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Author
Mang, H.J.

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

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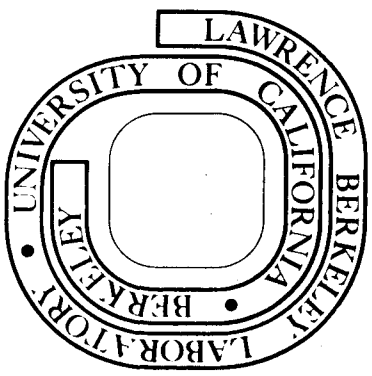

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ON THE SOLUTION OF CONSTRAINED HARTREE-FOCK-BOGOLYUBOV EQUATIONS

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}Er and ^{168}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 $c(\hat{Q} - Q_o)^2$, 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

$$\langle \hat{J}_x \rangle = J(J+1) - \langle J_z^2 \rangle \qquad (I.1)$$

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

$$\alpha^{\dagger}_{\nu} = \sum_{k} A_{k\nu}\, C^{+}_{k} + B_{k\nu}\, C_{k} \qquad \text{(II.1)}$$

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 $\alpha^{\dagger}_{\nu}$, α_{ν}. To each set of Fermi operators $\alpha^{\dagger}{}_{\nu}$, α_{ν} belongs a uniquely defined vacuum state $|\Phi\rangle$ with the property

$$\alpha_{\nu}|\Phi\rangle = 0 \qquad \text{(II.2)}$$

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*

$$H = Ho + H_{11} + H_{20} + H_{22} + H_{31} + H_{40}$$

with

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* In order to simplify matters A and B will be taken as real from now on.

$$H_o = \langle \phi | H | \phi \rangle$$

$$H_{11} = \sum_{\nu\mu} (H_{11})_{\nu\mu} \alpha_\nu^+ \alpha_\mu$$

$$H_{20} = \sum_{\nu\mu} (H_{20})_{\nu\mu} (\alpha_\nu^+ \alpha_\mu^+ + \alpha_\mu \alpha_\nu) \qquad \text{(II.3)}$$

$$H_{22} = \sum_{\nu\mu\lambda\rho} (H_{22})_{\nu\mu\lambda\rho} \alpha_\nu^+ \alpha_\mu^+ \alpha_\rho \alpha_\lambda$$

$$H_{31} = \sum_{\nu\mu\lambda\rho} (H_{31})_{\nu\mu\lambda\rho} (\alpha_\nu^+ \alpha_\mu \alpha_\rho \alpha_\lambda + \alpha_\lambda^+ \alpha_\rho^+ \alpha_\mu^+ \alpha_\nu)$$

$$H_{40} = \sum_{\nu\mu\lambda\rho} (H_{40})_{\nu\mu\lambda\rho} (\alpha_\nu^+ \alpha_\mu^+ \alpha_\lambda^+ \alpha_\rho^+ + \alpha_\rho \alpha_\lambda \alpha_\mu \alpha_\nu)$$

where $(H_{11})_{\nu\mu}$ and $(H_{20})_{\nu\mu}$ are given by:

$$(H_{11})_{\nu\mu} = \langle \Phi | \alpha_\nu \, H \, \alpha_\mu | \, \Phi \rangle \qquad \text{(II.4)}$$

$$(H_{20})_{\nu\mu} = \frac{1}{2} \langle \Phi \, | \alpha_\mu \alpha_\nu \, H | \Phi \rangle$$

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 $A_{k\nu}$, $B_{k\nu}$ and the Hamiltonian $H = t + v$.

$$(H_{11})_{\nu\mu} = (A^+ hA - B^+ hB + A^+ \Delta B - B^+ \Delta A)_{\nu\mu}$$

$$(H_{20})_{\nu\mu} = (A^+ hB - B^+ hA + A^+ \Delta A - B^+ \Delta B)_{\nu\mu} \qquad \text{(II.5)}$$

with $h = t + \Gamma$

Γ and Δ 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[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

$$\langle\chi|\phi\rangle \neq 0 \tag{II.6}$$

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

$$|\chi\rangle = K \exp\left(\tfrac{1}{2} \sum_{\mu\nu} C_{\mu\nu}\, \alpha_\mu^\dagger\, \alpha_\nu^\dagger\right)|\phi\rangle \tag{II.7}$$

