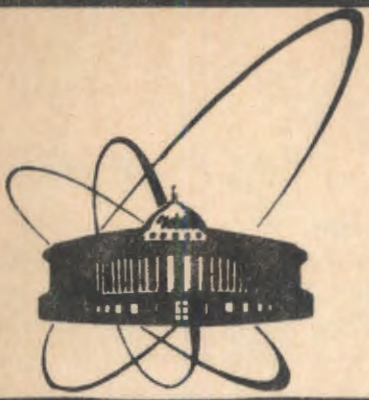

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E4-90-98

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ON A NEW APPROACH TO THE MICROSCOPIC SUBSTANTIATION OF THE INTERACTING BOSON MODEL-1

I. Microscopic determination of IBM-1 Hamiltonian parameters and application to even-even Zn isotopes

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1990

1. INTRODUCTION

The Interacting Boson Model (IBM)[1], under the influence of which the area of low energy excitations of nuclei has blossomed into an active and exciting field[2-4], was advanced by Iachello and Arima at first as purely phenomenological theory. Much of the appeal of the original version of the model, referred to as IBM-1 (IBM stands for IBM-1 and all its derivatives), stems from its overtly algebraic structure, which enables classification (according to the IReps of SU(6) group) of the boson basic states, to be exploited in conjunction with dynamical symmetries of the SU(6) boson Hamiltonian[1,3,4].

The impressive impact of the "new phenomenology" on the studies in nuclear structure and spectroscopy[3] has naturally raised the question about the link of IBM to the admittedly more fundamental nuclear Shell Model (SM). In particular, the microscopic substantiation of IBM in context of spherical SM, has indeed been put on the agenda and, despite the formidable work done in this direction[5] has not been removed eversince[2,4,6]. This problem has been investigated by several authors utilizing a variety of methods (Cf., e.g.: Table I in Ref. 6; Ch. 15 of Ref. 4 and vol. 2, part III, Sec. VIII of Ref. 2). A few problems encountered in the implementation of these microscopic approaches have also been remarked[2,6,7]:

(i) The mapping of the "giant" SM fermionic space into the small IBM boson subspace is, understandably, in no way unique.

(ii) The mapping procedure can be carried out explicitly in schematic cases only. In realistic cases the mapping procedures yield very complicated expressions. This is the crux of the matter, since the mapping lies in the heart of any attempt to derive IBM-like Hamiltonian starting from the SM.

(iii) The construction of the boson images of the IBM Hamiltonian and physical operators (which is based on equating matrix elements of the appropriate operators in the fermion space with those in the boson space for lowest generalized seniority states) can be effected in a closed form again only in particular cases.

(iv) Attempts to provide microscopic foundation of IBM-1 assume that the total number of s- and d-bosons, N, equals to the number of valence pairs ("IBM counting rule"). Such being the case, this is a phenomenological step, which can be avoided if one makes the best use of the underlying SU(6) symmetry. Moreover, fuller enlisting of symmetry considerations helps to resolve some of the problems mentioned above (Cf. Sec. 2).

This is by far not a complete list of predicaments of present-day IBM microscopy. They are only being mentioned as a rationale for the claim that additional efforts be directed to synthesizing of a theoretical framework which, exploiting maximally the inherent algebraic properties, accommodates sound microscopic support for the IBM-1.

In this connection we note that an alternative approach to arrive from the SM to collective SU(6)-model (referred to as Truncated Quadrupole Phonon Model (TQM)[8]) has been chosen by Janssen,

Jolos and Dönau as early as in Refs. 9-11. The TQM Hamiltonian has been constructed as the first set out on the basis of a sufficiently generic microscopic Hamiltonian[9-11]. With their seminal work[9] the authors of TQM have set the method for microscopic treatment of the collective quadrupole degree of freedom to enroll approximate bifermion SU(6) algebra, referred to as Quadrupole Collective Algebra (QCA)[12]. Since exact boson realization of QCA are available (Cf., e.g. Ref. 12), the passage to bosons is straightforward what made it possible to obtain the TQM Hamiltonian and physical operators directly, without having to resort to mapping of matrix elements. However, this approach encounters problems too. In particular, since the SU(6) symmetry has been enforced[9-11], this necessarily lays down conditions on the amplitudes of the collective pairs, composing QCA. The authors of TQM have pointed out that the relevant constraints, to be referred to as SU(6)-enforcing conditions (SU(6)-EC), can be inferred from the Jacobi identities what is, as a matter of fact, an intricate problem to solve. This fact might have been the reason that the further development of the approach, based on enforced symmetries, remained dormant for some time.

Due to recent publications[13-16], the enforced symmetry approach has been increasing brought to bear on the problem of microscopic foundation of IBM-1. Rigorous derivation of the ensuing SU(6)-EC and explicit microscopic contribution of Dyson, Holstein-Primakoff and Schwinger (SR) realization of QCA (each of them interrelated with the SU(6)-EC) have been itemized in Ref. 13. The developments presented in Refs. 13-16 have enabled us to advance a new approach to the microscopic substantiation of IBM-1, to be referred to as SU(6)-Boson Extended Random Phase Approximation (SU(6)-B-ERPA). While we shall return to this point in Sec. 2, it suffices for the moment to characterize SU(6)-B-ERPA as follows. The key role in this approach is played by the collective RPA quadrupole phonon operators subjected to SU(6)-EC. Substituting the SR of the constrained RPA quadrupole phonon operators and their commutators into the Quasiparticle Phonon Model[17] (QPM) Hamiltonian (an established microscopic model) we derive a genuine IBM-1 Hamiltonian with coefficients, depending on known microscopic quantities and on the amplitudes of the constrained phonons. This microscopically deduced IBM-1 Hamiltonian will be referred to as SU(6)-B-ERPA Hamiltonian. The unknown phonon amplitudes have been determined from a variational principle with constraints that ensures minimum of the SU(6)-B-ERPA Hamiltonian in the collective subspace in conjunction with fulfillment of the SU(6)-EC (Cf. Sec. 2).

The consistent treatment of the symmetry governed dynamics and of the SU(6)-EC, that go with it, constitutes the major innovation of the SU(6)-B-ERPA, being a part and parcel of the entire theoretical edifice.

The purpose of the present paper is twofold:

(i) to present an outline of the SU(6)-B-ERPA approach to the microscopic justification of IBM-1 (Sec. 2) and its computational realization (Sec. 3);

(ii) to apply SU(6)-B-ERPA in an illustrative microscopic calculation of IBM-1 Hamiltonian

parameters for the $^{64-70}Zn$ isotopes (Sec. 4). Experimental data, pertaining to the energies of low-lying collective states in these isotopes are available[18]. The parameters of IBM-1 Hamiltonian have been previously fitted to this chain of isotopes[19]. To the best of our knowledge, microscopic calculations of IBM-1 parameters for Zn isotopes have not been reported. These are the reasons behind our choice of these nuclei as object of our illustrative numerical investigations. Microscopic calculation of IBM-1 parameters in Pt isotopes are now in progress and will be reported elsewhere. In addition we plan to perform calculations within the SU(6)-B-ERPA for nuclei in the region of Sm isotopes.

In keeping with all, that has been discussed thus far, the subsequent treatment will provide the outline of SU(6)-B-ERPA as one possible way towards meeting the demands for a sound microscopic theory of IBM-1.

2. AN OUTLINE OF THE PRESENT APPROACH

As was stated in the Introduction, partial contributions to the development of the SU(6)-B-ERPA are contained in a series of papers[13-16]. In this section, for the first time, we present the full account of the theoretical underpinning of SU(6)-B-ERPA. A detailed expose is presented with purpose to publicize more widely the basic ideas and the mathematical apparatus of this alternative approach to the microscopic foundation of IBM-1.

Prior to setting up the SU(6)-B-ERPA, we recall a few items pertaining to the IBM-1 Hamiltonian (whose microscopic derivation is the ultimate end of the SU(6)-B-ERPA). The standard form of the latter reads[1,4]:

$$\begin{aligned} H_{IBM} &= \bar{h}\sum_{\mu}(d^{+}_{2\mu}d_{2\mu}) + C_{h_1}(\frac{1}{2}s^{+}s^{+}ss) + C_{h_2}(\sum_{\mu} d^{+}_{2\mu}d_{2\mu}s^{+}s) \\ &+ \sum_{L=0,2,4} \bar{C}_L(\frac{1}{2}\sqrt{2L+1}[[d^{+}_2 \otimes d^{+}_2]_{(L)} \otimes [\tilde{d}_2 \otimes \tilde{d}_2]_{(L)}]_{(00)} \\ &+ F[[d^{+}_2 \otimes d^{+}_2]_{(2)} \otimes [\tilde{d}_2 \otimes s]_{(2)}]_{(00)} + h.c. \\ &+ G[[d^{+}_2 \otimes d^{+}_2]_{(0)} \otimes [s \otimes s]_{(0)}]_{(00)} + h.c. \end{aligned} \tag{2.1}$$

Performing the needed recoupling in the tensor products featuring in (2.1), one can represent the IBM-1 Hamiltonian as an SO(3)-scalar, built from the generators $(d^{+}_{2\mu}s, s^{+}d_{2\mu}, d^{+}_{2\mu}d_{2\nu},\ \mu,\nu = 0,\pm1,\pm2)$ of the canonical SU(6) algebra in Schwinger realization (Cf., e.g. Ref. 12). The Hamiltonian (2.1) conserves the total number of s- and d-bosons, N, which, for a given nucleus, is postulated to be equal to the number of pairs of valence nucleons ("IBM-counting rule"). This is in essence a free parameter. The parameters in IBM-1 Hamiltonian are usually determined by the least square

fit to observed nuclear properties[1-4]. The variation of these parameters with mass number is smooth and fits are remarkable.

