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Correlations Beyond the Mean Field: Towards Variation After Projection Solutions

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General Remarks

1. Self-Consistent Mean Field Methods

- ✓ Variational space of wave functions $\{|\Phi\rangle\}$ made of product of single (quasi)particles operators acting on the vacuum.
- ✓ To include correlations within a product-type w.f. ⇒ **Breaking of the symmetries**
- ✓ Fails in weakly correlated regimes ⇒ Methods **Beyond the Mean Field**

2. Restoration of the symmetries

- ✓ *Exact* w.f. is an eigenstate of the operators associated to the symmetries ⇒ Improvement of the MF w.f. by restoring the broken symmetries
- ✓ Projection techniques: From a mean field w.f. (product-type) $|\Phi\rangle \Rightarrow |\Psi^S\rangle = P^S|\Phi\rangle$ where P^S is the projector onto the subspace of w.f. with the proper quantum numbers.

3. Projection techniques

- ✓ *Projection After Variation* (PAV)
- ✓ ***Variation After Projection* (VAP)**

→

Approximations to VAP solution:

- **Restricted VAP method**
- **(Projected) Lipkin-Nogami prescriptions**

Pairing Correlations. Particle Number Projection

1. Mean Field (BCS or HFB)

$\{|\Phi\rangle\}$ product of quasiparticle operators

$$\delta\left(\frac{\langle\Phi|\hat{H}-\lambda_1\hat{N}|\Phi\rangle}{\langle\Phi|\Phi\rangle}\right)_{|\Phi_0\rangle}=0$$

$$\lambda_1 \Rightarrow \langle\Phi|\hat{N}|\Phi\rangle = N$$

$$E_0^{MF}=\frac{\langle\Phi_0|\hat{H}|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle}$$

2. Projection After Variation (PAV)

$$|\Psi^N_{PAV}\rangle = P^N|\Phi_0\rangle \Rightarrow$$

$$E_0^{PAV}=\frac{\langle\Psi^N_{PAV}|\hat{H}|\Psi^N_{PAV}\rangle}{\langle\Psi^N_{PAV}|\Psi^N_{PAV}\rangle}$$

3. Variation After Projection (VAP)

$\{|\Psi^N\rangle = P^N|\Phi\rangle\}$ projected product-type w.f.

$$\delta\left(\frac{\langle\Psi^N|\hat{H}|\Psi^N\rangle}{\langle\Psi^N|\Psi^N\rangle}\right)_{|\Psi^N\rangle=|\Psi^N_{VAP}\rangle}=0 \Rightarrow$$

$$E_0^{VAP}=\frac{\langle\Psi^N_{VAP}|\hat{H}|\Psi^N_{VAP}\rangle}{\langle\Psi^N_{VAP}|\Psi^N_{VAP}\rangle}$$

Towards the VAP solution

Kamlah expansion of the projected (VAP) energy provides the most relevant degrees of freedom:

$$E_0^{VAP} \approx \langle \hat{H} \rangle - k_2 \langle (\Delta \hat{N})^2 \rangle - k_4 \langle (\Delta \hat{N})^4 \rangle - \ldots$$

1. Restricted VAP 1 (RVAP$_1$)

$\{ |\Phi(\Delta N^2)\rangle \}$ product of quasiparticle operators

$$\left.\left.\begin{array}{l} \delta\left(\dfrac{\langle \Phi(\Delta N^2)|\hat{H} - \lambda_1 \hat{N} - \lambda_{\Delta N^2} \Delta \hat{N}^2 |\Phi(\Delta N^2)\rangle}{\langle \Phi(\Delta N^2)|\Phi(\Delta N^2)\rangle} \right)_{|\Phi\rangle = |\Phi_0\rangle} = 0 \\ \lambda_1 \Rightarrow \langle \Phi(\Delta N^2)|\hat{N}|\Phi(\Delta N^2)\rangle = N \\ \lambda_{\Delta N^2} \Rightarrow \langle \Phi(\Delta N^2)|\Delta \hat{N}^2|\Phi(\Delta N^2)\rangle = \Delta N^2 \end{array}\right\} \Rightarrow E^{MF}(\Delta N^2) = \frac{\langle \Phi(\Delta N^2)|\hat{H}|\Phi(\Delta N^2)\rangle}{\langle \Phi(\Delta N^2)|\Phi(\Delta N^2)\rangle}\right.$$

$$|\Psi^N(\Delta N^2)\rangle = P^N |\Phi(\Delta N^2)\rangle \Rightarrow E^N(\Delta N^2) = \frac{\langle \Phi(\Delta N^2)|\hat{H} P^N|\Phi(\Delta N^2)\rangle}{\langle \Phi(\Delta N^2)|P^N|\Phi(\Delta N^2)\rangle}$$

Defines a Projected Potential Energy Surface (PPES) which is a reduced variational space

$$E_0^{RVAP_1} = \min\left(E^N(\Delta N^2) \right)$$

Towards the VAP solution

$$E_0^{VAP} \approx \langle \hat{H} \rangle - k_2 \langle (\Delta \hat{N})^2 \rangle - k_4 \langle (\Delta \hat{N})^4 \rangle - \ldots$$