(K normalization constant)

$$\gamma_\mu = \sum_\nu S_{\nu\mu}\left(\alpha_\nu + \sum_\rho C_{\rho\nu}\, \alpha_\rho^+\right) \tag{II.8}$$

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

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

$$\gamma_\mu = \sum_\nu P_{\nu\mu}\, \alpha_\nu + R_{\nu\mu}\, \alpha_\nu^+ \tag{II.9}$$

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

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

Consider now:

$$\frac{\langle\chi|H|\chi\rangle}{\langle\chi|\chi\rangle} = \frac{\langle\Phi|e^{\frac{1}{2}\sum_{\lambda\rho} C^{*}_{\lambda\rho}\alpha_{\rho}\alpha_{\lambda}} H\, e^{\frac{1}{2}\sum_{\mu\nu} C_{\mu\nu}\alpha^{+}_{\mu}\alpha^{+}_{\nu}}|\Phi\rangle}{\langle\Phi|e^{\frac{1}{2}\sum_{\lambda\rho} C^{*}_{\lambda\rho}\alpha_{\rho}\alpha_{\lambda}}\, e^{\frac{1}{2}\sum_{\mu\nu} C_{\mu\nu}\alpha^{+}_{\mu}\alpha^{+}_{\nu}}|\Phi\rangle} \qquad \text{(II.11)}$$

$$= E\,(\{C_{\mu\nu}\})$$

Obviously one has:

$$\frac{\partial}{\partial C^{*}_{\mu\nu}} H \Big|_{\{C_{\mu\nu}=0\}} = \langle\Phi|\alpha_{\nu}\alpha_{\mu}\, H\,|\,\Phi\rangle = (H_{20})_{\mu\nu} \qquad \text{(II.12)}$$

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 $\langle\phi|\hat{Q}|\phi\rangle$ (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

$$\frac{\partial}{\partial C_{\mu\nu}} \langle \Phi | H | \Phi \rangle = (H_{20})_{\mu\nu}$$

$$\frac{\partial}{\partial C_{\mu\nu}} \langle \Phi | \hat{J} | \Phi \rangle = (J_{20})_{\mu\nu} \qquad \text{(III.1)}$$

$$\Delta E = \sum_{\mu\nu} C_{\mu\nu} (H_{20})_{\mu\nu} + O(C_{\mu\nu}^2) \qquad \text{(III.2)}$$

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

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

$$C_{\mu\nu} = - \eta (H_{20})_{\mu\nu} \qquad \eta > 0 \qquad \text{(III.3)}$$

Then ΔJ is given by

$$\Delta J = -\eta \sum_{\mu\nu} (H_{20})_{\mu\nu} \quad (J_{20})_{\mu\nu} \tag{III.4}$$

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

$$\begin{aligned} \Delta E &= -\eta \ (H_{20})^2 \\ \Delta J &= -\eta \ (H_{20} \cdot J_{20}) \end{aligned} \tag{III.5}$$

Of course ΔJ should vanish provided the expectation value $\langle \phi | \hat{J} | \phi \rangle$ equals J_o, the desired value. If this is not the case on sets

$$C_{\mu\nu} = \frac{(J_o - \langle \hat{J} \rangle}{(J_{20})^2} \quad J_{\mu\nu} \tag{III.6}$$

and repeats this procedure if necessary until $\langle \hat{J} \rangle$ equals J_o.
From now on one decreases the energy without changing $\langle \hat{J} \rangle$ by setting

$$C_{\mu\nu} = -\eta \left[(H_{20})_{\mu\nu} - \frac{(H_{20} \cdot J_{20})}{(J_{20})^2} (J_{20})_{\mu\nu} \right] \tag{III.7}$$

With the coefficients $C_{\mu\nu}$ from Eqn. III.7 the new quasi-particle operators γ_μ follow from equation II.8. The quantities $S_{\nu\mu}$ are determined by the requirement that the operators γ_μ fulfill Fermi commutation relations. In practice this is achieved by orthogonalisation of a set of vectors g'_μ.

