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 $\Psi_j$ made of product of single (quasi)particles operators acting on the vacuum.
✓ To include correlations within a product-type w.f. $\Rightarrow$ Breaking of the symmetries
✓ Fails in weakly correlated regimes $\Rightarrow$ Methods Beyond the Mean Field

2. Restoration of the symmetries

✓ Exact w.f. is an eigenstate of the operators associated to the symmetries $\Rightarrow$ Improvement of the MF w.f. by restoring the broken symmetries
✓ Projection techniques: From a mean field w.f. (product-type) $\Psi_j$ $\Rightarrow$ $S_i = P^S_j$ 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)

\[ \pm \frac{\hbar j \hat{H} i - \hat{N} j \hat{N} i}{\hbar j \hat{N} i} = 0 \]

\[ \prod_{j=0}^{\infty} \left( \begin{array}{c} \hbar \hat{N} j \hat{N} i \\ \hbar j \hat{N} i \end{array} \right) = N \]

2. Projection After Variation (PAV)

\[ j^a_{PAV} N i = P^N j \hat{C}_0 i \]

\[ E_{PAV}^0 = \frac{\hbar^a N_{PAV} j \hat{H} j^a_{PAV} N_{PAV} i}{\hbar^a N_{PAV} j^a_{PAV} N_{PAV} i} \]

3. Variation After Projection (VAP)

\[ j^a N i = P^N j \hat{C}_i g \]

\[ \prod_{j=0}^{\infty} \left( \begin{array}{c} \hbar j \hat{H} j^a N_i \\ \hbar j^a N_i \end{array} \right) = 0 \]

\[ j^a N i = j^a N_{VAP} i \]

\[ E_{VAP}^0 = \frac{\hbar^a N_{VAP} j \hat{H} j^a N_{VAP} i}{\hbar^a N_{VAP} j^a N_{VAP} i} \]
Towards the VAP solution

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

\[ E_{0}^{\text{VAP}} = \frac{1}{4} h\hat{A}i \hat{i} \quad k_{2} h(\hat{c} \hat{N})^{2}i \hat{i} \quad k_{4} h(\hat{c} \hat{N})^{4}i \hat{i} \quad \cdots \]

### 1. Restricted VAP 1 (RVAP₁)

A product of quasiparticle operators

\[ \hat{\mathcal{A}} \quad \frac{\mathcal{H}(\hat{c} \hat{N}^{2}) j \hat{\mathcal{H}} i}{\mathcal{H}(\hat{c} \hat{N}^{2}) j \mathcal{H}(\hat{c} \hat{N}^{2}) i} = 0 \]

\[ \mathcal{H}(\hat{c} \hat{N}^{2}) j \hat{\mathcal{H}} i \mathcal{T} \mathcal{H}(\hat{c} \hat{N}^{2}) i = N \]

\[ \mathcal{H}(\hat{c} \hat{N}^{2}) j \mathcal{H}(\hat{c} \hat{N}^{2}) i = \mathcal{H}(\hat{c} \hat{N}^{2}) \]

\[ j^{a} N (\hat{c} \hat{N}^{2}) i = \mathcal{H}(\hat{c} \hat{N}^{2}) j \mathcal{T}(\hat{c} \hat{N}^{2}) i \]

\[ E^{\text{MF}} (\hat{c} \hat{N}^{2}) = \frac{\mathcal{H}(\hat{c} \hat{N}^{2}) j \mathcal{H}(\hat{c} \hat{N}^{2}) i}{\mathcal{H}(\hat{c} \hat{N}^{2}) j \mathcal{T}(\hat{c} \hat{N}^{2}) i} \]

**1. Introduction**

2. Results

3. Conclusions

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**Abstract**

**Keywords**

**Introduction**

**Methods**

**Results**

**Discussion**

**Conclusions**
Towards the VAP solution

\[ E_{0}^{\text{VAP}} = \frac{1}{4} \hbar A_{i}^{\phantom{i}j} + k_{2}\hbar (\xi N)^{2i} j + k_{4}\hbar (\xi N)^{4i} j \cdots \]

2. Restricted VAP 2 (RVAP₂)

\[ \sum_{i} \frac{\hbar \xi j \hat{A}_{i}^{\phantom{i}j} \xi N_{i} \xi N_{i} \xi N_{i} \xi N_{i} \xi N_{i} \xi N_{i} \xi N_{i} \xi N_{i}}{\hbar \xi j \xi i} = 0 \quad \text{if } \xi j = \xi i \]

\[ \begin{align*}
&1 \quad \hbar \xi j \xi N_{i} \xi N_{i} = N \\
&\xi N_{i} \quad \hbar \xi j \xi N_{i} \xi i = \xi N_{i} \\
&\xi N_{i} \quad \hbar \xi j \xi N_{i} \xi i = \xi N_{i} \\
&\xi N_{i} \quad \hbar \xi j \xi N_{i} \xi i = \xi N_{i} \\
\end{align*} \]

\[ E_{M}^{\text{MF}} (\xi N_{i} ; \xi N_{i}) \]