2. Restricted VAP 2 (RVAP$_2$) $\{ |\Phi(\Delta N^2; \Delta N^4)\rangle \}$ product of quasiparticle operators

$$\delta \left(\frac{\langle \Phi | \hat{H} - \lambda_1 \hat{N} - \lambda_{\Delta N^2} \Delta \hat{N}^2 - \lambda_{\Delta N^4} \Delta \hat{N}^4 | \Phi \rangle}{\langle \Phi | \Phi \rangle} \right)_{|\Phi\rangle = |\Phi_0\rangle} = 0$$

$$\lambda_1 \Rightarrow \langle \Phi | \hat{N} | \Phi \rangle = N$$

$$\lambda_{\Delta N^2} \Rightarrow \langle \Phi | \Delta \hat{N}^2 | \Phi \rangle = \Delta N^2$$

$$\lambda_{\Delta N^4} \Rightarrow \langle \Phi | \Delta \hat{N}^4 | \Phi \rangle = \Delta N^4$$

$$\Rightarrow E^{MF}(\Delta N^2; \Delta N^4)$$

$$|\Psi^N(\Delta N^2; \Delta N^4)\rangle = P^N |\Phi_0(\Delta N^2; \Delta N^4)\rangle \Rightarrow E^N(\Delta N^2; \Delta N^4)$$

Defines a two dimensional Projected Potential Energy Surface (PPES) which is a reduced variational space

$$E_0^{RVAP_2} = \min \left(E^N(\Delta N^2; \Delta N^4) \right)$$

Towards the VAP solution

3. Lipkin-Nogami (LN) Prescrition

$\{|\Phi\rangle\}$ product of quasiparticle operators

$$\delta\left(\frac{\langle\Phi|\hat{H}-\lambda_1\hat{N}-h_2\Delta\hat{N}^2|\Phi\rangle}{\langle\Phi|\Phi\rangle}\right)_{|\Phi\rangle=|\Phi_{LN}\rangle}=0$$

$$\lambda_1 \Rightarrow \langle\Phi|\hat{N}|\Phi\rangle = N$$

$$h_2=\frac{\langle\hat{H}\Delta\hat{N}^2\rangle-\langle\hat{H}\rangle\langle\Delta\hat{N}^2\rangle-\frac{\langle\hat{H}\Delta\hat{N}\rangle\langle\Delta\hat{N}^3\rangle}{\langle\Delta\hat{N}^2\rangle}}{\langle\Delta\hat{N}^4\rangle-\langle\Delta\hat{N}^2\rangle^2-\frac{\langle\Delta\hat{N}^3\rangle^2}{\langle\Delta\hat{N}^2\rangle}}$$

$$\Rightarrow\ E_0^{LN}=\frac{\langle\Phi_{LN}|\hat{H}|\Phi_{LN}\rangle}{\langle\Phi_{LN}|\Phi_{LN}\rangle}-h_2\frac{\langle\Phi_{LN}|\Delta\hat{N}^2|\Phi_{LN}\rangle}{\langle\Phi_{LN}|\Phi_{LN}\rangle}$$

4. Projected Lipkin-Nogami (PLN)

$$|\Psi^N_{PLN}\rangle = P^N|\Phi_{LN}\rangle \Rightarrow$$

$$E_0^{PLN}=\frac{\langle\Psi^N_{PLN}|\hat{H}|\Psi^N_{PLN}\rangle}{\langle\Psi^N_{PLN}|\Psi^N_{PLN}\rangle}$$

Towards the VAP solution

5. (P)Lipkin-Nogami and Restricted VAP methods

- Lipkin-Nogami w.f. belongs to the set of wave functions constrained to ΔN^2

$$|\Phi_{LN}\rangle \in \left\{ |\Phi(\Delta N^2)\rangle \right\} \Rightarrow \boxed{h_2 = \lambda \Delta N^2}$$

The above condition can be deduced in a variational way:

- We evaluate with the set of constrained wave function $\left\{ |\Phi(\Delta N^2)\rangle \right\}$ the approximate projected energy as a function of ΔN^2

$$E_0^{LN}(\Delta N^2) = \langle \hat{H} \rangle - h_2 \langle (\Delta \hat{N})^2 \rangle$$

- We minimize $E_0^{LN}(\Delta N^2)$ along the (ΔN^2) direction assuming that:

$$\left.\begin{array}{l} \dfrac{\partial \langle \hat{H} \rangle}{\partial (\Delta N^2)} \equiv \lambda \Delta N^2 \\ h_2 \neq h_2(\Delta N^2) \end{array}\right\} \qquad \frac{\partial E_0^{LN}(\Delta N^2)}{\partial (\Delta N^2)} = 0 \Rightarrow \boxed{h_2 = \lambda \Delta N^2}$$

Towards the VAP solution

5. (P)Lipkin-Nogami and Restricted VAP methods

- LN method provides results as good as $RVAP_1$ whenever the second order expansion of the projected energy will be a good approach to the exact projected energy.

- LN solution will coincide to the minimum of $E_0^{LN}(\Delta N^2) = \langle \hat{H} \rangle - h_2 \langle (\Delta \hat{N})^2 \rangle$ curve whenever $h_2 \neq h_2(\Delta N^2)$

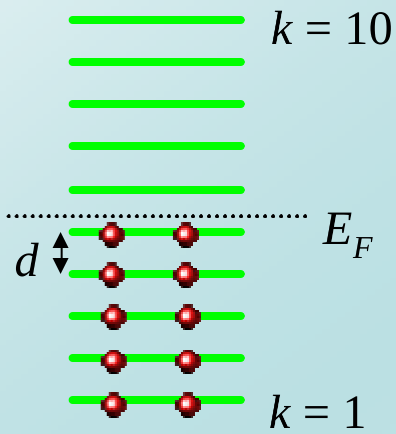
- PLN solution will be as good as $RVAP_1$ only. $\left(|\phi^N_{PLN}\rangle \in \left\{ P^N |\phi(\Delta N^2)\rangle \right\} \right)$