These are related to the operators γ'_μ which fulfill the relations

$$\gamma'_\mu = \alpha_\nu + \sum_\rho C_{\rho\nu}\, \alpha^\dagger_\rho$$

$$\{\gamma'^\dagger_\nu\ \gamma'_\sigma\} = \delta_{\nu\sigma} + \sum_\rho C_{\rho\nu}\, C_{\rho\sigma} \qquad \text{III.8}$$

by

$$(\vec{g}'_\nu\ \vec{g}'_\sigma) = \{\gamma'^\dagger_\nu\ \gamma'_\sigma\} \qquad \text{III.9}$$

If the orthogonal vectors g_μ are

$$g_\mu = \Sigma\, S_{\nu\mu}\, g'_\nu \qquad \text{III.10}$$

then the operators γ_ν are

$$\gamma_\mu = \Sigma\, S_{\nu\mu}\, \gamma'_\nu \qquad \text{III.11}$$

This implies for the new coefficients $A'_{k\mu}$, $B'_{k\mu}$

$$A'_{k\mu} = \sum_{\nu\rho} S_{\nu\mu}\, (A_{k\nu} + \sum_\rho C_{\rho\nu}\, B_{k\rho})$$

$$B'_{k\mu} = \sum_{\nu\rho} S_{\nu\mu}\, (B_{k\mu} + \sum_\rho C_{\rho\nu}\, A_{k\rho})$$

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

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

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

$$\langle \phi | \hat{J}_x | \phi \rangle = J(JH) - \langle J_z^2 \rangle \qquad \text{(angular momentum)} \qquad \text{IV. 3}$$

$$\langle \phi | \phi_o \rangle = 0 \quad \text{(for excited states } |\phi\rangle) \qquad \text{IV. 4}$$

In the case of Equ. IV. 4, $|\phi_o\rangle$ is the wavefunction of the energetically lowest state with the same quantum numbers as $|\phi\rangle$. It should be noted at this point that the relation

$$\frac{\partial}{\partial C_{\mu\nu}} \langle \phi | \phi_o \rangle \Big|_{\{C_{\mu\nu} = 0\}} = \langle \phi | \alpha_\mu \alpha_\nu | \phi_o \rangle = 0_{\mu\nu} \qquad \text{IV. 5}$$

holds. The requirement on H_{20} is in this case

$$(O \cdot H_{20}) = 0 \qquad \text{IV. 6}$$

in every step of the iterative solution of the constrained HFB - equations. Calculations were performed for ^{164}Er and ^{168}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 $\Theta_{core} = 6\ MeV^{-1}$. 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 Θ_{core} requires the knowledge of the angular frequency ω which is obtained from the relation

$$\omega = \frac{\partial E}{\partial (J_x)} = \frac{(H'_{20} \cdot J'_{20})}{(J'_{20})^2}.$$

Here H'_{20} and J'_{20} 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

1) P. Quentin, H. Flocard and D. Vautherin, in: Proc. Intern. Conf. on Nucl. Phys., Munich 73, Vol. 1, p. 41

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

3) D. J. Thouless, The quantum mechanics of many-body systems (Academic Press, New York and London, 1961).

4) F. S. Stephens and R. Diamond, private communication.

Table 1

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

PROTONS		NEUTRONS	
State	Energy	State	Energy
1g g/2	-5.4792	1h 11/2	-6.5503
1g 7/2	-0.7415	1g g/2	-0.8651
2d 5/2	0.0000	2f 7/2	-1.7303
1h 11/2	1.0464	1i 13/2	0.5200
2d 3/2	2.6531	3p 3/2	1.6067
3S 1/2	2.9662	2f 5/2	2.1010
1h g/2	6.7975	3p 1/2	3.2134
		2g 9/2	7.1930

Table 2

Strength constants of the interaction used. These constants are to be multiplied by dimension-less matrix elements like $\langle n\ l\ j\ m \mid \left(\frac{r}{r_o}\right)^2 r^o_2 | nl'j'm' \rangle\ Y^o_2$ Here r_o 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.