The main aim of any microscopic approach to the "SU(6) phenomenology" is to relate the free parameters of H_{IBM-1}, featuring in (2.1),to the microscopic quantities of an established fermionic Hamiltonian. Developing the SU(6)-B-ERPA, we have utilized as reference the Quasiparticle-Phonon Model Hamiltonian for spherical nuclei. Detailed presentation of QPM and its applications can be found in Ref. 17. (The QPM has been successfully used for description of the fragmentation of quasiparticle and collective (phonon) states in wide excitation energy interval). Within the QPM Bogolubov's quasiparticles and phonons are being used as simple modes of excitations, instead of the nucleon degrees of freedom (hence the name QPM has come into being). More specifically, we employ a particular QPM Hamiltonian including an average nuclear field as the Saxon-Woods potential, superconducting pairing interactions and isoscalar quadrupole-quadrupole forces (Cf. eq. (1) of Ref. 17):

$$H_{micr} = \sum_{\tau} \left\{ \sum_{jm}^{\tau} (E_j - \lambda_\tau) a^+_{jm} a_{jm} - \frac{G_\tau}{4} (P^+_0 \cdot P_0)^\tau - \frac{\kappa}{2} : (M^+_2 \cdot M_2)^\tau : \right\} . \qquad (2.2)$$

The notation $\{\tau = (n,p)\}$ is used; the summation $\{\sum^\tau\}$ for $\{\tau = n\}$ is over the neutron and for $\{\tau = p\}$ over proton states. The single-particle states are specified (if there is not ambiguity) by the quantum numbers jm; E_j are the single-particle energies; λ is the chemical potential;G and κ are the respective strengths of the monopole pairing and quadrupole-quadrupole interactions. The pair creation and quadrupole operators entering in the scalar products in (2.2) are defined in a standard fashion:

$$P^+_0 = \sum_{jm} (-1)^{j-m} a^+_{jm} a^+_{j-m} \qquad (2.3)$$

$$M^+_{2\mu} = \frac{1}{\sqrt{5}} \sum_{jj'mm'} f_{jj'} (jmj'm' \mid 2\mu) a^+_{jm} a_{j'm'} . \qquad (2.4)$$

Where $f_{jj'}$ stand for the reduced single particle matrix elements of the operator $(ir)^2 Y_{2\mu}(\Omega)$[17].

In reality H_{micr} given by (2.2) is nothing else, but the schematic spherical single particle pairing-plus-quadrupole Hamiltonian, which constitutes the main part of the QPM Hamiltonian (Cf. eq. (1) of Ref. 17).

By performing the canonical Bogolubov transformation

$$a^+_{jm} = u_j \alpha^+_j + (-1)^{j-m} v_j \alpha_{j-m} \qquad (2.5)$$

and introducing subsequently multipole phonon operators[17]

$$Q^+_{\lambda\mu i} = \frac{1}{2}\sum_{jj'}[\psi^{\lambda i}_{jj'}(jmj'm' \mid \lambda\mu)\alpha^+_{jm}\alpha^+_{j'm'} - (-1)^{\lambda-\mu}\phi^{\lambda i}_{jj'}(jmj'm' \mid \lambda-\mu)\alpha_{j'm'}\alpha_{jm}]$$

$$Q_{\lambda\mu i} = \frac{1}{2}\sum_{jj'}[\psi^{\lambda i}_{jj'}(jmj'm' \mid \lambda\mu)\alpha_{j'm'}\alpha_{jm} - (-1)^{\lambda-\mu}\phi^{\lambda i}_{jj'}(jmj'm' \mid \lambda-\mu)\alpha^+_{jm}\alpha^+_{j'm'}] \qquad (2.6)$$

we cast H_{micr} into the usual quasiparticle-phonon representation:

$$H'_{micr} = \sum_j \varepsilon_j\sqrt{2j+1}B(jj;00) - \frac{\kappa}{20}\sum_{\mu=-2}^{2}\sum_{i,i'=1}^{i_{max}} Z_{1i}Z_{1i'}Q^+_{2\mu i}Q_{2\mu i'} - \frac{\kappa}{40}\sum_{\mu=-2}^{2}\sum_{i,i'=1}^{i_{max}} Z_{1i}Z_{1i'}(Q^+_{2\mu i}Q^+_{2-\mu i'}$$
$$+ \ h.c.) - \frac{\kappa}{20}\sum_{\mu=-2}^{2}(\sum_{i=1}^{i_{max}} Z_{1i}[(-1)^\mu Q^+_{2\mu i} + Q_{2-\mu i}]\sum_{j_1j_2} f_{j_1j_2}v^{(-)}_{j_1j_2}B(j_1j_2;2-\mu) + h.c.)$$
$$- \frac{\kappa}{10}\sum_{\mu=-2}^{2}(-1)^\mu \sum_{j_1j_2j_3j_4} f_{j_1j_2}v^{(-)}_{j_1j_2}f_{j_3j_4}v^{(-)}_{j_3j_4}B(j_1j_2;2\mu)B(j_3j_4;2-\mu)\ , \qquad (2.7)$$

where: in the definition of $Q^+_{\lambda\mu i}$ the index λ denotes multipolarity, μ denotes z-projection in the laboratory system, and i is the label of the solution of the RPA dynamical equation;

$$B(jj';\lambda\mu) \equiv \sum_{mm'}(-1)^{j'+m'}(jmj'm' \mid \lambda\mu)\alpha^+_{jm}\alpha_{j'-m'} \qquad (2.8)$$

$$Z_{1i} \equiv \sum_{jj'} f_{jj'}u^{(+)}_{jj'}(\psi^{2i}_{jj'} + \phi^{2i}_{jj'}) \qquad (2.9)$$

$$u^{(+)}_{jj'} = u_jv_{j'} + u_{j'}v_j,\ v^{(-)}_{jj'} = u_ju_{j'} - v_jv_{j'},\ \varepsilon_j = [(E_j-\lambda_\tau)^2 + \Delta^2_\tau]^{\frac{1}{2}},\ \Delta_\tau = G_\tau\sum_j u_jv_j\ . \qquad (2.10)$$

[6]The chemical potential λ_τ and correlation function Δ_τ are calculated according to the known equations[20]. We note that the fragment of the monopole pairing interaction that does not contribute to the formation of ε_j (Cf. eq. (2.10)), featuring in H_{micr}, has been cast aside. Short of the first term in eq. (2.6), the rest originates from the quadrupole-quadrupole force, involving the normal product of $:(M^+_2\cdot M_2):$. As to the quadrupole operator, its explicit form in the quasiparticle-phonon representation reads:

$$M^+_{2\mu} = \frac{(-1)^\mu}{\sqrt{5}}\sum_{i=1}^{i_{max}} Z_{1i}[Q^+_{2\mu i} + (-1)^\mu Q_{2-\mu i}] + \sum_{jj'} f_{jj'}v^{(-)}_{jj'}B(jj';2\mu)\ . \qquad (2.11)$$

Note that the first term includes summation over collective (i=1) and noncollective phonons ($i = 2,...,i_{max}$).

It is evident from eqs. (2.1) and (2.7) that phenomenological and reference Hamiltonian are in different representations, which makes it difficult to compare them. Since direct construction of the boson image of H'_{micr} (employing standard boson expansion techniques) does not automatically yield H_{IBM-1} one has to elaborate a special procedure which allows to single out from H'_{micr} the fragment with a boson structure, identical to that of the H_{IBM-1} defined by (2.1). The essence of this

procedure, which was formulated in principle and used by the creators of TQM[9-11], can be stated as follows. It has been assumed[9-11], that there exists a subspace of quadrupole collective states, which are weakly connected with the rest of states. Such being the case, the set of operators, which generate this class of states, are bound to constitute, at least approximately, a closed algebra (which has turned out to be isomorphic to SU(6)[9,10]). The possibility to use known boson realizations (Dyson, Holstein-Primakoff and Schwinger, see Ref. 12) of the latter greatly facilitates the bosonization of the reference Hamiltonian and produces a genuine SU(6) boson Hamiltonian if SR of QCA is used.

We now turn to the choice of the collective subspace in SU(6)-B-ERPA. From eqs. (2.7) and (2.11), it is apparent that the Hamiltonian H'_{micr} and the quadrupole operator $M^+_{2\mu}$ are built out of the set of operators $Q_{2\mu i}$, $Q^+_{2\mu i}$, $B(jj';2\mu)$, $\mu = 0, \pm 1, \pm 2$; $i = 1, 2, ..., i_{max}$. The latter set of operators constitutes the building blocks of the reference Hamiltonian. In addition, by acting with the $Q^+_{2\mu 1}$ operators on the phonon vacuum one generates quadrupole collective (i=1) and noncollective ($i = 2, ..., i_{max}$) phonon states. It is thus natural to choose as collective subspace the set of states, generated by the $Q^+_{2\mu 1}$-operators acting on the vacuum. Such a choice is further supported by observation (established in Ref. 13) that if we assume, according to Janssen, Jolos and Dönau[9-11], that this collective subspace is weakly coupled with the states of another nature, then the set of operators $Q_{2\mu 1}$, $Q^+_{2\mu 1}$, $[Q_{2\mu 1}, Q^+_{2\mu 1}]$ approximately closes the ensuing SU(6) algebra QCA. Indeed it has been shown[13] that:

$$[Q^+_{2\mu 1}, [Q_{2\nu 1}, Q^+_{2\sigma 1}]] = 2 \sum_{\rho=-2}^{2} (Q^+_{2\rho 1} C_{\mu\nu\sigma\rho} + Q_{2\rho 1} D_{\mu\nu\sigma\rho}) \tag{2.12}$$

plus sums involving $[(\lambda = 2,\ i \geq 2)]$ "scattering" terms,

$$[Q_{2\mu 1}, [Q_{2\nu 1}, Q^+_{2\sigma 1}]] = -2 \sum_{\rho=-2}^{2} (Q_{2\rho 1} C_{\mu\nu\sigma\rho} + Q^+_{2\rho 1} D_{\mu\nu\sigma\rho}) \tag{2.13}$$

plus sums involving $[(\lambda = 2,\ i \geq 2)]$ "scattering" terms.