Pairing hamiltonians

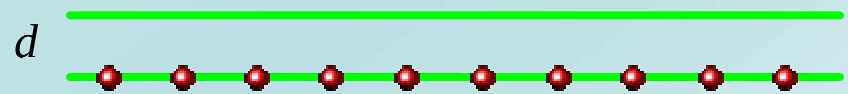
$$\hat{H} = \sum_{k=1}^{N} \varepsilon_k \left(c_k^\dagger c_k + c_{\bar{k}}^\dagger c_{\bar{k}} \right) - G \sum_{k,q=1}^{N} c_k^\dagger c_{\bar{k}}^\dagger c_{\bar{q}} c_q$$

✓ *Multilevel pairing hamiltonian*

- Single particle levels are equally spaced an doubly-degenerated (Ω=2).
- *N* = number of particles = number of levels



✓ *Two level pairing hamiltonian*



✓ *Condensation energy*

$$E_{cond} = E_0 - \left(2 \sum_{k=1}^{N/2} \varepsilon_k - G \frac{N}{2} \right)$$

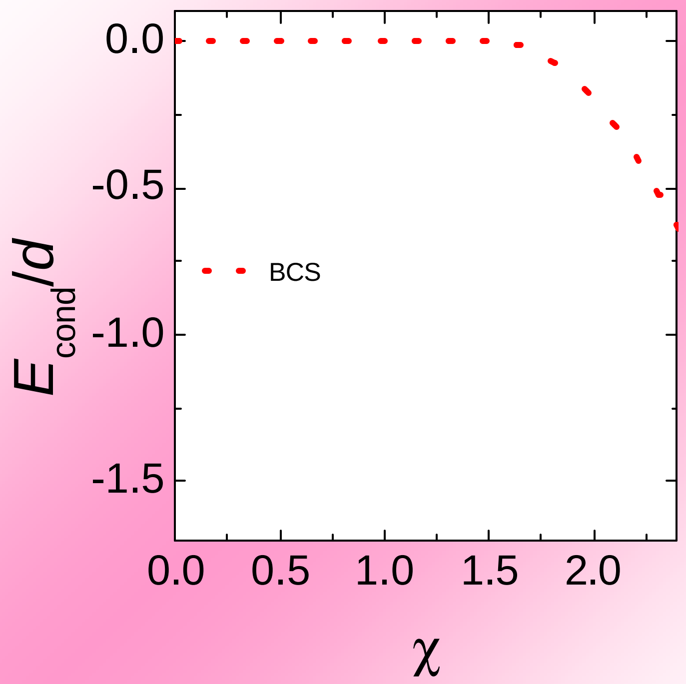
Ground state energy

✓ *Normalized interaction strength*

$$\lambda = \frac{G}{d} (\Omega - 1)$$

Multilevel Pairing hamiltonian

✓ ***Mean Field* (BCS)**

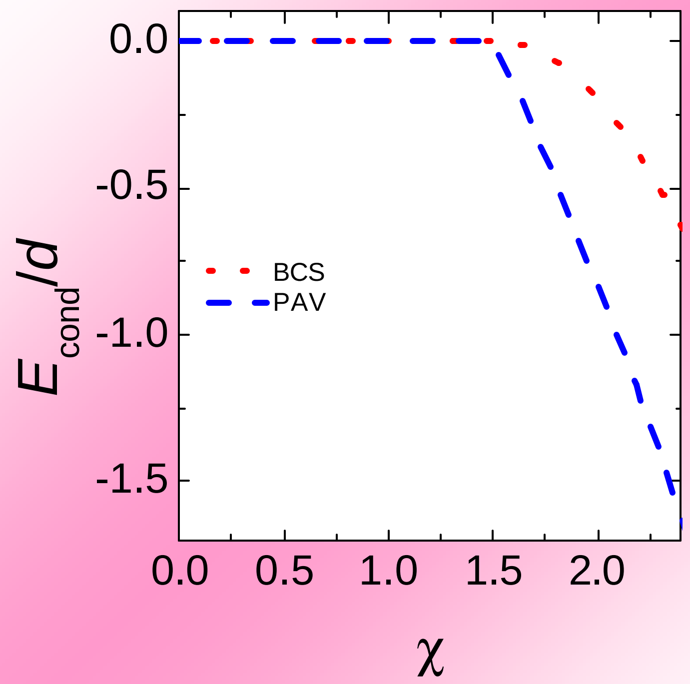


✓ There is a phase transition between non-correlated and correlated regimes at the mean field level, associated to the breaking of the particle number symmetry.

