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Author
Mang, H.J.

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H. J. Mang, B. Samadi, and P. Ring

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ON THE SOLUTION OF CONSTRAINED
HARTREE-FOCK-BOGOLYUBOV EQUATIONS

H.J. Mang
Nuclear Science Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California

B. Samadi and P. Ring
Technische Universitat Munchen
Physik Department
D8046 GARCHING BRD

ABSTRACT

A method is described to solve constrained HFB-equations without
introduction of a Lagrangian multiplier. To demonstrate the versatility
of the method rotational bands in $^{164}\text{Er}$ and $^{168}\text{Yb}$ are calculated.
I. Introduction

The interest in solutions of the HFB-equations stems mainly from the success of the theory in the calculation of energy surfaces\(^1\) and properties of rotational states.\(^2\). In the first case the expectation value of the quadrupole operator \(\hat{Q}\), and if necessary of higher multipole operators, must be constrained whereas in the second case the expectation value of the angular momentum operator must be fixed at a given value.

The conventional technique for solving such problems is to introduce a Lagrangian multiplier i.e. to add a term \(-\omega \hat{J}_x\) or \(-\eta \hat{Q}\) to the Hamiltonian. Difficulties arise if the expectation value is not a single valued function of the Lagrangian multiplier. They can be overcome by using a quadratic constraint like \(c(\hat{Q} - Q_0)^2\), which is added to the energy expression to be varied. In this paper a method is described which also circumvents such difficulties and has moreover the advantage that the energy is only calculated for a single given value of the expectation value of the constraining operator. For instance, in the case of rotational states one obtains solutions which exactly fulfill

\[
\langle \hat{J}_x \rangle = J(J+1) - \langle J_z^2 \rangle \\
\tag{I.1}
\]

And these are the only physically significant solutions. There is no need to do a calculation for several values of the Lagrangian multiplier and then interpolate between them.
II. Review of HFB-Theory

For the convenience of the reader the important equations of HFB-theory are given once more. Details can be found in reference 2 and the literature cited there.

A Bogolyubov transformation is defined by

\[ \alpha^+_\nu = \sum_k A_{k\nu} C^+_k + B_{k\nu} C_k \]  

(II.1)

The coefficients \( A_{k\nu} \) and \( B_{k\nu} \) are only restricted by the requirement that the set of Fermi operators \( C^+_k, C_k \) are transformed into a new set of Fermi operators \( \alpha^+_\nu, \alpha_\nu \). To each set of Fermi operators \( \alpha^+_\nu, \alpha_\nu \) belongs a uniquely defined vacuum state \( |\phi\rangle \) with the property

\[ \alpha_\nu |\phi\rangle = 0 \]  

(II.2)

Given a Hamiltonian \( H \) one may now ask the question which vacuum state \( |\phi\rangle \) minimizes the expectation value \( \langle \phi | H |\phi\rangle \). The equations of this variation principle are most conveniently formulated by transforming the Hamiltonian \( H \) into the quasi-particle representation:

\[ H = H_0 + H_{11} + H_{20} + H_{22} + H_{31} + H_{40} \]

with

* In order to simplify matters \( A \) and \( B \) will be taken as real from now on.
\[ H_0 = \langle \phi | H | \phi \rangle \]
\[ H_{11} = \sum_{\nu \mu} (H_{11})_{\nu \mu} \alpha^+_\nu \alpha^+_\mu \]
\[ H_{20} = \sum_{\nu \mu} (H_{20})_{\nu \mu} (\alpha^+_\nu \alpha^+_\mu + \alpha^+_{\bar{\nu}} \alpha_{\bar{\mu}}) \]
\[ H_{22} = \sum_{\nu \mu \lambda \rho} (H_{22})_{\nu \mu \lambda \rho} \alpha^+_\nu \alpha^+_\mu \alpha^+_\lambda \alpha^+_\rho \]
\[ H_{31} = \sum_{\nu \mu \lambda \rho} (H_{31})_{\nu \mu \lambda \rho} (\alpha^+_\nu \alpha^+_\mu \alpha^+_\lambda \alpha^+_\rho + \alpha^+_{\bar{\nu}} \alpha^+_{\bar{\mu}} \alpha^+_{\bar{\lambda}} \alpha^+_{\bar{\rho}}) \]
\[ H_{40} = \sum_{\nu \mu \lambda \rho} (H_{40})_{\nu \mu \lambda \rho} (\alpha^+_\nu \alpha^+_\mu \alpha^+_\lambda \alpha^+_\rho + \alpha^+_{\bar{\nu}} \alpha^+_{\bar{\mu}} \alpha^+_{\bar{\lambda}} \alpha^+_{\bar{\rho}}) \]

where \((H_{11})_{\nu \mu}\) and \((H_{20})_{\nu \mu}\) are given by:
\[ (H_{11})_{\nu \mu} = \langle \phi | \alpha^+_\nu H \alpha^+_\mu | \phi \rangle \]
\[ (H_{20})_{\nu \mu} = \frac{1}{2} \langle \phi | \alpha^+_\mu \alpha^+_\nu H | \phi \rangle \]