The explicit form of $C_{\mu\nu\tau\rho}$ and $D_{\mu\nu\tau\rho}$ is given in Ref. 13 (Cf. eqs.(22) and (23)) and will be of no use further. We stress that, if the "scattering" terms in commutation relations (2.12) and (2.13) are cast aside, the set of operators

$$\{Q_{2\mu 1}, Q^+_{2\mu 1}, [Q_{2\mu 1}, Q^+_{2\nu 1}], [Q^+_{2\mu 1}, Q^+_{2\nu 1}], [Q_{2\mu 1}, Q_{2\nu 1}]\} \tag{2.14}$$

will compose a closed algebra, but not necessarily the Lie algebra. It has been proved[13], that the necessary and sufficient conditions that the above set of operators form a Lie algebra, are given by:

$$W^{(k)}_{j_1 j_2} \equiv \sum_{j_3} (-1)^{j_1 + j_3} \begin{Bmatrix} 2 & 2 & k \\ j_1 & j_2 & j_3 \end{Bmatrix} \phi^{21}_{j_1 j_3} \psi^{21}_{j_2 j_3} = 0 \tag{2.15}$$

for k=0,1,2,3,4, and any $j_1 j_2$,

$$D_k \equiv \frac{25}{2} \sum_{j_3 j_4 j_5 j_6} (-1)^{j_5 - j_6} \begin{Bmatrix} j_4 & j_3 & 2 \\ j_2 & j_1 & 2 \\ 2 & 2 & k \end{Bmatrix} (\psi^{21}_{j_1 j_3} \psi^{21}_{j_3 j_5} \psi^{21}_{j_5 j_4} \phi^{21}_{j_3 j_6} - \phi^{21}_{j_1 j_3} \phi^{21}_{j_3 j_5} \phi^{21}_{j_5 j_4} \psi^{21}_{j_3 j_6}) = 0 \qquad (2.16)$$

for k=0,1,2,3,4,

and

$$C_1 = C_3 = 0 \qquad (2.17)$$

$$C_0 = C_2 = C_4 = C \qquad (2.18)$$

$$C_k \equiv \frac{25}{2} \sum_{j_3 j_4 j_5 j_6} (-1)^{j_5 - j_6} \begin{Bmatrix} j_4 & j_3 & 2 \\ j_2 & j_1 & 2 \\ 2 & 2 & k \end{Bmatrix} (\psi^{21}_{j_1 j_3} \psi^{21}_{j_3 j_5} \psi^{21}_{j_5 j_4} \psi^{21}_{j_3 j_6} - \phi^{21}_{j_1 j_3} \phi^{21}_{j_3 j_5} \phi^{21}_{j_5 j_4} \phi^{21}_{j_3 j_6}) = 0 \,. \qquad (2.19)$$

Constraints (2.15)-(2.19) constitute the so called SU(6)-EC.

In virtue of eq. (2.15), the commutators $[Q_{2\mu 1}, Q_{2\nu 1}]$ and $[Q^+_{2\mu 1}, Q^+_{2\nu 1}]$ vanish identically (Cf. eq. (34) in Ref. 13), thus ensuring the elimination of redundant operators in the set (2.14). While it is by no means a trivial matter to infer constraints (2.15)-(2.19) from the condition that the operators set (2.14) forms a Lie algebra (sufficiency), it is easy to show that, if eqs. (2.15)-(2.19) are satisfied, then the set of operators $\left\{Q_{2\mu 1}, Q^+_{2\nu 1}, [Q_{2\mu 1}, Q^+_{2\nu 1}]\right\}$ composes a Lie algebra (necessity). The exploit form of the Lie algebra under consideration, the so called QCA reads (Cf. eqs. (36)-(38) in Ref.13):

$$[Q^+_{2\mu 1}, [Q_{2\nu 1}, Q^+_{2\sigma 1}]] = C\delta_{\mu\nu} Q^+_{2\sigma 1} + C\delta_{\nu\sigma} Q^+_{2\mu 1} \qquad (2.20)$$

$$[Q_{2\mu 1}, [Q_{2\nu 1}, Q^+_{2\sigma 1}]] = -C\delta_{\mu\sigma} Q_{2\nu 1} - C\delta_{\nu\sigma} Q_{2\mu 1} \qquad (2.21)$$

$$[[Q_{2\mu 1}, Q^+_{2\nu 1}], [Q_{2\sigma 1}, Q^+_{2\rho 1}]] = C\delta_{\sigma\nu} [Q_{2\mu 1}, Q^+_{2\rho 1}] - C\delta_{\mu\rho} [Q_{2\sigma 1}, Q^+_{2\nu 1}] \,. \qquad (2.22)$$

QCA is isomorphic to the Cartan-Weyl SU(6) algebra (Cf. Sec. VII of Ref. 13). The explicit isomorphism QCA$\Leftrightarrow$SU(6) in conjunction with the SU(6)-EC have permitted to construct microscopic Schwinger boson realization of QCA, which is directly associated[12] with the IBM-1. The SR under consideration can be written as (Cf. eqs. (51)-(53) in Ref. 13):

$$Q^{+SR}_{\mu} = N^{-1/2} d^+_{2\mu} s \qquad (2.23)$$

$$Q^{SR}_{\mu} = N^{-1/2} s^+ d_{2\mu} \qquad (2.24)$$

$$[Q_\mu, Q^+_\nu]^{SR} = N^{-1} (\delta_{\mu\nu} s^+ s - d^+_{2\nu} d_{2\mu}) \qquad (2.25)$$

$$N \equiv Int\left[\frac{1}{C}\right] \,, \qquad (2.26)$$

where the quantity C is defined by eqs. (2.18) and (2.19).

This quantity has been shown[12] to measure the deviation of the two-phonon norm from unity. It reflects the fact that the constraint operators $\{Q_\mu^{+SR}, Q_\mu^{SR}\}$, which are an SU(6)-approximation image of the two-quasiparticle RPA phonon operators (2.6), account for Pauli principle in average, since in virtue of eqs. (2.18) the quantities C_k should not depend on the angular momentum of the phonon state. We intend to undertake in the future in-deep investigation of the nagging question of spurious states associated with violation of antisymmetry[21-25] as it stands in the SU(6)-B-ERPA.

We see from eq. (2.26) within the SU(6)-B-ERPA the total number of bosons can be associated with the integer number, nearest to C^{-1}.

To emphasize the fact that eqs. (2.23)-(2.25) represent the SR of the enforced QCA, the notation Q_μ^{SR}, Q_μ^{+SR} has been used for the constraint RPA phonon operators. Exact boson representations for the operators $B(jj';LM)$, needed to bosonize the reference Hamiltonian H'_{micr}, have been also constructed in Ref. 13 (Cf. eqs. (67) and (69)):

$$(2j+1)^{1/2}B(jj';00) = \sum_{j'}[(\psi_{jj'}^{21})^2 + (\phi_{jj'}^{21})^2] \sum_{\mu=-2}^{2} d_{2\mu}^{+} d_{2\mu} \tag{2.27}$$

$$B(j_1 j_2;LM) = 5\sum_{j_3}(-1)^{j_1+j_3} \left\{ \begin{array}{ccc} 2 & 2 & L \\ j_1 & j_2 & j_3 \end{array} \right\} (\psi_{j_1 j_3}^{21}\psi_{j_2 j_3}^{21} + \phi_{j_1 j_3}^{21}\phi_{j_2 j_3}^{21})[d_2^{+} \otimes \tilde{d}_2]_{(LM)}, \; L = 2,4\,. \tag{2.28}$$

We are ready now to deduce from H'_{micr} the fragment with the IBM-1 boson structure. To this end we first separate the collective part of H'_{micr}, i.e. the part including the collective operators $Q_{2\mu 1}, Q_{2\mu 1}^{+}$. This in fact amounts to restricting the summations in rhs of eq. (2.7) to $i_{max} = 1$. Upon replacement of the operators $\{B(jj;00), B(jj';2\mu), Q_{2\mu 1}, Q_{2\mu 1}^{+}\}$, featuring in the collective part of H'_{micr}, by their boson equivalents (given by (2.27),(2.23),(2.24) and (2.28), respectively), the collective part of H'_{micr} acquires precisely the form of the IBM-1 Hamiltonian (2.1).