✓ After the phase transition the condensation energy decreases with increasing interaction strength

Multilevel Pairing hamiltonian

✓ ***Projection After Variation* (PAV)**

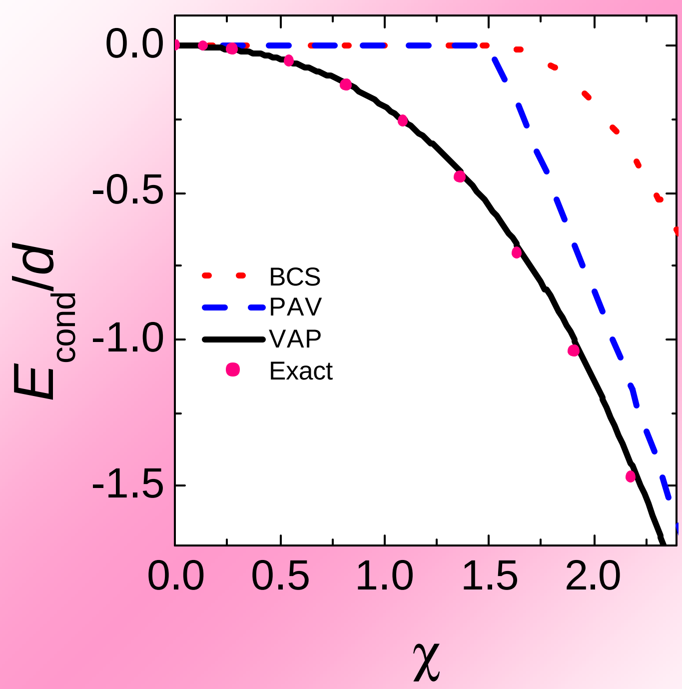


✓ The phase transition remains in the PAV approach.

✓ There is not any energy gain in the non-correlated regime.

Multilevel Pairing hamiltonian

✓ ***Variation After Projection* (VAP)**



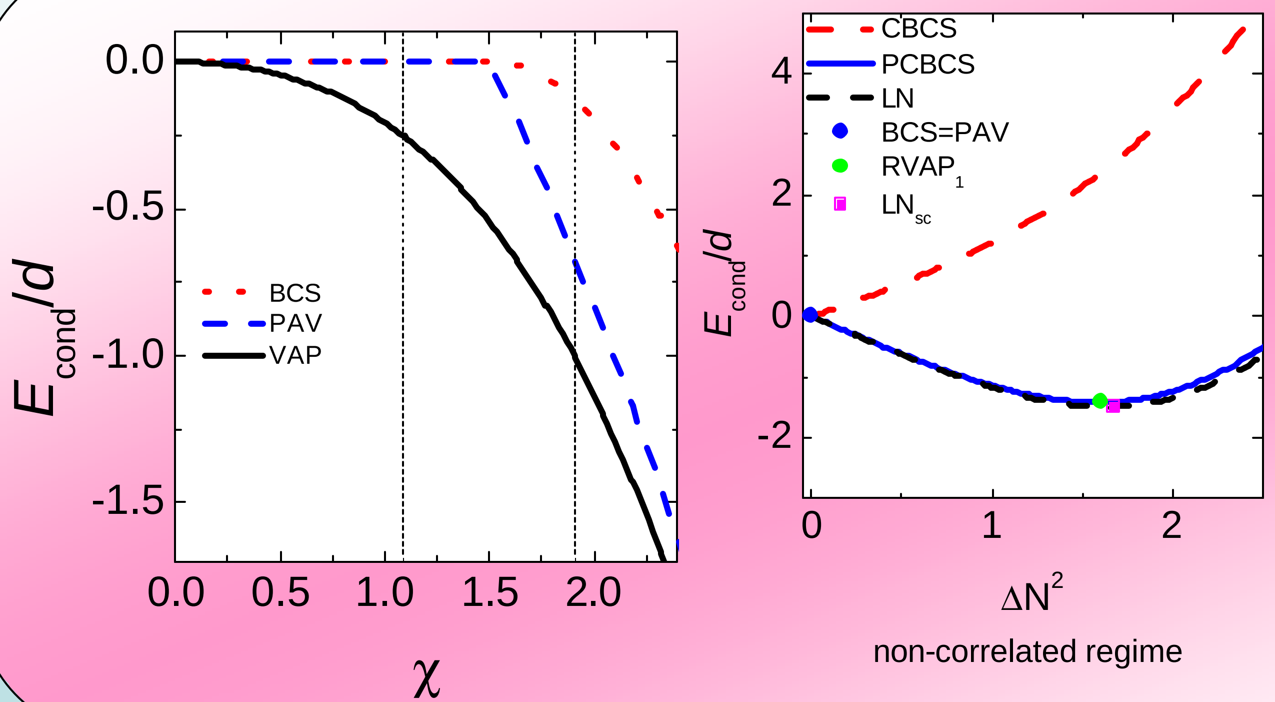
✓ No phase transition is observed in the VAP approach.

✓ Correlated solutions are obtained for the whole range of interaction strengths.

✓ Best approximation to the exact solution (Richardson).

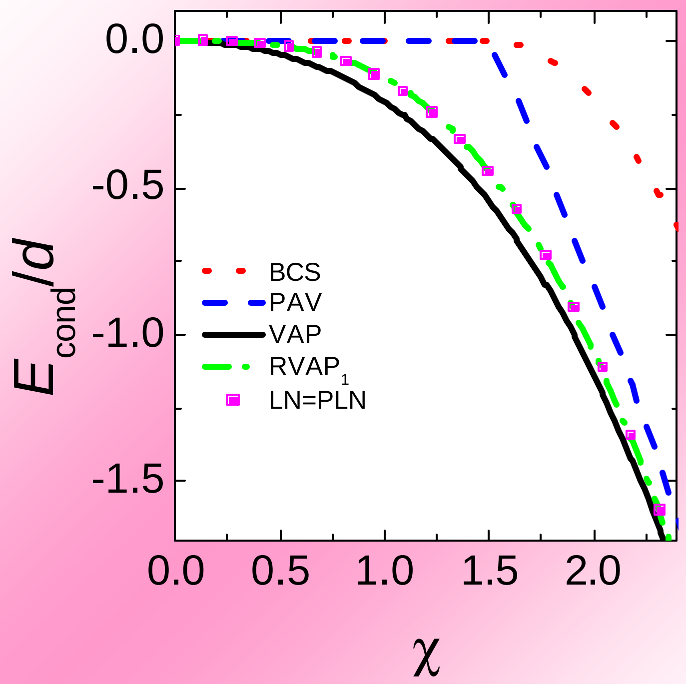
Multilevel Pairing hamiltonian

✓ ***Restricted Variation After Projection 1 (RVAP$_1$) and Lipkin-Nogami methods***