The terms with four quasi-particle operators are defined analogously but are not needed here. \((H_{11})_{\nu \mu}\) and \((H_{20})_{\nu \mu}\) can be expressed in terms of the coefficients \(A_{kv}, B_{kv}\) and the Hamiltonian \(H = t + v\).

\[ (H_{11})_{\nu \mu} = (A^+ B^+ h A - A^+ B^+ A^+ B^+ A A)_{\nu \mu} \]
\[ (H_{20})_{\nu \mu} = (A^+ h B - B^+ h A + A^+ A A^+ B - B^+ A A^+ B)_{\nu \mu} \]

with \(h = t + \Gamma\)

\(\Gamma\) and \(\Lambda\) are the self-consistent single particle potential and pairing potential respectively. (For details see ref. 2 eqn. 3.61)
Next a theorem on HFB-functions (vacuum states) due to Thouless\textsuperscript{3}) is used. The theorem is stated without proof, which is given in reference 2. Any two vacuum states $|\phi\rangle$ and $|\chi\rangle$ whose scalar product is non zero

$$\langle \chi | \phi \rangle \neq 0 \quad \text{(II.6)}$$

and the corresponding sets of quasi-particle operators $\{\gamma^{+}_{\mu}, \gamma_{\mu}\}$ and $\{\alpha^{\dagger}_{\nu}, \alpha_{\nu}\}$ are related as follows:

$$|\chi\rangle = K \exp \left( \frac{i}{\hbar} \sum_{\mu \nu} C^{\dagger}_{\mu \nu} \alpha_{\mu}^{\dagger} \alpha^{\dagger}_{\nu} \right) |\phi\rangle \quad \text{(II.7)}$$

(K normalization constant)

$$\gamma_{\mu} = \Sigma_{\nu} S_{\nu \mu} (\alpha_{\nu}^{\dagger} + \Sigma_{\rho} C_{\rho \nu} \alpha^{\dagger}_{\rho}) \quad \text{(II.8)}$$

$$\alpha_{\nu} |\phi\rangle = 0$$

$$\gamma_{\mu} |\chi\rangle = 0$$

$$\gamma_{\mu} = \Sigma_{\nu} P_{\nu \mu} \alpha_{\nu} + R_{\nu \mu} \alpha^{\dagger}_{\nu} \quad \text{(II.9)}$$

$$C_{\mu \nu} = (RP^{-1})_{\mu \nu} \quad \text{(II.10)}$$

Equations II.7 and II.8 give $|\chi\rangle$ and $\gamma_{\mu}$ in terms of $C_{\mu \nu}$ whereas in Equations II.9 and II.10 $C_{\mu \nu}$ is given in terms of $\alpha_{\nu}$, $\alpha_{\nu}^{\dagger}$, and $\gamma_{\mu}$, $\gamma_{\mu}^{\dagger}$. 
Consider now:

\[
\frac{\langle \chi | H | \chi \rangle}{\langle \chi | \chi \rangle} = \frac{\frac{1}{2} \sum \lambda \rho \rho^* \lambda^*}{\frac{1}{2} \sum \lambda \rho \rho^* \lambda^*} \frac{1}{e^2} \frac{\sum \mu \nu \alpha_\mu^+ \alpha_\nu}{\sum \mu \nu \alpha_\mu^+ \alpha_\nu} \]

\[
= E \{C_{\mu \nu}\} \tag{II.11}
\]

Obviously one has:

\[
\frac{\partial}{\partial C_{\mu \nu}} H \bigg|_{\{C_{\mu \nu} = 0\}} = \langle \phi | \alpha_\nu \alpha_\mu^+ H | \phi \rangle = (H_{\mu \nu}^{20})_{\mu \nu} \tag{II.12}
\]

Because Equations II.7 and II.8 establish the most general variation of \(|\phi\rangle\), Equations II.12 gives the variation of any expectation value \(\langle \phi | Q | \phi \rangle\) (just replace \(H\) by \(Q\) in II.11 and II.12). This variation or the derivative with respect to \(C_{\mu \nu}\) is determined by the coefficients \(A_{k\nu}\) and \(B_{k\nu}\) through Equations II.3 to EE.5. Therefore not only any expectation value but also its derivative is given in terms of these coefficients.

This forms the basis of a numerical method for the solution of constrained HFB-equations which is described in the following section.
III. Numerical Method of Solution.

