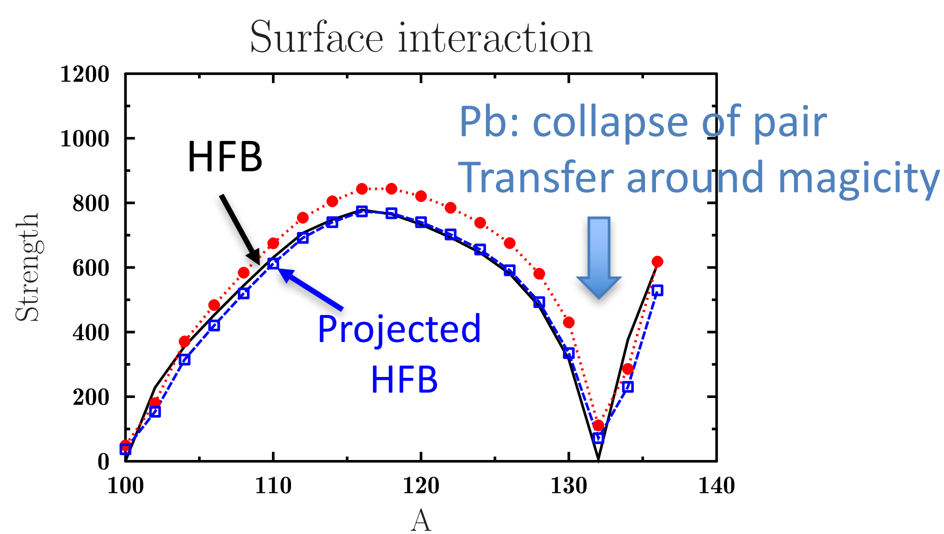


$$|N\rangle = P_N |QP\rangle$$

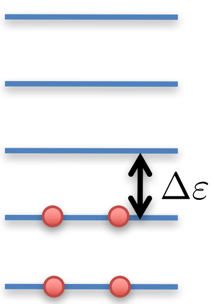
$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \;\; e^{i\varphi(\hat{N}-N)}$$