Multilevel Pairing hamiltonian

✓ ***Restricted Variation After Projection 1 ($RVAP_1$) and Lipkin-Nogami methods***



✓ The phase transition disappears.

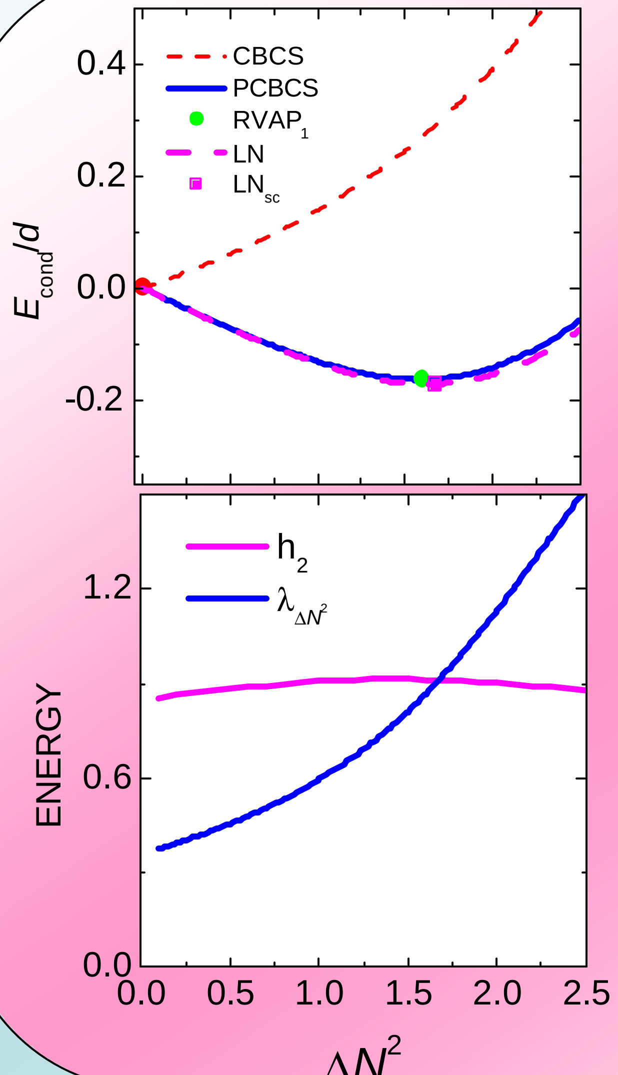
✓ Closer to the VAP solution than MF and PAV approaches

✓ LN and PLN almost coincide to the RVAP1 solution

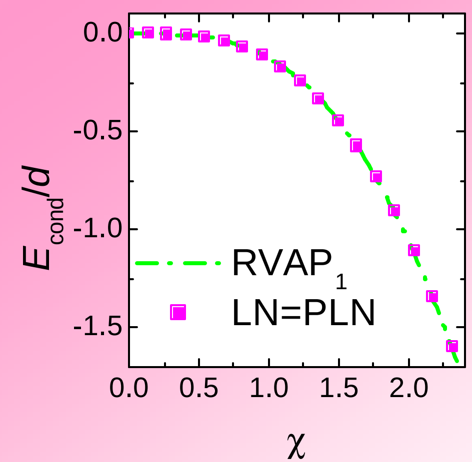
✓ There are still correlations that cannot be described by neither $RVAP_1$ nor (P)LN methods

Multilevel Pairing hamiltonian

✓RVAP$_1$ *vs.* (P)LN



- The Projected Energy expansion is a very good approximation to the exact projection

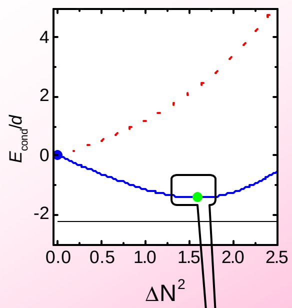


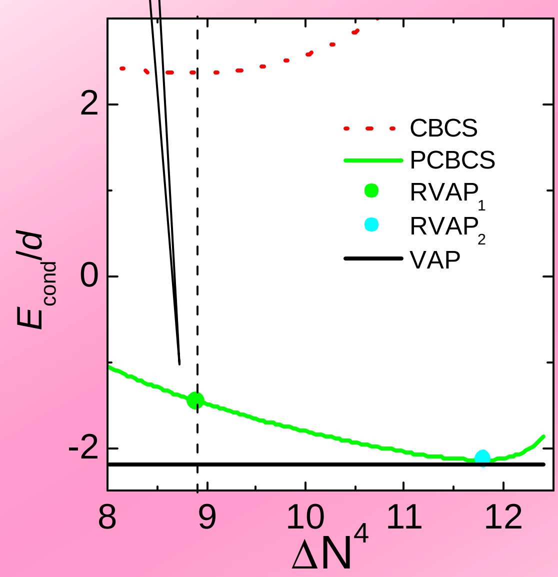
- ***h*$_2$** parameter is almost constant along DN^2 direction.