The term by term comparison of microscopically derived and the phenomenological IBM-1 Hamiltonian (2.1) leads to following microscopic expressions for the IBM-1 Hamiltonian parameters:

$$\bar{h} = \frac{1}{2}Z_{41} - \frac{\kappa}{20}Z_{11}^2 - \frac{5}{2}\kappa Z_{21}^2 \tag{2.29}$$

$$C_h = C_{h_1} = C_{h_2} = -\frac{\kappa}{10}Z_{11}^2/N \tag{2.30}$$

$$\bar{C}_L = -25\kappa Z_{21}^2 \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ 2 & 2 & L \end{array} \right\} \quad (L = 0,2,4) \tag{2.31}$$

$$F = -\frac{\kappa}{2}(5/N)^{1/2}Z_{11}Z_{21} \tag{2.32}$$

$$G = -\frac{\kappa}{8\sqrt{5}}Z_{11}^2/N \quad , \tag{2.33}$$

where:

$$Z_{21} \equiv \sum_{j_1 j_2 j_3} (-1)^{j_1+j_2} f_{j_1 j_2} v^{(-)}_{j_1 j_2} \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ j_1 & j_2 & j_3 \end{array} \right\} (\psi^{21}_{j_1 j_3} \psi^{21}_{j_3 j_2} + \phi^{21}_{j_1 j_3} \phi^{21}_{j_3 j_2}) \tag{2.34}$$

$$Z_{41} \equiv \sum_{j_1 j_2} (\epsilon_{j_1} + \epsilon_{j_2}) [(\psi^{21}_{j_1 j_2})^2 + (\phi^{21}_{j_1 j_2})^2] \tag{2.35}$$

the quantity Z_{11} has been defined before (Cf. eq. (2.9). With the aid of transformation $\bar{h}' = \bar{h} + (N-1)(C_{h_1} - C_{h_2})$, $\bar{C}'_L = \bar{C}_L + (C_{h_1} - 2C_{h_2})$, the most general IBM-1 Hamiltonian (2.1) can be transcribed to a six-parameter form. In the sequel we shall deal with the set of six parameters $\{\bar{h}', F, G, \bar{C}'_L\}$.

From eqs. (2.29)-(2.33) it is evident that all the parameters except $\bar{C}_2$ have correct signs ($Z_{11}, Z_{41} > 0; Z_{21} < 0$). However, we are not able to obtain a negative-valued $\bar{C}'_2$ in the present approach. The inclusion of the isovector part of the quadrupole-quadrupole force could hopefully resolve this "sign" problem[14].

We have seen that the physical assumption of the collective quadrupole degree of freedom being weakly connected to the other degrees of freedom amounts to a truncation of the shell-model space to the collective subspace generated by the constraint quadrupole phonon operators $\{Q^{+SR}_\mu\}$, given by eqs. (2.23) in conjunction with the SU(6)-EC. Decoupled collective subspace under consideration is, in fact, the totally symmetric IR $[N, O^4]$ of the SU(6) group. Acting repeatedly with the operator Q^{+SR}_μ on the highest weight state $\mid hws > \equiv \frac{(s^+)^N}{\sqrt{N!}} \mid 0)$ of $[N, O^4]$, one constructs the entire (N+5)!/(N!5!)-dimensional subspace, spanned by the monomials

$$\left\{ \frac{(s^+)^{n_s}}{(n_s!)^{1/2}} \prod_{\mu=-2}^{2} (d^+_\mu)^{n_\mu} \mid 0) \right\},$$

where $n_s + \sum_{\mu=-2}^{2} n_\mu = N$ (Cf. Ref. 12).

It is this decoupled subspace $[N, O^4]$ which has engendered H_{B-ERPA}, the IBM-1 Hamiltonian with microscopic expressions for the parameters given by eqs. (2.29)-(2.33). Once the closure of QCA has been enforced, the problem of the fermions to bosons mapping has a well defined solution, since a full scope exact boson realizations of QCA=SU(6) are known and can be directly used[12].

We emphasize that since the SU(6) based H_{B-ERPA} is an approximation to the QPM Hamiltonian, we do not impose the requirement on the H_{B-ERPA} spectrum to coincide exactly with the spectrum of the QPM Hamiltonian. This procedure differs from the ones in Refs. 26,27.

We have succeeded to derive microscopically a Hamiltonian which possesses the ensuing SU(6) sd-boson form (2.1). This is a crucial step, but as seen from expressions (2.29)-(2.35), the coefficients of our microscopic IBM-1 Hamiltonian depend on (ψ, ϕ)-amplitudes, which are not defined as yet. In order to determine the coefficients of the derived Hamiltonian (so that it can be used in microscopic calculations), we need a procedure to determine the unknown phonon amplitudes.

However, no consensus seems to exist as to how to proceed in general case. Klein and Vallieres have proposed[28] that the collective pairs be determined by a variational condition on the trace of the Hamiltonian. On one hand, in the case under consideration it is natural to determine (ψ, ϕ) from variational principle which ensures that the collective isoscalar quadrupole phonon states lie lowest in the energy spectrum, and thus are maximally separated from the rest of the states (Cf. Ref. 29). On the other hand the SR of QCA and hence the resulting microscopic IBM-1 Hamiltonian are to be considered in interconnection with the SU(6)-EC, since $\{Q_{2\mu 1}, Q^{+}_{2\mu 1}, [Q_{2\mu 1}, Q^{+}_{2\mu 1}]\}$ close the QCA if and only if the constraints (2.15)-(2.18) are fulfilled.

Therefore we should formulate the variational principle in question in such a way that it ensures simultaneously: a minimum of the obtained microscopic Hamiltonian H_{B-ERPA} in the collective one -phonon states space and fulfillment of the SU(6)-EC.

Translating this condition in mathematical terms we can write[15]:

$$\delta\{(hws \mid Q^{SR}_{\mu} H_{B-ERPA} Q^{+SR}_{\mu} \mid hws) - \frac{1}{2} w Z_{31} - \sum_{k=0,2,4} \lambda_k D_k$$

$$- \sum_{k=0,2} \lambda_{4k}(C_4 - C_k) - \lambda_{2N}(C_2 - 1/N_{ph})\} = 0 \tag{2.36}$$

$$Z_{31} \equiv \sum_{jj'} [(\psi^{21}_{jj'})^2 - (\phi^{21}_{jj'})^2] = r \tag{2.37}$$

$$D_k = 0 \quad k = 0, 2, 4 \tag{2.38}$$

$$C_4 - C_k = 0 \quad k = 0, 2 \tag{2.39}$$

$$C_2 - 1/N_{ph} = 0 \ . \tag{2.40}$$

In eq. (2.36) symbol $\delta\{...\}$ implies differentiation upon the independent variables ψ and ϕ. In the variational problem (2.36)-(2.40) the phonon amplitudes ψ and ϕ are normalized to an arbitrary constant r (r = 2 in the case of RPA). The necessity of a generalized normalization and its effect on the B-ERPA solutions will be discussed in more detail in Sect. IV.

We note that SU(6)-boson image of the third term in H'_{micr} gives no contribution to the expectation value $(hws \mid Q^{SR}_{\mu} H_{B-ERPA} Q^{SR+}_{\mu} \mid hws)$, because it changes phonon number (see eqs. (2.7), (2.23) and (2.28)).

As already stated in Refs.15,16, a part of the SU(6)-EC: $D_1 = D_3 = C_1 = C_3 = 0$ are trivially satisfied and for this reason they do not appear in the variational problem with constraints expressed by eqs. (2.36)-(2.40).

If SU(6)-symmetry governed dynamical problem (2.36)-(2.40) is solved, the quantity C (and hence $N = Int[C^{-1}]$) defined by eqs. (2.18) and (2.19), is determined. However, it might be useful to introduce an additional requirement $C = N^{-1}_{ph}$, where, in particular, N_{ph} can be the total number of bosons prescribed by the "IBM counting rule". The constraint (2.40) reflects just this additional requirement.

The unknown amplitudes $\{\psi, \phi\}$ needed to specify completely the microscopic SU(6)-sd boson Hamiltonian H_{B-ERPA} can be determined by solving numerically the above mentioned problem.

Carrying out the requisite differentiations upon $\psi_{jj'}$ and $\phi_{jj'}$ we cast eq. (2.36) into a more explicit form:

$$(\varepsilon_{j_1 j_2} \mp \omega) \begin{pmatrix} \psi^{21}_{j_1 j_2} \\ \phi^{21}_{j_1 j_2} \end{pmatrix} - \frac{\kappa}{10} Z_{11} f_{j_1 j_2} u^{(+)}_{j_1 j_2} - \frac{10}{7} \kappa Z_{21} \frac{\partial Z_{21}}{\partial \begin{pmatrix} \psi \\ \phi \end{pmatrix}_{j_1 j_2}} + \frac{40}{7} \kappa Z_{51} \frac{\partial Z_{51}}{\partial \begin{pmatrix} \psi \\ \phi \end{pmatrix}_{j_1 j_2}}$$

$$- \sum_{k=0,2,4} \lambda_k \frac{\partial D_k}{\partial \begin{pmatrix} \psi \\ \phi \end{pmatrix}_{j_1 j_2}} - \sum_{k=0,2} \lambda_{4k} \frac{\partial (C_4 - C_k)}{\partial \begin{pmatrix} \psi \\ \phi \end{pmatrix}_{j_1 j_2}} - \lambda_{2N} \frac{\partial C_2}{\partial \begin{pmatrix} \psi \\ \phi \end{pmatrix}_{j_1 j_2}} = 0 \quad , \qquad (2.41)$$

where $\varepsilon_{j_1 j_2} = \varepsilon_{j_1} + \varepsilon_{j_2}$,

$$Z_{51} \equiv \sum_{j_1 j_2} f_{j_1 j_2} v^{(-)}_{j_1 j_2} W^{(2)}_{j_1 j_2}$$

Omitting all the terms which are nonlinear in ψ or ϕ, we obtain:

$$\begin{cases} (\varepsilon_{j_1 j_2} - \omega)\psi^{21}_{j_1 j_2} = \frac{\kappa}{10} Z_{11} f_{j_1 j_2} u^{(+)}_{j_1 j_2} \\ (\varepsilon_{j_1 j_2} + \omega)\phi^{21}_{j_1 j_2} = \frac{\kappa}{10} Z_{11} f_{j_1 j_2} u^{(+)}_{j_1 j_2} \end{cases} .$$