$Q_{pp} = -0.0418$

$Q_{pn} = -0.110$

$Q_{nn} = -0.0418$

$G_{pp} = -0.2200$

$G^{++}_{nn} = -0.1980$

$G^{+-}_{nn} = -0.1870$

$G^{--}_{nn} = -0.1727$

FIGURE CAPTIONS

1. Experimental[4] and calculated energy levels of ^{164}Er.
2. Experimental and calculated energy levels of ^{168}Yb.
3. Calculated intrinsic quadropole moments of ^{164}Er. g.s. = ground state band, ex.b. = excited state band, - = negative parity band.
4. Calculated intrinsic quadrapole moments of ^{168}Yb.

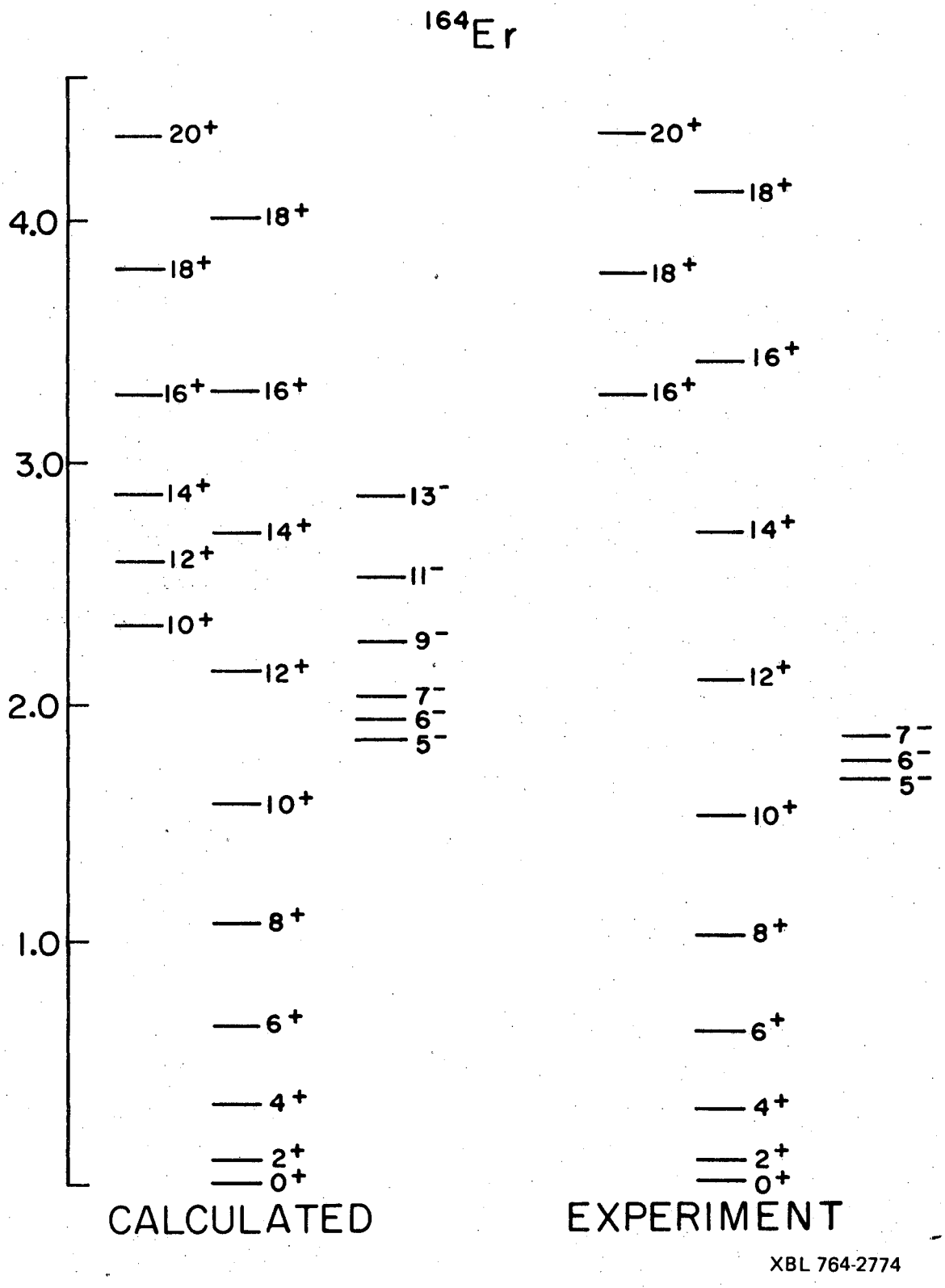

Fig. 1

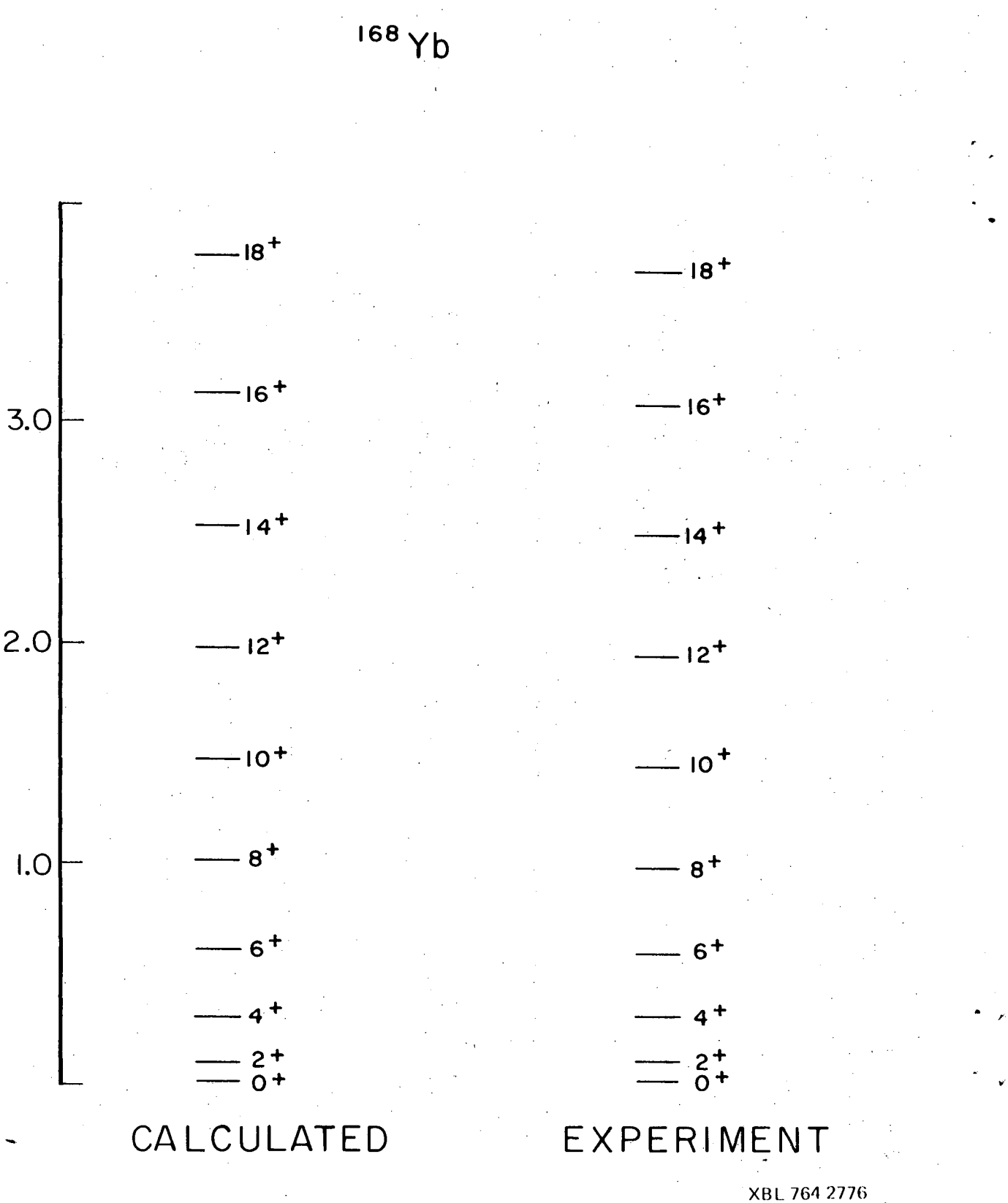
168 Yb
18+
16+
14+
12+
10+
8+
6+
4+
2+
0+
3.0
2.0
1.0
CALCULATED
EXPERIMENT
XBL 764 2776