Multilevel Pairing hamiltonian

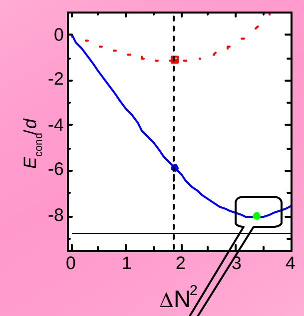
✓ ***Restricted Variation After Projection 2* (RVAP$_2$)**

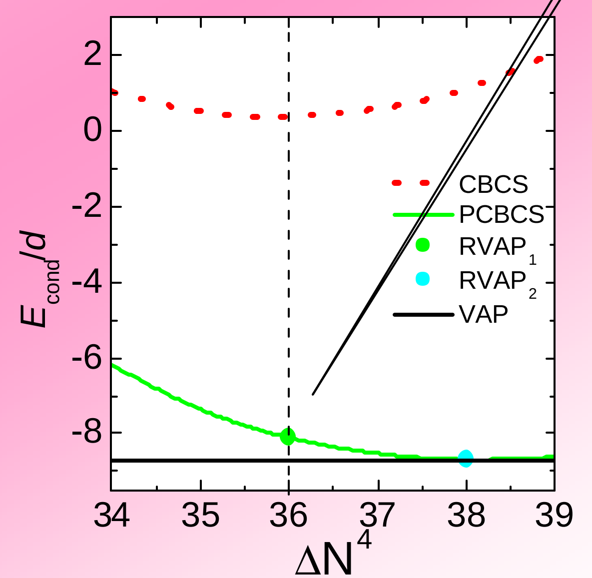
Exploring the ¢ N^4 at the minima of the PPES along the ¢ N^2 direction