This system can easily be solved analytically:

$$\begin{pmatrix} \psi^{21}_{j_1 j_2} \\ \phi^{21}_{j_1 j_2} \end{pmatrix} = \frac{\kappa}{10} Z_{11} f_{j_1 j_2} u^{(+)}_{j_1 j_2} \begin{pmatrix} (\varepsilon_{j_1 j_2} - \omega)^{-1} \\ (\varepsilon_{j_1 j_2} + \omega)^{-1} \end{pmatrix} . \qquad (2.42)$$

Substituting these expressions into the definition Z_{11}, given by eq. (2.9) we get:

$$\frac{\kappa}{5} \sum_{j_1 j_2} (f_{j_1 j_2} u^{(+)}_{j_1 j_2})^2 (\varepsilon^2_{j_1 j_2} - \omega^2)^{-1} = 1 \ . \qquad (2.43)$$

Equation (2.43) is nothing else but the RPA secular equation (Cf., e.g. Ref. 17), while eqs. (2.42) give the standard RPA solutions for (ψ, ϕ) amplitudes for a separable force.

The full problem (2.36)-(2.40) is an extension of RPA (ERPA) in boson representation with SU(6)-constraints. (That is why the abbreviation SU(6)-B-ERPA has been introduced.). An inherent feature of the SU(6)-B-ERPA is the consideration of the SU(6) symmetry governed dynamics in interconnection with the constraints dictated by the enforcement of SU(6) symmetry. As a matter of fact this pattern is not unfamiliar in other selfconsistent schemes. As pointed out in Ref. 30, in the framework of SU(6)-B-ERPA the SU(6)-EC play a role similar to that of the optimized RPA boundary condition, introduced in Ref. 31; the purpose was to extend the Selfconsistent Collective Coordinate Method[32] in such a way that it becomes applicable in the vicinity of RPA critical point too.

3. COMPUTATIONAL ASPECTS OF THE PROBLEM

The symmetry governed dynamical problem, formulated in the previous section, is essentially a non-linear problem with respect to the unknown amplitudes ψ and ϕ and can in principle be stated in different forms: as an overdetermined system of equations; as a Lagrange problem with constraints and so on. In Ref. 30 a formally equivalent mathematical problem has been treated approximately by simple scaling of phonon amplitudes, but with no guarantee that the SU(6)-EC are fulfilled.

Proceeding as in Ref. 15 we choose the way of direct generalization of the RPA problem regarding it as a minimization problem with constraints in form of equalities in the sense of classical non-linear programming (see e.g. Ref. 33, ch. 1). Thus the dynamical problem results explicitly in a system of non-linear equations which expresses the necessary condition for optimization of the Lagrange function (2.41), formed by the energy expectation value in one-phonon states, the normalization condition (2.37) and the SU(6)-EC (2.38)-(2.40):

$$\begin{aligned}
&(\varepsilon_{j_1 j_2} \mp \omega) \begin{pmatrix} \psi^{21}_{j_1 j_2} \\ \phi^{21}_{j_1 j_2} \end{pmatrix} - \frac{\kappa}{10} Z_{11} f_{j_1 j_2} u^{(+)}_{j_1 j_2} - \frac{10}{r} \kappa (Z_{21} - 2Z_{61}) P_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} \\
&- 4 \sum_{k=0,2,4} \lambda_{4k} \left[S^{(4)}_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} - S^{(k)}_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} \right] \\
&- \sum_{k=0,2,4} \lambda_k \tilde{G}^{(k)}_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} - \lambda_{2N} S^{(2)}_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = 0
\end{aligned} \tag{3.1}$$

$$Z_{31} - r \;=\; 0 \tag{3.2}$$

$$C_4 - C_k \;=\; 0\,; \quad k = 0, 2 \tag{3.3}$$

$$D_k \;=\; 0\,; \quad k = 0, 2, 4 \tag{3.4}$$

$$C_2 - N_{ph}^{-1} \;=\; 0 \tag{3.5}$$

The quantities P,S and $\tilde{G}$ featuring in eqs. (3.1) are defined as:

$$P_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} \equiv (-1)^{j_1 + j_2} \sum_{j_3} \begin{Bmatrix} 2 & 2 & 2 \\ j_1 & j_3 & j_2 \end{Bmatrix} \left[\begin{pmatrix} \psi^{21}_{j_1 j_3} \\ \phi^{21}_{j_1 j_3} \end{pmatrix} f_{j_3 j_2} v^{(-)}_{j_3 j_2} + f_{j_1 j_3} v^{(-)}_{j_1 j_3} \begin{pmatrix} \psi^{21}_{j_3 j_2} \\ \phi^{21}_{j_3 j_2} \end{pmatrix} \right]$$

$$S^{(k)}_{j_1 j_2} \begin{pmatrix} \psi \\ \phi \end{pmatrix} \equiv \frac{25}{2} \sum_{j_3 j_4} \begin{Bmatrix} j_4 & j_3 & 2 \\ j_2 & j_1 & 2 \\ 2 & 2 & k \end{Bmatrix} \begin{pmatrix} \psi^{21}_{j_1 j_3} \\ \phi^{21}_{j_1 j_3} \end{pmatrix} \begin{pmatrix} \psi^{21}_{j_3 j_4} \\ \phi^{21}_{j_3 j_4} \end{pmatrix} \begin{pmatrix} \psi^{21}_{j_2 j_4} \\ \phi^{21}_{j_2 j_4} \end{pmatrix} \quad .$$

$$\bar{G}^{(k)}_{j_1 j_2}\begin{pmatrix}\psi\\ \phi\end{pmatrix} \equiv G^{(k)}_{j_1 j_2}\begin{pmatrix}\psi\\ \phi\end{pmatrix} - S^{(k)}_{j_1 j_2}\begin{pmatrix}\phi\\ \psi\end{pmatrix} + \frac{25}{2}\sum_{j_3 j_4}\begin{Bmatrix} j_4 & j_3 & 2\\ j_2 & j_1 & 2\\ 2 & 2 & k\end{Bmatrix}\Bigg[\begin{pmatrix}\psi^{21}_{j_1 j_3}\\ \phi^{21}_{j_1 j_3}\end{pmatrix}\begin{pmatrix}\psi^{21}_{j_2 j_4}\\ \phi^{21}_{j_2 j_4}\end{pmatrix}\begin{pmatrix}\phi^{21}_{j_2 j_4}\\ \psi^{21}_{j_2 j_4}\end{pmatrix}$$

$$+ \begin{pmatrix}\phi^{21}_{j_1 j_2}\\ \psi^{21}_{j_1 j_3}\end{pmatrix}\begin{pmatrix}\psi^{21}_{j_2 j_4}\\ \phi^{21}_{j_2 j_4}\end{pmatrix}\begin{pmatrix}\psi^{21}_{j_2 j_4}\\ \phi^{21}_{j_2 j_4}\end{pmatrix}\Bigg]$$

$$G^{(k)}_{j_1 j_2}\begin{pmatrix}\psi\\ \phi\end{pmatrix} \equiv \frac{25}{2}\sum_{j_3 j_4}\begin{Bmatrix} j_4 & j_3 & 2\\ j_2 & j_1 & 2\\ 2 & 2 & k\end{Bmatrix}\begin{pmatrix}\psi^{21}_{j_1 j_3}\\ \phi^{21}_{j_1 j_3}\end{pmatrix}\begin{pmatrix}\phi^{21}_{j_2 j_4}\\ \psi^{21}_{j_2 j_4}\end{pmatrix}\begin{pmatrix}\psi^{21}_{j_2 j_4}\\ \phi^{21}_{j_2 j_4}\end{pmatrix} .$$

They stem from the derivatives of quantities Z_{21}, Z_{51}, C_k and D_k in $\begin{pmatrix}\psi^{21}_{j_1 j_3}\\ \phi^{21}_{j_1 j_3}\end{pmatrix}$, what can easily be checked with the aid of eqs. (2.16) and (2.19), written in a modified form:

$$C_k \equiv \sum_{j_1 j_2}\left[S^{(k)}_{j_1 j_2}(\psi)\,\psi_{j_1 j_2} - S^{(k)}_{j_1 j_2}(\phi)\,\phi_{j_1 j_2}\right]$$

$$D_k \equiv \sum_{j_1 j_2}\left[G^{(k)}_{j_1 j_2}(\psi)\,\psi_{j_1 j_2} - G^{(k)}_{j_1 j_2}(\phi)\,\phi_{j_1 j_2}\right] .$$

In the numerical method we employ the vector of unknowns contains on an equal footing the vector of Lagrange multipliers (ω, λ). We solve numerically the problem iterating simultaneously, all the components $(\psi, \phi, \omega, \lambda)$. In principle, the condition for local convexity of the Lagrange function in the optimization point should be checked, but this requirement can not be met directly in practice.