The equations to start with are

\[ \frac{\partial}{\partial C_{\mu
u}} \langle \phi | H | \phi \rangle = (H_{20})_{\mu
u} \]
\[ \frac{\partial}{\partial C_{\mu
u}} \langle \phi | J | \phi \rangle = (J_{20})_{\mu
u} \]  

(III.1)

\[ \Delta E = \sum_{\mu\nu} C_{\mu\nu} (H_{20})_{\mu\nu} + O(C_{\mu\nu}^2) \]

(III.2)

\[ \Delta J = \sum_{\mu\nu} C_{\mu\nu} (J_{20})_{\mu\nu} + O(C_{\mu\nu}^2) \]

From now only the terms linear in \( C_{\mu\nu} \) will be taken into account. Clearly \( \Delta E \) is negative and has its greatest absolute value if one sets

\[ C_{\mu\nu} = - \eta (H_{20})_{\mu\nu} \quad \eta > 0 \]  

(III.3)

Then \( \Delta J \) is given by
\[ \Delta J = -n \sum_{\mu \nu} (H_{20})^{\mu \nu} (J_{20})^{\mu \nu} \]  \hspace{1cm} (III.4)

An expression like \( \sum_{\mu \nu} (H_{20})^{\mu \nu} (J_{20})^{\mu \nu} \) can be interpreted as a scalar product of two vectors \( H_{20} \) and \( J_{20} \). With this simplified notation \( \Delta E \) and \( J_{20} \) take the form

\[ \Delta E = -n (H_{20})^2 \]  \hspace{1cm} (III.5)

\[ \Delta J = -n (H_{20} \cdot J_{20}) \]

Of course \( \Delta J \) should vanish provided the expectation value \( \langle \phi \mid \hat{J} \mid \phi \rangle \) equals \( J_0 \), the desired value. If this is not the case on sets

\[ C_{\mu \nu} = \frac{(J_0 - \langle \hat{J} \rangle)}{(J_{20})^2} J_{\mu \nu} \]  \hspace{1cm} (III.6)

and repeats this procedure if necessary until \( \langle \hat{J} \rangle \) equals \( J_0 \).

From now on one decreases the energy without changing \( \langle \hat{J} \rangle \) by setting

\[ C_{\mu \nu} = -n \left[ (H_{20})^{\mu \nu} - \frac{(H_{20} \cdot J_{20})}{(J_{20})^2} (J_{20})^{\mu \nu} \right] \]  \hspace{1cm} (III.7)

With the coefficients \( C_{\mu \nu} \) from Eqn. III.7 the new quasi-particle operators \( \gamma_{\mu} \) follow from equation II.8. The quantities \( S_{\nu \mu} \) are determined by the requirement that the operators \( \gamma_{\mu} \) fulfill Fermi commutation relations. In practice this is achieved by orthogonalisation of a set of vectors \( \hat{v}_\mu \).
These are related to the operators $\gamma^\mu_\nu$ which fulfill the relations

\[
\gamma^\mu_\nu = \alpha_\nu + \sum_\rho C^\rho_\nu \alpha^{\dagger}_\rho
\]

\[
\{\gamma^\mu_\nu, \gamma^\sigma_\sigma\} = \delta^\nu_\sigma + \sum_\rho C^\rho_\nu C^\rho_\sigma
\]

by

\[
(\tilde{g}^\gamma_\nu, \tilde{g}^\gamma_\sigma) = \{\gamma^\mu_\nu, \gamma^\mu_\sigma\}
\]

If the orthogonal vectors $g^\mu_\mu$ are

\[
g^\mu_\mu = \sum_\nu S^\nu_\mu g^\nu_\nu
\]

then the operators $\gamma^\mu_\nu$ are

\[
\gamma^\mu_\nu = \sum_\nu S^\nu_\mu \gamma^\nu_\nu
\]

This implies for the new coefficients $A^\prime_\mu_\nu$, $B^\prime_\mu_\nu$

\[
A^\prime_\mu_\nu = \sum_\nu S^\nu_\mu (A^\nu_\mu + \sum_\rho C^\rho_\nu B^\rho_\mu)
\]

\[
B^\prime_\mu_\nu = \sum_\nu S^\nu_\mu (B^\nu_\mu + \sum_\rho C^\rho_\nu A^\rho_\mu)
\]

It is clear that any number of constraints can be handled in the manner described. Only Equ. III.7 has to be generalized.
IV Applications