Fig. 2

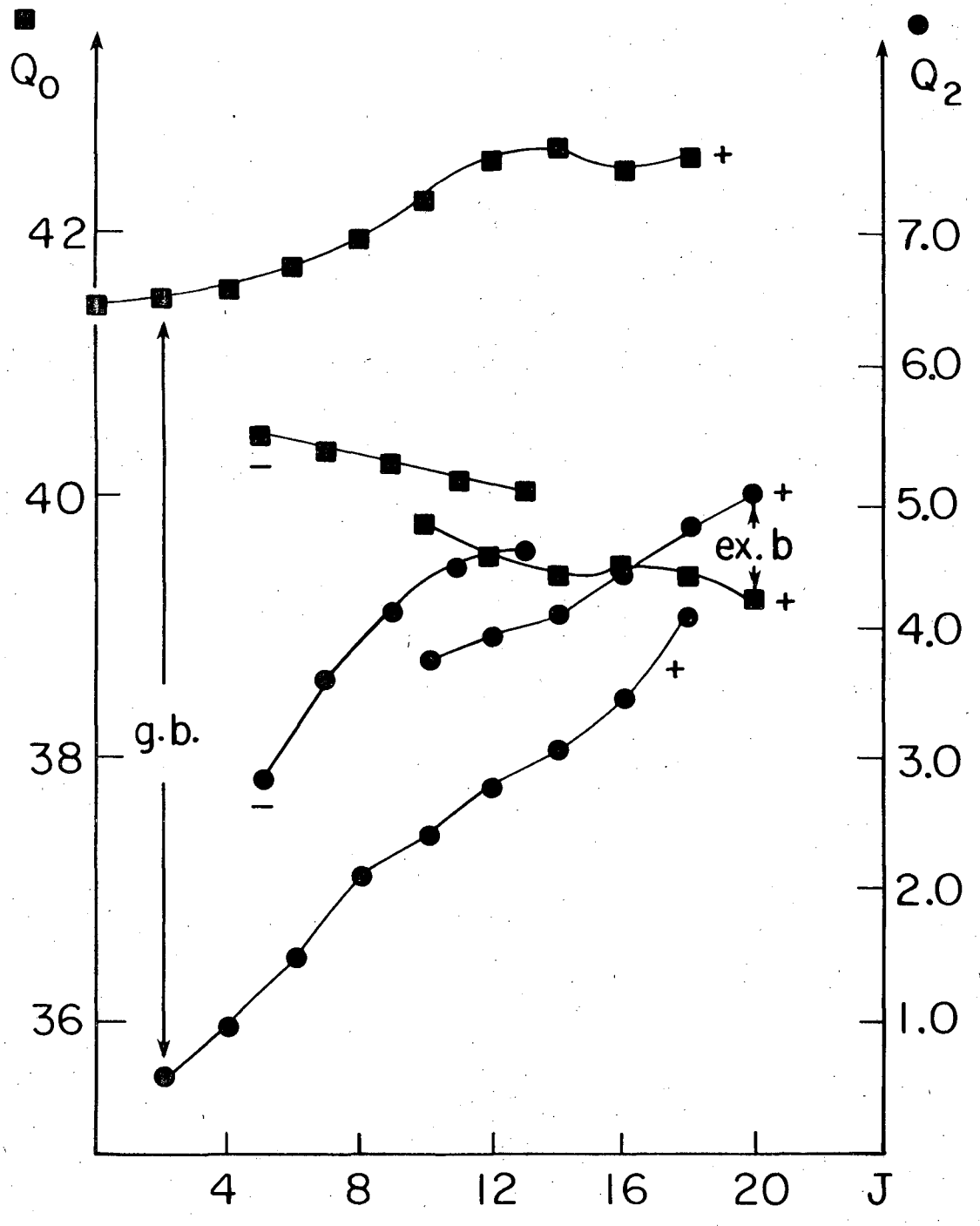

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Fig. 3