As we mentioned in Sect. 2 the first two terms in the l.h.s. of eqs. (3.1) together with eq. (3.2) form just the usual RPA problem. The inclusion of third term in eqs. (3.1) leads to a non-linear generalization of the RPA referred to as ERPA. The latter takes into account the BB-terms of the Hamiltonian H'_{mier} (2.7). In solving the general problem of SU(6)-B-ERPA we use two options: (i) the B-ERPA-option, where the total number of bosons is not fixed (it includes all the terms in eq. (3.1) but not the last one and all constraint conditions excluding eq. (3.5)), and (ii) the BN-ERPA-option in which the total system of equations (3.1)-(3.5) is treated.

The BN-ERPA non-linear system of equations is solved numerically by means of an auto-regularized Gauss-Newton iteration process[34,35], executed by the program-package REGN[36]. Because the gradients of the constraint conditions go to zero in the vicinity of the solution so that problems becomes strongly ill-conditioned, we have used a new (unpublished) version of the program REGN, which realizes an iteration process scaled according to Marquardt[37] and then auto-regularized (see Ref. 35, eq. (18)). We employ as initial approximations the RPA-values of (ψ, ϕ, ω) given by eqs. (2.42) and (2.43) and zero values for the Lagrange multipliers (λ).

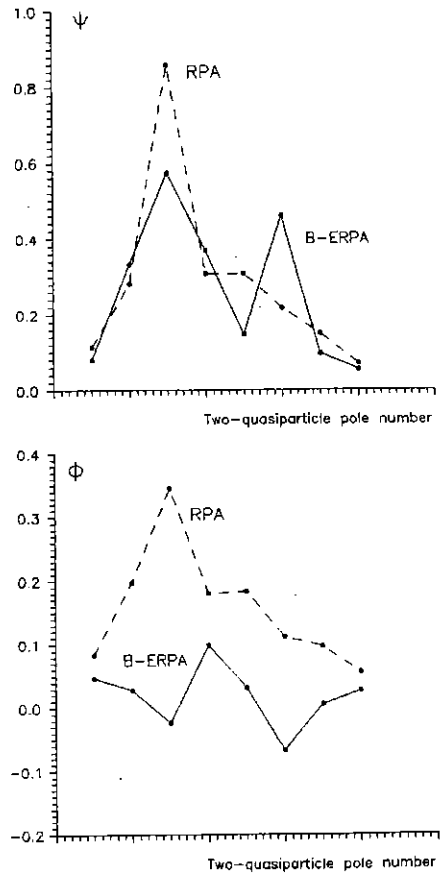

Figure 1: Comparision of the leading components of the phonon amplitudes (ψ, ϕ) calculated in RPA and B-ERPA.

The dimension of the system (3.1)-(3.5) is [2 × (the number of $f_{j_1 j_2}$ m.e.) + 7] in the general (BN-ERPA) case. Practically it includes 70-150 unknowns/equations when all the $f_{j_1 j_2}$ matrix elements in one sub-shell around the Fermi-surface are taken into account. Solutions are constructed with high accuracy: the maximal defect in satisfying every single equation is not greater than 10^{-10}.

Solutions of the system (3.1)-(3.5), which realizes the "bosonized collective phonons", keep generally some common features (the number and position of the leading components) with the usual RPA solutions, but at the same time some distinguishable differences can be observed (see fore more details Fig. 1). In particular, it is evident that the BN-ERPA solutions are not result of a simple operation (like scaling) on the RPA ones. The picture shown on Fig.1 changes from isotope to isotope. As to the question about the total number of BN-ERPA solutions in the collective sub-space (for RPA there is only one solution), we are unable to give a definite answer. From the general point of view the number of solutions of a non-linear problem (ERPA, B-ERPA, BN-ERPA) should be more than one what is demonstrated (for the case of ERPA) on Fig. 2. In this case we have found a second branch of solutions which approaches the first (RPA-like) branch in a point, where ERPA solution become complex. The same can be observed for the B-ERPA solutions (on Fig. 2): they also become complex for a definite value of the quadrupole strength κ. In the B-ERPA and BN-ERPA cases we have not found a second solution of the system (3.1)-(3.5), but the only one which originates from the usual RPA solution.

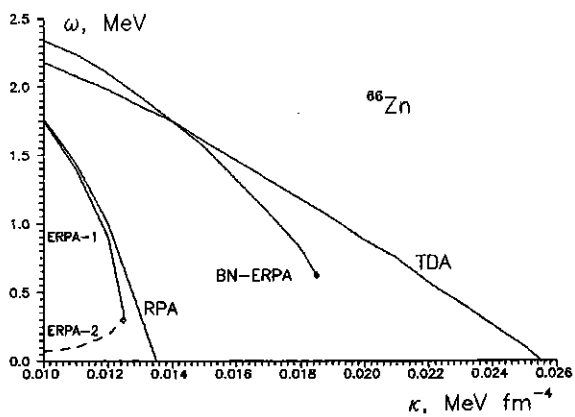

Figure 2: Dependence of the energy of 2_1^+ state on the strength of quadrupole-quadrupole interaction within TDA, RPA, ERPA and BN-ERPA.

4. DISCUSSION OF NUMERICAL RESULTS FOR Zn ISOTOPES

To carry out the microscopic calculations of the IBM-1 Hamiltonian parameters (Cf. eqs. (2.29-(2.33)) we have employed the values of Woods-Saxon potential parameters published in Ref. 38. These prameters have been chosen in such a way that the resulting level scheme and wave functions give reasonable description of the properties of low-lying states and mean square radii in the region of Zn isotopes. The values of monopole pairing interaction strengths $G_n = 0.260MeV$ and $G_p = 0.264MeV$ are fixed so as to reproduce the even-odd mass differences. In Table I we present the single particle levels, used in our calculations. The total number of quadrupole matrix elements $f_{j_1 j_2}$ (Cf. eq. (2.4)) between the s.p. states (Table I) amounts to 98. Among these 49 are neutron and 49 are proton matrix elements. Methodical calculations have indicated that in fact only 28 matrix elements (14 proton and 14 neutron m.e.) for s.p. levels around the Fermi surface play a significant role. Therefore only these have been used in our calculations.

Table I: Single particle energies for Zn isotopes

nlj	neutron energies, MeV	proton energies, MeV
$1s_{1/2}$	-37.39918	-38.12718
$1p_{3/2}$	-29.95807	-30.54278
$1p_{1/2}$	-28.67243	-28.79809
$1d_{5/2}$	-21.66252	-21.97828
$1d_{3/2}$	-18.79695	-18.12351
$2s_{1/2}$	-18.28062	-17.65574
$1f_{7/2}$	-12.76614	-12.70211
$2p_{3/2}$	-8.83229	-7.46996
$1f_{5/2}$	-7.96067	-6.20901
$2p_{1/2}$	-7.19289	-5.17669
$1g_{9/2}$	-3.50583	-2.91440
$2d_{5/2}$	-0.58232	1.91519
$3s_{1/2}$	-0.38138	3.13661
$2d_{3/2}$	1.09788	4.94147
$1g_{7/2}$	3.00672	6.25283
$1h_{11/2}$	5.66360	7.13096

The values of the constant of the isoscalar quadrupole-quadrupole interaction satisfying the condition $\omega_{RPA} = E^{expt}_{2^+_1}$, or $\omega_{TDA} = E^{expt}_{2^+_1}$ are denoted κ_R, or κ_T, respectively.

In the first place we have verified to what extend the SU(6)-EC given by eqs. (2.15)-(2.18) are satisfied within the conventional RPA and TDA. From the results presented in Table II, it can be seen, that strictly speaking, neither the "equality" part, (Cf. eqs. (2.18)) nor the "vanishing" part (Cf. eqs. (2.15) and (2.16) in the case of RPA) of SU(6)-EC are automatically fulfilled. It is also seen, that if we define $\bar{N} \equiv Int\{\bar{C}^{-1}\}$, where $\bar{C} = \frac{1}{3}(C_0 + C_2 + C_4)$, the values of $\bar{N}$ agree quite well with the "IBM-counting rule". In general outline it seems reasonable to utilize RPA as a starting approximation in solving the SU(6) symmetry governed dynamical problem defined by eqs. (3.1)-(3.5).