Projection After Variation applied to pair transfer

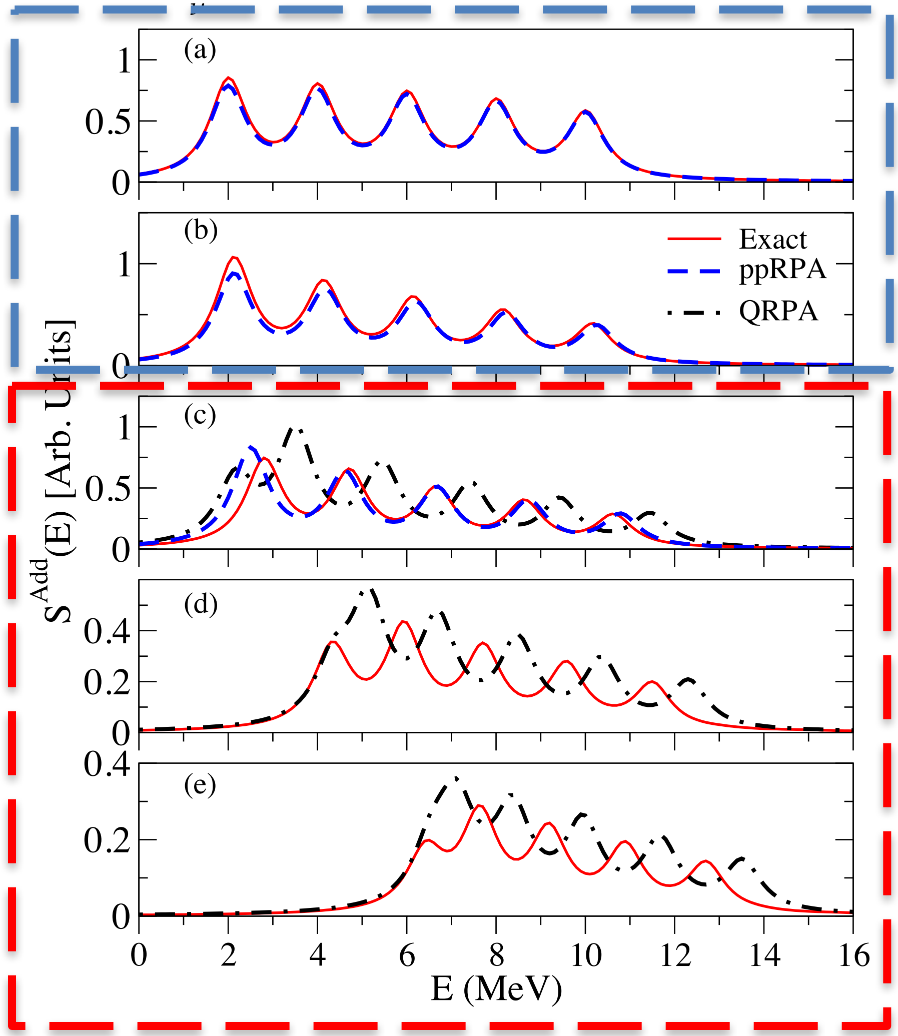


Grasso, Lacroix, Vitturi, PRC85 (2012)



$$H = \sum_{i=1}^{\Omega} \varepsilon_i a_i^\dagger a_i + g \sum_{i \neq j}^{\Omega} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

$$\sum_\nu |\langle N+2,\nu|\hat{T}|N,0\rangle|^2 \delta\left(E - \Delta E_\nu^{N+2}\right)$$



QRPA applied to pair transfer

$$|\nu\rangle = Q_\nu^\dagger|0\rangle$$

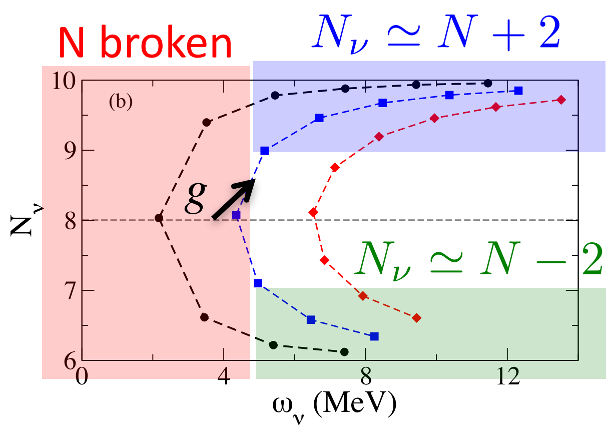
Normal phase: $$Q_\nu^\dagger = \sum_p X_p^\nu a_p^\dagger a_{\bar{p}}^\dagger + \sum_h Y_h^\nu a_h^\dagger a_{\bar{h}}^\dagger,$$

Superfluid phase: $$Q_\nu^\dagger = \sum_i (X_j^\nu \alpha_i^\dagger \alpha_{\bar{i}}^\dagger - Y_j^\nu \alpha_{\bar{i}} \alpha_i)$$

- ppRPA very good
- QRPA is *globally* good

Role of particle number non-conservation?

$$N_\nu = \langle \nu|\hat{N}|\nu\rangle$$



Gambacurta and Lacroix, PRC86 (2012).

Including particle number conservation

Recipe:

Take all 2QP states + GS

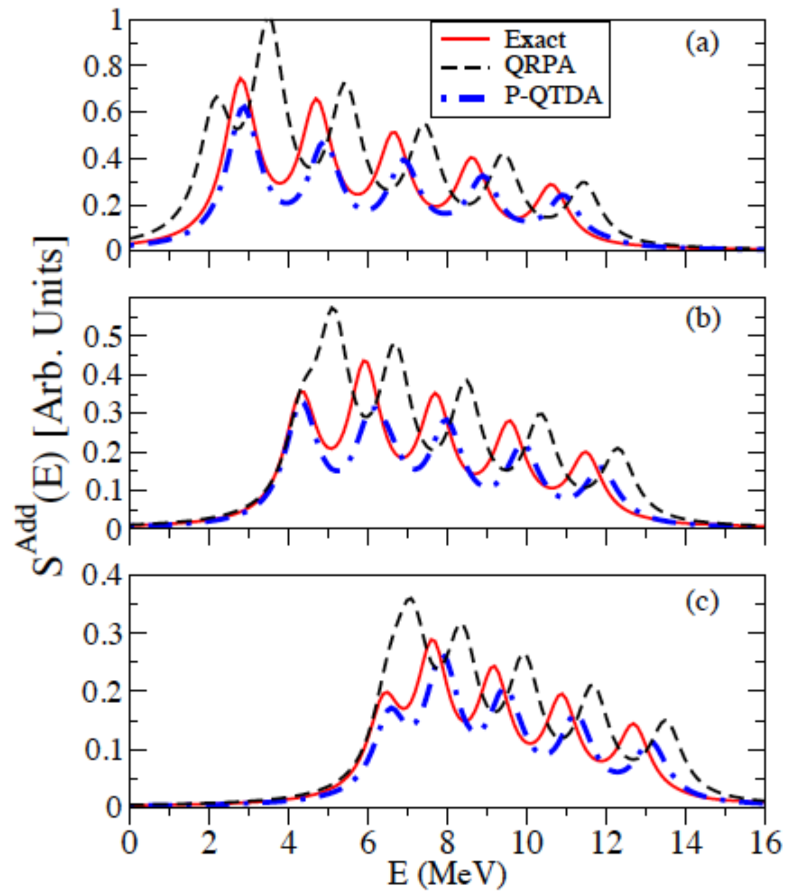
$$|\Phi_k\rangle = \hat{P}_{N+2}\alpha^\dagger_k \alpha^\dagger_{\bar{k}}|0, QP\rangle$$

↓

orthonormalization

↓

Diagonalize H in the reduced space



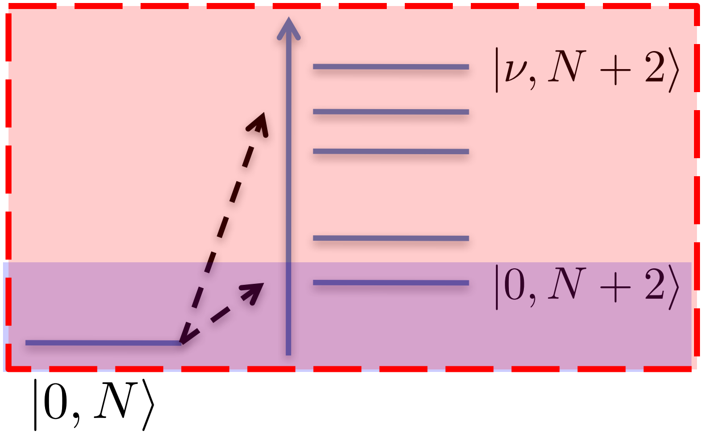
(a) $G/\Delta\varepsilon = 0.5$, (b) 0.7, (c) 0.9

➡ Confirms the role of U(1) sym. breaking

➡ Improve the QRPA

➡ Directly applicable in existing HFB codes

Gambacurta and Lacroix, PRC86 (2012).



Improved description pair transfer to excited states.
(Projected QRPA like)

Improved description of ground state
(QP perturbation theory)

Present status:

- Directly applicable on existing HFB codes
- Application to nuclei
- Need to couple to reactions codes

Other strategy:

- Perform nuclear structure and reaction in a unique framework

- CI combined with symmetry breaking + restoration has some potentialities
- Application to the pairing model is quite encouraging
- Excited states: still to be explored is the possibility to use RPA, QRPA states

Current development (J. Ripoche PhD)

- Implementation in HFB code with bare interaction
- Compare with other techniques (MBPT, CC, …)
- Exploring now the use with other symmetries