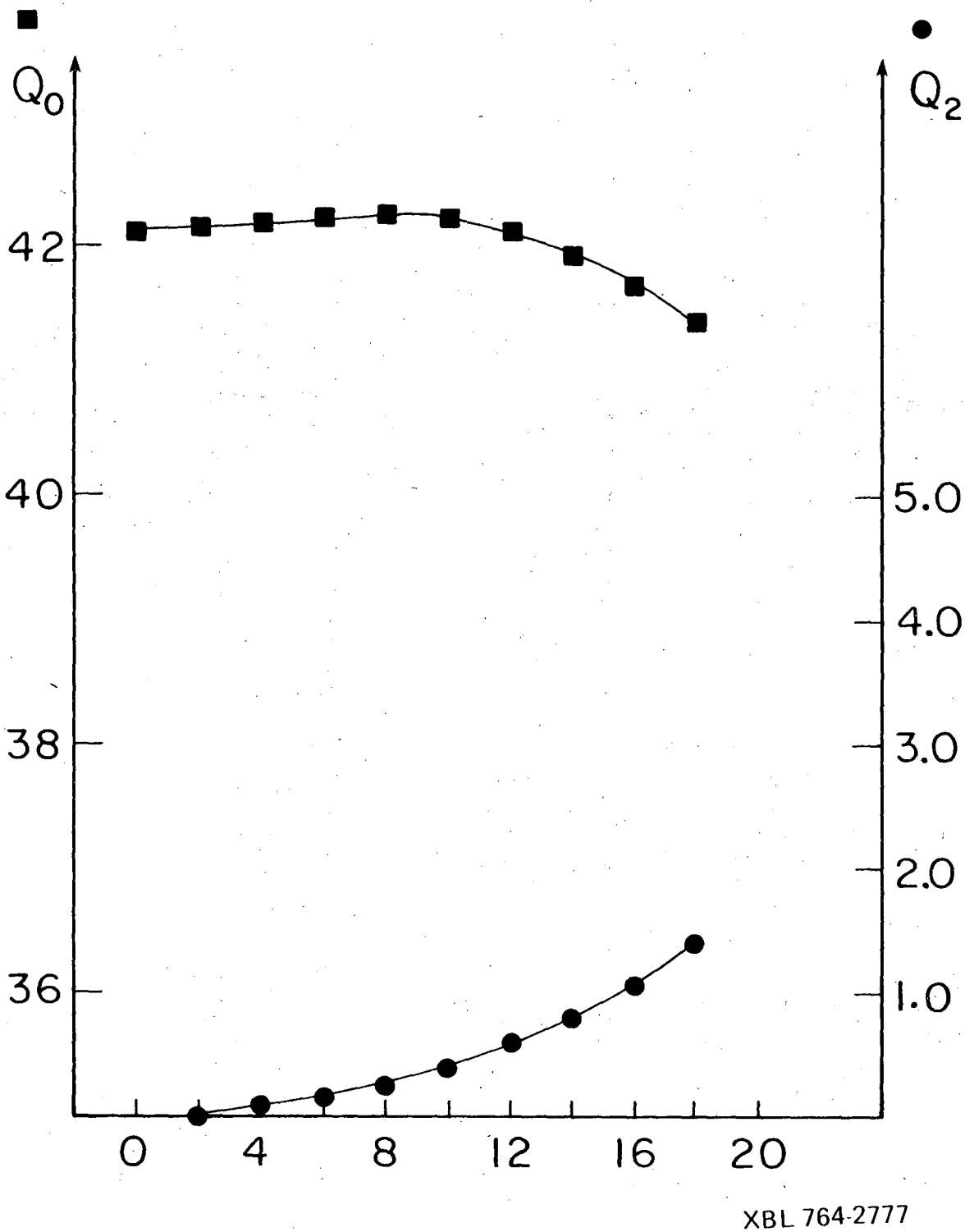

Fig. 4

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