Table II: Degree of fulfilment of the "SU(6)-EC" within RPA and TDA

Nucleus	Approach	N_{IBM}	$\bar{N}$	C_0	C_2	C_4	D_0	D_2	D_4	$W^{(k)}_{max}$
^{64}Zn	RPA	4	3	0.43	0.19	0.40	0.19	0.08	0.16	0.08
	TDA		4	0.22	0.09	0.20	0.00	0.00	0.00	0.00
^{66}Zn	RPA	5	3	0.42	0.21	0.39	0.18	0.08	0.16	0.08
	TDA		4	0.22	0.11	0.20	0.00	0.00	0.00	0.00
^{68}Zn	RPA	6	3	0.27	0.25	0.41	0.13	0.10	0.16	0.098
	TDA		6	0.15	0.13	0.21	0.00	0.00	0.00	0.00
^{70}Zn	RPA	6	3	0.10	0.45	0.67	0.07	0.19	0.28	0.098
	TDA		7	0.07	0.18	0.27	0.00	0.00	0.00	0.00

In Table III we present the values of the IBM-1 Hamiltonian parameters evaluated microscopically by using expressions (2.29)-(2.33), alongside with the fitted[19] IBM-1 parameters in ^{68}Zn. The amplitudes (ψ, ϕ) featuring in these microscopic expressions have been computed without taking into account the SU(6)-EC (RPA and ERPA cases, Cf. Sec. 3), and with the SU(6)-EC "switched on" (B-ERPA and BN-ERPA cases, Cf. Sec. 3). In the latter case where these conditions are satisfied by construction, the maximal value of $W^{(k)}_{jj'}$ decreases considerably, as required by eqs. (2.15). From Table III it follows that the neglecting of the SU(6)-EC destroys the overall agreement between the calculated and fitted parameters: the values of $(F, G, \bar{C}'_L)$, calculated in B-ERPA, or BN-ERPA are closer to the phenomenological ones, than the values of $(F, G, \bar{C}'_L)$ computed in RPA or ERPA. As to the d-boson energy $\bar{h}'$, the bosonized theories B-ERPA, or BN-ERPA yield larger values than RPA, or ERPA (for the same values of the quadrupole-quadrupole strength $\kappa = \kappa_R$). The value of N, calculated according to eq. (2.26) in conjunction with SU(6)-EC, i.e. in B-ERPA, is quite close to the value, prescribed by the "IBM-1 counting rule".

Table III: Values of IBM-1 Hamiltonian parameters in different microscopical approaches in ^{68}Zn for $\kappa = \kappa_r$ and r = 2

	N	$\bar{h}'$	F	G	$\bar{C}'_0$	$\bar{C}'_2$	$\bar{C}'_4$	$W^{(k)}_{max}$
IBM-1	6	1.17±0.04	0.084	-0.085±0.038	-0.63±0.07	-0.40±0.06	0.11±0.04	
RPA	3	1.04	0.829	-1.85	3.20	3.30	3.30	0.098
ERPA	4	1.06	0.892	-1.65	2.94	2.94	2.94	0.088
B-ERPA	5	2.07	0.471	-0.472	0.70	0.80	0.80	0.011
BN-ERPA	6	2.13	0.350	-0.394	0.60	0.69	0.68	0.008

As we have already mentioned (Cf. Sec. 2, eqs. (2.29)-(2.35)) since we use only the isoscalar quadrupole-quadrupole force, we fail to reproduce the signs of $\bar{C}'_L$.

All conclusions, stemming from Table III, hold for the other isotopes as well. Using the calculated values of IBM-1 parameters as input in program PHINT[39] we have obtained spectra of low-lying states in $^{64-70}Zn$, which are too stretched compared to the experimental ones. This is not surprising at all, because, as stated in Sec. 2, in the course of derivation of the IBM-1 parameters we have related only the collective quadrupole phonon subspace ($\lambda = 2, i = 1$) (Cf. eqs. (2.12)-(2.13)). Clearly, whenever the space has been truncated, one naturally expects the occurrence of renormalization effects, which will affect the values of the computed parameters. We have found out (at first time heuristically) a mechanism that leads to compression of the theoretical spectra. This mechanism consists in reduction of the normalization constant r, featuring in eq. (2.37). A case in point is shown on Fig. 3. One sees that by renormalizing the value of r from r = 2 to r = 0.73, we achieve a reasonable agreement between theoretical and experimental spectrum.

A conceivable way to justify theoretically the ensuing reduction of r would be to account, in some effective way, for the role of the degrees of freedom, which have been ignored in the course of the enforcement of QCA (Cf. eqs. (2.12)-(2.13)). These were, at first place, the noncollective quadrupole degrees of freedom ("scattering terms" with $\lambda = 2, i \geq 2$) and the degrees of freedom other than the quadrupole one ("scattering terms" with $\lambda \geq 3$ and $i \geq 1$). To illustrate the procedure, it suffices to confine ourselves to the noncollective quadrupole degrees of freedom. To avoid needless complications we consider Tamm-Dankoff quadrupole phonon operators:

$$T^+_{2\mu i} \equiv \frac{1}{2} \sum_{jmj'm'} \psi^{2i}_{jj'}(jmj'm'|2\mu)\alpha^+_{jm}\alpha^+_{j'm'} \tag{4.1}$$

$$T_{2\mu i} \equiv \frac{1}{2} \sum_{jmj'm'} \psi^{2i}_{jj'}(jmj'm'|2\mu)\alpha_{j'm'}\alpha_{jm} \quad . \tag{4.2}$$

Utilizing for $\alpha^+\alpha^+$ and $\alpha\alpha$ exact bosons realizations in terms of antisymmetric ideal bosons $b_{jmj'm'}$

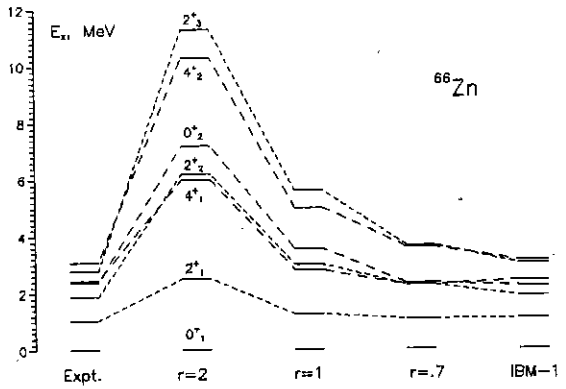

Figure 3. Dependence of the energies of the low-lying 0^+, 2^+, 4^+ states in ^{66}Zn on the one-phonon state normalization $Z_{31} = r$

and $b^+_{jmj'm'}$[40,41] we derive the following representation for $T^+_{2\mu i}$ and $T_{2\mu i}$ in terms of collective ($d^+_{2\mu 1}$) and noncollective ($d^+_{2\mu i}, i > 1$) quadrupole bosons:

$$T^+_{2\mu i} = \frac{1}{2}\left[\sum_{jj'}\psi^{2i}_{jj'}\right] d^+_{2\mu i} - \sum_{\mu_1\mu_2\mu_3}\sum_{i_1i_2i_3} C^T_{2\mu i 2\mu_1 i_1 2\mu_2 i_2 2\mu_3 i_3}\, d^+_{2\mu_1 i_1} d^+_{2\mu_2 i_2} d_{2\mu_3 i_3} \tag{4.3}$$

$$T_{2\mu i} = \frac{1}{2}\left[\sum_{jj'}\psi^{2i}_{jj'}\right] d_{2\mu i} \equiv \frac{r_T}{2} d_{2\mu i} \quad . \tag{4.4}$$

Here: $d^+_{2\mu i} \equiv \sum_{jmj'm'}\psi^{2i}_{jj'}\langle jmj'm' \mid 2\mu\rangle b^+_{jmj'm'}$ by definition and the quantity $C^T_{2\mu i 2\mu_1 i_1 2\mu_2 i_2 2\mu_3 i_3}$ has been computed to be given by:

$$C^T_{2\mu i 2\mu_1 i_1 2\mu_2 i_2 2\mu_3 i_3} = \sum_{k=0}^{4} C^T_{k i i_1 i_2 i_3} \sum_{K=-k}^{k} (2\mu 2\mu_2 \mid Kk)(2\mu_3 2\mu_1 \mid Kk) \tag{4.5}$$

with:

$$C^T_{k i i_1 i_2 i_3} = \frac{25}{2}\sum_{j_1 j_2 j_3 j_4}(-1)^{j_3 - j_1}\begin{Bmatrix} j_4 & j_3 & 2 \\ j_2 & j_1 & 2 \\ 2 & 2 & k \end{Bmatrix} \psi^{2i}_{j_1 j_2}\psi^{2i_3}_{j_3 j_1}\psi^{2i_2}_{j_2 j_4}\psi^{2i_3}_{j_3 j_4} \quad . \tag{4.6}$$

If we set $i = i_1 = i_2 = i_3 = 1$, from eq. (4.6) we go back to the familiar "collective" quantity C^T_k, defined by eq. (2.19) in which all $\phi_{jj'} = 0$.

Let us introduce now the following quantity:

$$Inv = \sum_{i=1}^{i_{max}} \sum_{\mu=-2}^{2} \langle 0 \mid \left[T_{2\mu i}, \left[T_{2\mu i}, T^{+}_{2\mu i}\right]\right] \left[T^{+}_{2\mu i}, \left[T_{2\mu i}, T^{+}_{2\mu i}\right]\right] \mid 0 \rangle \ . \tag{4.7}$$

With the aid of eqs. (4.3) and (4.4) we readily obtain:

$$\widetilde{Inv} = -4 \left(\frac{r_T}{2}\right)^4 \sum_{i=1}^{i_{max}} \sum_{\mu=-2}^{2} \left(C^T_{2\mu i 2\mu i 2\mu i 2\mu i}\right)^2 . \tag{4.8}$$

If we keep only the collective degree of freedom, we have to calculate the double commutators in eq. (4.7) according to the QCA commutation relations (2.20)-(2.22). Using them we get an approximate value for Inv:

$$\widetilde{Inv} = -20\, C^2 \ . \tag{4.9}$$

Comparing eqs. (4.8) and (4.9) we find that a possibility presents itself to effectively take into account the neglecting of the noncollective degrees of freedom. Indeed, we can preserve the approximately computed quantity Inv, requiring that $\widetilde{Inv} = Inv$. This conservation of $\widetilde{Inv}$ will be compensated by a replying renormalization of r_T which, in virtue of eqs. (4.8) and (4.9) is given by:

$$r_T = 2 \left[5\, C^2 / \left(5\, C^2 + \sum_{i=2}^{i_{max}} \sum_{\mu=-2}^{2} \left(C^T_{2\mu i 2\mu i 2\mu i 2\mu i} \right)^2 \right) \right]^{1/4} . \tag{4.10}$$

In the same fashion we can incorporate the other neglected degrees of freedom ($\lambda > 2$, $i \geq 1$). These results can be generalized to the case of RPA phonon operators. The generalization reduces merely to replacement of $C^T_{\lambda_1\mu_1 i_1 \lambda_2\mu_2 i_2 \lambda_3\mu_3 i_3}$ by their RPA-extensions (Cf. eq. (2.19)). We have thus illustrated that the reduction of r_T which we have used heuristically to obtain better agreement between the experimental and theoretical spectra, can be interpreted as an effective way to include within SU(6)-B-ERPA, in an algebraic manner again, the noncollective quadrupole degrees of freedom.