non-correlated regime



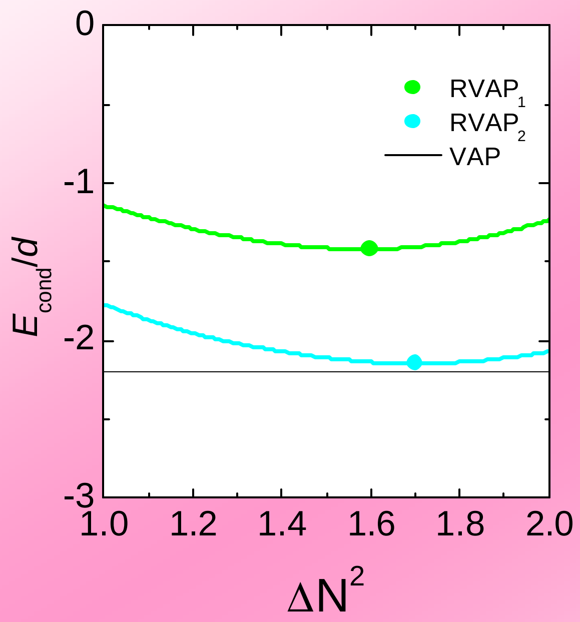


correlated regime

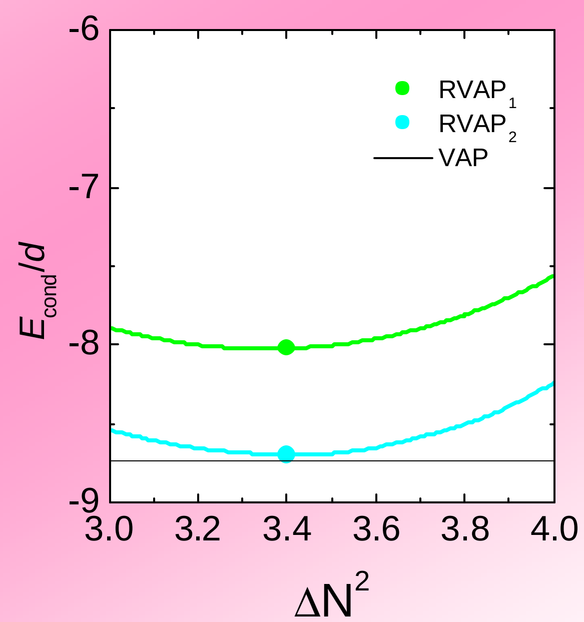
Multilevel Pairing hamiltonian

✓ ***Restricted Variation After Projection 2* (RVAP$_2$)**

Choosing the minima of © ¢ N^2; ¢ N^4 ª



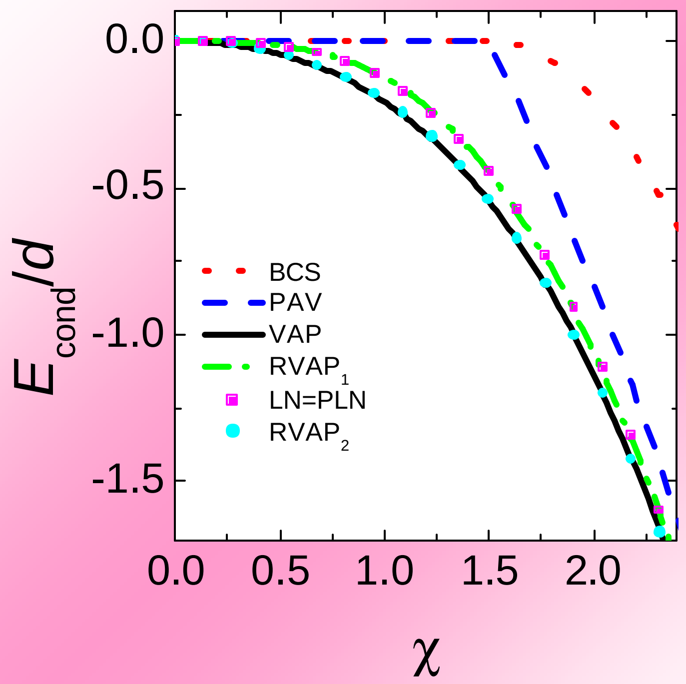
non-correlated regime



correlated regime

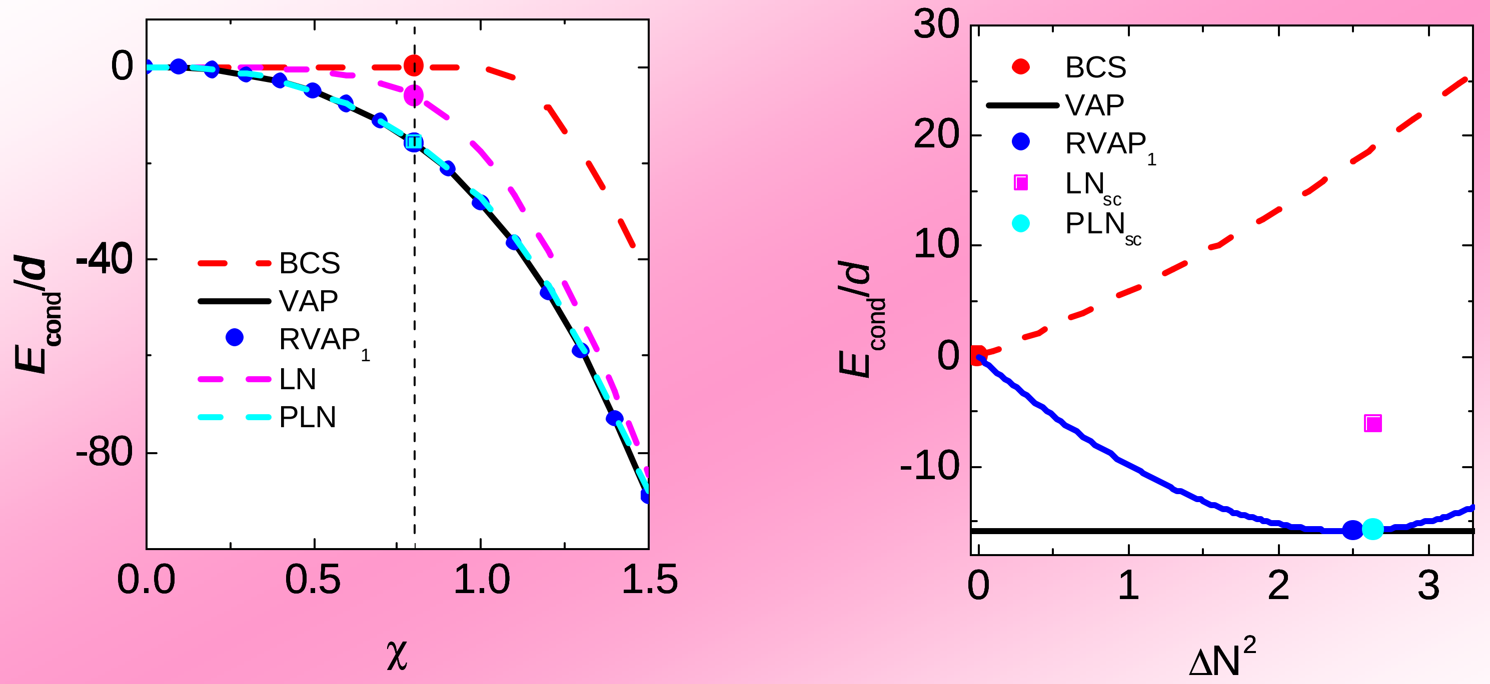
Multilevel Pairing hamiltonian

✓ ***Restricted Variation After Projection 2* (RVAP$_2$)**



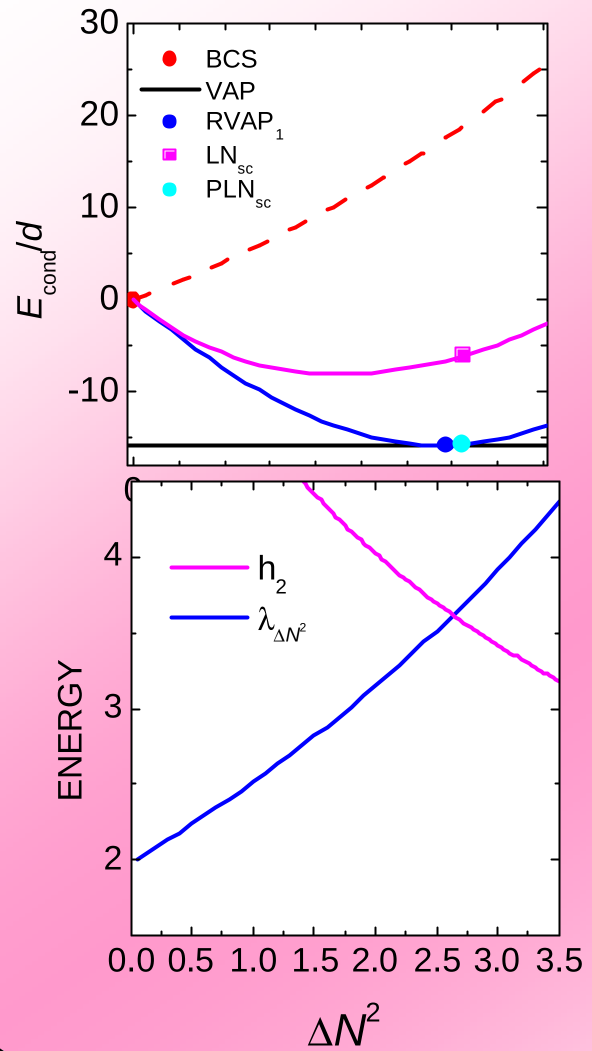
✓ RVAP$_2$ solution is almost on top of VAP one testing the ability of the RVAP method.