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

\[ E_{0}^{\text{RVAP}_{2}} = \min \sum_{i} E_{N} (\xi N_{i} ; \xi N_{i}) \]
Towards the VAP solution

3. Lipkin-Nogami (LN) Prescription

\[
\hat{A} = \frac{h \hat{j} \hat{A} \hat{j} \hat{i} - \hat{N} \hat{i}}{h \hat{j} \hat{i}} + \frac{h \hat{j} \hat{N} \hat{j} \hat{i} - \hat{N} \hat{i}}{h \hat{j} \hat{i}} = 0
\]

\( j \hat{j} \hat{i} = j \hat{j} \hat{i} = 0 \)

\[
h_2 = \frac{h \hat{N} \hat{j} \hat{N} \hat{j} \hat{i} - \hat{N} \hat{j} \hat{i}}{h \hat{j} \hat{i}}
\]

\[
h_2 = \frac{h \hat{N} \hat{j} \hat{N} \hat{j} \hat{i} - \hat{N} \hat{j} \hat{i}}{h \hat{j} \hat{i}}
\]

4. Projected Lipkin-Nogami (PLN)

\[
j^a \hat{N} \hat{j} \hat{i} = P \hat{j} \hat{j} \hat{i}
\]

\[
E_0^{LN} = \frac{h \hat{j} \hat{j} \hat{j} \hat{i} \hat{j} \hat{j} \hat{i}}{h \hat{j} \hat{j} \hat{i}}
\]

\[
E_0^{PLN} = \frac{h \hat{j} \hat{j} \hat{j} \hat{i} \hat{j} \hat{j} \hat{i}}{h \hat{j} \hat{j} \hat{i}}
\]
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 $\psi N^2$

$$\text{j} \overset{\circ}{\otimes}_{LN} \text{i} 2 \text{j} \overset{\circ}{\otimes} (\psi N^2) \text{i}$$

$$\implies h_2 = \cdot \psi N^2$$

The above condition can be deduced in a variational way:

- We evaluate with the set of constrained wave function $\text{j} \overset{\circ}{\otimes} (\psi N^2) \text{i}$ the approximate projected energy as a function of $\psi N^2$

$$E_{0}^{LN}(\psi N^2) = h^A i \text{i} h_2 h(\psi N)^2 i$$

- We minimize $E_{0}^{LN}(\psi N^2)$ along the $(\psi N^2)$ direction assuming that:

$$\left\{ \frac{\partial E_{0}^{LN}(\psi N^2)}{\partial \psi N^2} \cdot \psi N^2, h_2 \notin h_2(\psi N^2) \right\} = 0 \implies h_2 = \cdot \psi N^2$$
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 \(E_{0}^{LN}(\psi N^2) = h^4 i \; i \; h_2(\psi N^2)\) curve whenever \(h_2 \not\in h_2(\psi N^2)\)

- PLN solution will be as good as RVAP\(_1\) only.
Circular Hamiltonians

**Multilevel pairing Hamiltonian**

- Single particle levels are equally spaced and doubly-degenerate ($\Omega = 2$).
- $N = \text{number of particles} = \text{number of levels}$

**Normalized interaction strength**

$\hat{\mathcal{A}} = \frac{G}{d} \left( -i \right)^1$
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.
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 (RVAP₁) 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 RVAP₁ 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 $\Delta N^2$ direction.
**Multilevel Pairing Hamiltonian**

- **Restricted Variation After Projection 2 (RVAP₂)**

Exploring the $\mathcal{C} N^4$ at the minima of the PPES along the $\mathcal{C} N^2$ direction

- **CBCS**
- **PCBCS**
- **RVAP₁**
- **RVAP₂**
- **VAP**

**Graphs**
- Non-correlated regime
- Correlated regime
Choosing the minima of $\mathcal{C} \propto N^2; \propto N^4$
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

Diagram showing the energy $E_{\text{cond}/d}$ as a function of $\chi$ and $\Delta N^2$ for different models: BCS, VAP, RVAP, LN, and PLN.
Two Level Pairing Hamiltonian

\[ \text{RVAP}_2 \text{ vs. (P)LN} \]

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

- The \( h_2 \) parameter has a strong dependence on \( \Delta N^2 \) direction.
1. Introduction

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Relative Errors

- LN method fails in weakly correlated regimes
- PLN is as good as RVAP₁ although in weakly correlated regimes could fail
- In the Multilevel model PLN and RVAP₁ have a poor performance in the weak pairing region and RVAP₂ 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 $\Delta N^2$ 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.