The constraints used in applying HFB-theory to the problem of nuclear rotations were the following:

\[ \langle \phi | \hat{N}_p | \phi \rangle = Z \quad \text{(proton number)} \quad \text{IV. 1} \]

\[ \langle \phi | \hat{N}_n | \phi \rangle = N = A - Z \quad \text{(neutron number)} \quad \text{IV. 2} \]

\[ \langle \phi | \hat{J}_x | \phi \rangle = J(J_H) - \langle J_z^2 \rangle \quad \text{(angular momentum)} \quad \text{IV. 3} \]

\[ \langle \phi | \phi_0 \rangle = 0 \quad \text{(for excited states |ϕ⟩)} \quad \text{IV. 4} \]

In the case of Eqn. IV. 4, |ϕ₀⟩ is the wavefunction of the energetically lowest state with the same quantum numbers as |ϕ⟩. It should be noted at this point that the relation

\[ \frac{\partial}{\partial C_{\mu \nu}} \langle \phi | \phi_0 \rangle \big|_{C_{\mu \nu} = 0} = \langle \phi | \alpha_\mu | \alpha_\nu \rangle |_{\phi_0} = 0 \quad \text{IV. 5} \]

holds. The requirement on H₂₀ is in this case

\[ (0 \cdot H_{20}) = 0 \quad \text{IV. 6} \]

in every step of the iterative solution of the constrained HFB - equations. Calculations were performed for \(^{164}\text{Er}\) and \(^{168}\text{Yb}\). The single particle configuration space was the same as used earlier\(^2\). The strength constants of the quadrupole-quadrupole force (Q) plus pairing force (G)
were slightly changed compared to the earlier work in order to give somewhat more quantitative agreement with experimental data. Besides that, a moment of inertia of the core was introduced. The core consists of 40 protons and 70 neutrons in single particle states not taken into account explicitly. The magnitude of this moment of inertia was chosen as \( \Theta_{\text{core}} = 6 \, \text{MeV}^{-1} \). Single particle energies and force constants are given in Table 1 and 2. This establishes the Hamiltonian and the expression for the energy to be used in the variational principle. It should be mentioned that the use of \( \Theta_{\text{core}} \) requires the knowledge of the angular frequency \( \omega \) which is obtained from the relation

\[
\omega = \frac{\partial E}{\partial \langle J \rangle} = \frac{(H_{20}^1 \cdot J_{20}^1)}{(J_{20}^1)^2}.
\]

Here \( H_{20}^1 \) and \( J_{20}^1 \) are those parts of the vectors \( H_{20} \) and \( J_{20} \) that are orthogonal to \( N_{p20} \) and \( N_{n20} \) (compare Equs. III.4 to III.7 and the notation introduced there).

Calculated and experimental results are shown in Figs. 1 to 4. It is evident that the calculation reproduces the general trend of the experimental data. In particular, the two 16\(^+\) states lie very close. This indicates that in this approach the Coriolis matrix elements are automatically reduced to a sufficient degree in order to have states of the same angular momentum and parity very close to each other\(^4\).

The results on \(^{168}\)Yb indicate that at least within a limited range of mass numbers experimental data are reproduced by the same simple effective interaction.
The results are encouraging enough to warrant the use of more sophisticated effective interactions in calculations of the type described here.
Acknowledgements

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References


2) H. J. Mang, Phys. Reports Vol 18C No. 6 (1975)


Table 1
Quantum numbers of single-particle states and their energies in MeV

<table>
<thead>
<tr>
<th>State</th>
<th>Energy</th>
<th>State</th>
<th>Energy</th>
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<td>1g g/2</td>
<td>-5.4792</td>
<td>1h 11/2</td>
<td>-6.5503</td>
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<td>1g 7/2</td>
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<td>1g g/2</td>
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<tr>
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<td>0.0000</td>
<td>2f 7/2</td>
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<td>3p 3/2</td>
<td>1.6067</td>
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Table 2
Strength constants of the interaction used. These constants are to be multiplied by dimension-less matrix elements like $\langle n' j' m' | \frac{1}{r_0^2} r_0^2 | n j m \rangle Y^0_2$

Here $r_0$ is the oscillator length. $G^{++}_{nn}$ is the pairing force constant acting between neutron states of positive parity $G^{+-}_{nn}$ and $G^{-+}_{nn}$ are analogous.

<p>| | | | |</p>
<table>
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<td>$G^{+-}_{nn}$</td>
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FIGURE CAPTIONS

1. Experimental\textsuperscript{(4)} and calculated energy levels of $^{164}$Er.
2. Experimental and calculated energy levels of $^{168}$Yb.
3. Calculated intrinsic quadrupole moments of $^{164}$Er. g.s. = ground state band, ex.b. = excited state band, - = negative parity band.
4. Calculated intrinsic quadrupole moments of $^{168}$Yb.
CALCULATED EXPERIMENT

Fig. 1
$^{168}$Yb

CALCULATED EXPERIMENT

Fig. 2
Fig. 4
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