Two Level Pairing hamiltonian



Two Level Pairing hamiltonian

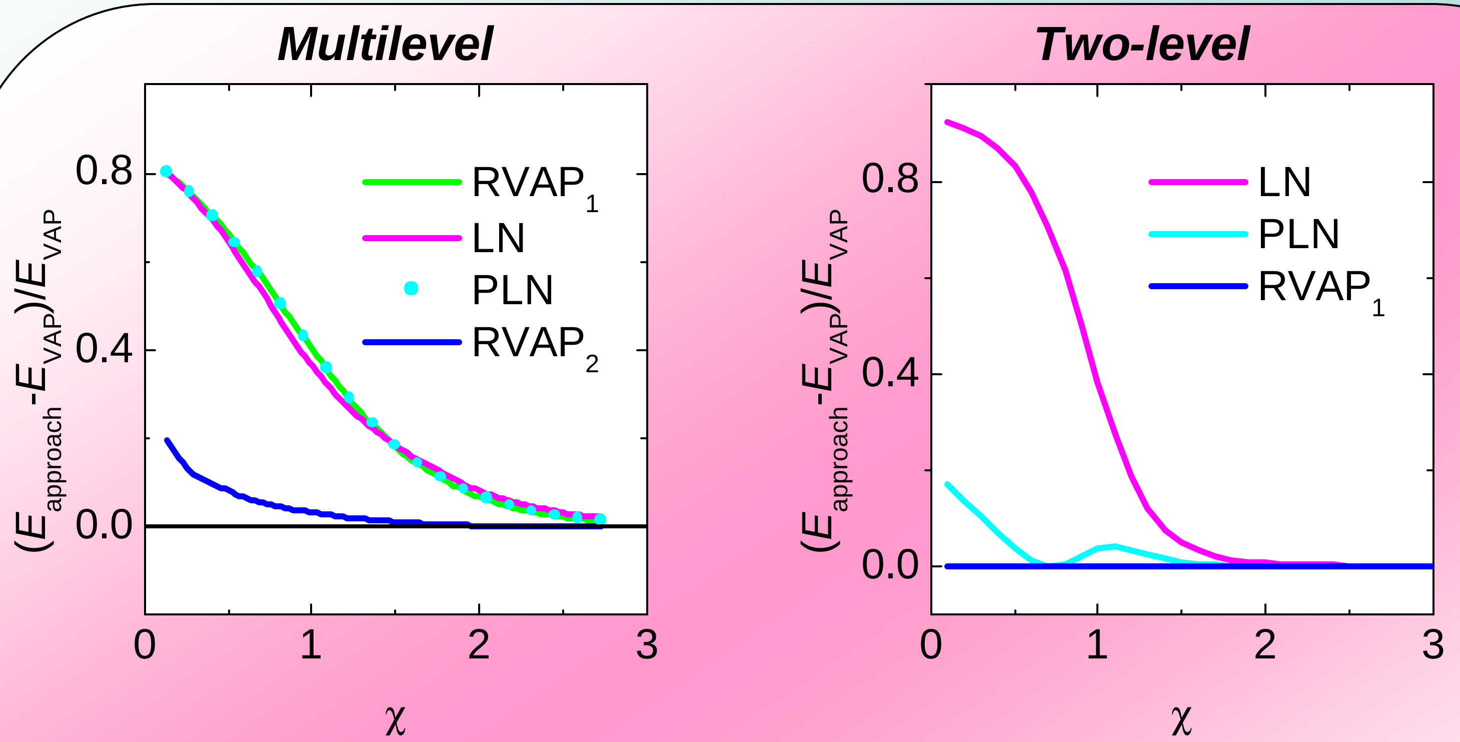
✓$RVAP_2$ *vs.* (P)LN



➢ The Projected Energy expansion is not a good approximation to the exact projection

➢ h_2 parameter has a strong dependence on ΔN^2 direction.

Relative Errors



- LN method fails in weakly correlated regimes
- PLN is as good as $RVAP_1$ although in weakly correlated regimes could fail
- In the Multilevel model PLN and $RVAP_1$ have a poor performance in the weak pairing region and $RVAP_2$ is necessary

Conclusions

- ✓ **Variation After Projection solutions can be approximated by the Restricted Variation After Projection method in a general and computationally feasible procedure.**

- ✓ **The Lipkin-Nogami method can be deduced in a variational context where an approximate projected energy is minimized along DN^2 direction.**

- ✓ **Whenever the Lipkin-Nogami and Projected Lipkin-Nogami fails (weak pairing regions) the Restricted Variation After Projection method is a perfect candidate to approximate VAP solutions.**