From eq. (4.10) it follows that taking into account the noncollective degrees of freedom, e.g. by including the quantities $C^T_{2\mu i 2\mu i 2\mu i 2\mu i}$ with $2 \leq i \leq i_{max}$ in the calculation, indeed amounts to reduction of r_T, as desired. As evident from Fig. 3, for all values of r we obtained a picture of a moderate anharmonic vibrator. The scale is determined by $\tilde{h}'$. The order of the levels in the split multiplets depends on the relationship between the rest of the microscopically calculated parameters of IBM-1. One sees that the order of the levels is maintained with the decrease of r.

We note that the compression of microscopically calculated spectra due to renormalization effects, is a general trend established previously by other authors employing different techniques[20,42-45].

In Table IV we present the parameters of the IBM-1 Hamiltonian for $^{64-70}Zn$, calculated within SU(6)-BN-ERPA, what is one of the goals of present article. The values of κ and r have been chosen empirically so as to reach most reasonable agreement between the theoretical and the phenomenological sets of parameters. It is seen that the optimal values of κ and r are quite stable along the chain

Table IV: Phenomenologically and microscopically calculated parameters of IBM-1 Hamiltonian for $^{64-70}Zn$

Nucl.	Approach	$\bar{h}'$	F	G	$\bar{C}'_0$	$\bar{C}'_2$	$\bar{C}'_4$
^{64}Zn	IBM-1 N=4	0.89±0.0	0.112±0.03	-0.185±0.02	0.10±0.40	-0.34±0.03	0.32±0.04
	BN-ERPA N=4 r=0.6	0.89	0.005	-0.059	0.10	0.10	0.10
^{66}Zn	IBM-1 N=5	1.04±0.0	0.061±0.057	-0.138±0.03	0.69±0.47	-0.36±0.03	0.23±0.05
	BN-ERPA N=5 r=0.73	1.04	0.022	-0.075	0.13	0.13	0.13
^{68}Zn	IBM-1 N=6	1.17±0.04	0.084±0.0	-0.085±0.38	-0.63±0.07	-0.40±0.06	0.11±0.04
	BN-ERPA N=6 r=0.71	1.10	0.030	-0.054	0.09	0.10	0.10
^{70}Zn	IBM-1 N=10	1.08±0.0	0.106±0.02	-0.047±0.02	-0.44±0.0	-0.35±0.05	0.17±0.06
	BN-ERPA N=10 r=0.7	1.08	0.049	-0.069	0.10	0.13	0.11

of isotopes (Cf. column II of Table IV). It is worth to mention that a relatively strong reduction of r (from r = 2 to r = 0.7) is required for the whole chain $^{64-70}Zn$, which implies a rather massive renormalization effects. Such a renormalization leads to fairly good theoretical values of $\bar{h}'$. The theory reproduces correctly the signs and the order of magnitude of F,G,$\bar{C}'_4$-parameters.

Summarizing the results given in Table IV, one is led to the conclusion that as a rule, the SU(6)-B-ERPA produces quite reasonable values of IBM-1 parameters. Of course, the comparison of phenomenological and microscopic parameters does not give complete idea about the goodness of the theoretically calculated parameters. Therefore, the latter have been used as input in program PHINT[39] to produce the corresponding energy spectra of $I^\pi = 0^+, 2^+, 4^+, 6^+$-states in $^{64-70}Zn$. The results are summarized in Table V together with the experimental and phenomenological IBM-1 spectra. Table V reveals the following tendencies:

(i) Ensuring excellent reproduction of the first $I^\pi = 2^+$ states energies (by a proper choice of r)

Table V: Experimental and calculated energies in Zn-isotopes

$I_i^\pi(band)$		Nucleus			
		^{64}Zn	^{66}Zn	^{68}Zn	^{70}Zn
$0_2^+(\beta_1)$	Exp.	1.9103	2.3726	1.6559	1.0507
	IBM-1	1.9241	2.2201	1.6124	1.0773
	BN-ERPA	1.9500	2.3363	2.3601	2.4081
$0_3^+(\beta_2)$	Exp.	2.6092	3.1055		2.1390
	IBM-1	2.5851	3.1413		1.9627
	BN-ERPA	3.0137	3.5952		3.7578
$2_1^+(g)$	Exp.	0.9915	1.0394	1.0774	0.8848
	IBM-1	0.9886	1.0909	1.1042	0.8669
	BN-ERPA	0.9059	1.0635	1.1086	1.0638
$2_2^+(\gamma)$	Exp.	1.7994	1.8730	1.8832	1.7539
	IBM-1	1.7482	1.8733	1.9294	1.6054
	BN-ERPA	1.9127	2.2657	2.3297	2.3268
$2_3^+(\beta_1)$	Exp.	2.7937	2.7804	2.3384	1.9574
	IBM-1	2.7263	3.0058	2.4868	1.9597
	BN-ERPA	3.0413	3.6543	3.6754	3.7774
$4_1^+(g)$	Exp.	2.3070	2.4490	2.4174	1.7865
	IBM-1	2.3172	2.4262	2.3297	1.8309
	BN-ERPA	1.9126	2.2636	2.3247	2.2696
$4_2^+(\gamma)$	Exp.	2.7367	3.0800	2.9594	
	IBM-1	3.0116	3.1106	3.0613	
	BN-ERPA	3.0137	3.5931	3.6492	
$6_1^+(g)$	Exp.	3.9937	4.1820	3.6876	
	IBM-1	3.9495	3.9864	3.7042	
	BN-ERPA	3.0136	3.5909	3.6432	

we attain satisfactory description of the behavior of the second $I^\pi = 2^+$ state energies. In ^{70}Zn, which exhibits the largest discrepancy, the calculated energies differ by 0.5 MeV. As to third $I^\pi = 2^+$ states, we see that the energies are poorly described. The same can be said about description of the second $I^\pi = 0^+$-state energies.

(ii) For the low-spin states $I^\pi = 0^+, 2^+$ the agreement between experimental and theoretical energies is better for the lighter isotopes $^{64,66}Zn$, while for the states with $I^\pi = 4^+, 6^+$ the agreement is better for the heavier isotopes $^{68-70}Zn$.

It should be kept in mind that the SU(6)-B-ERPA has a restricted range of validity. Strictly speaking, within this microscopic model one can treat only the quadrupole collective states. We emphasize, that while IBM-1 has 6 free parameters, we have at our disposal only 2 parameters, for the moment; one of them (r) will be calculated in future with the aid of eq. (4.10).

5. SUMMARY AND CONCLUSIONS

We have presented full account of an approach to the microscopic foundation of IBM-1, alternative to the traditionally employed approaches which are based on mapping procedures[2,4-6]. This approach is a further development of the approximate bifermion SU(6) algebra method[9-11] used in the derivation of the SU(6) boson Hamiltonian of TQM. The main novelty of our SU(6)-B-ERPA consists in the treatment, on equal footing, both the dynamics governed by the SU(6)-B-ERPA Hamiltonian (Cf. eqs. (2.36)-(2.37)) and the SU(6)-EC (Cf. eqs. (2.38)-(2.40)). Since the latter reflect the important fact that the QCA=SU(6) has been enforced, they have to be reckoned with in any kinds of approaches that claim to provide sound microscopic substantiation of IBM-1. Another merit of SU(6)-B-ERPA is that the total number of bosons is inferable from the basic framework of the approach (Cf. eqs. (2.26)). The computed values of N are, as a rule, close to the values given by the "IBM-counting rule".

We note that SU(6)-B-ERPA can be extended, so as to be adequate for providing microscopic foundation of the other versions of IBM, such as IBM-2, IBFM-1 and IBFM-2.

For the first time we have proved the existence of numerical solutions of the Lagrange minimization problem with constraints (Cf. eqs. (3.1)-(3.5)). This implies in particular that the SU(6)-EC are compatible with the SU(6)-B-ERPA dynamics.

The SU(6)-EC which are inalienable part of SU(6)-B-ERPA, have been totally neglected up to now. The illustrative numerical calculations carried out in Zn isotopes have confirmed the important role played by the SU(6)-EC: their neglecting deteriorates the overall agreement between the computed and fitted sets of IBM-1 parameters (Table III). The numerical calculations performed in Zn isotopes have indicated that in order to achieve reasonable values of the computed IBM-1 parameters, we have to reduce essentially the value of the normalization constant r, which indicates that the role of the neglected degrees of freedom is important. The renormalization of r enables quantitative description of the energies of the first and second $I^\pi = 2^+$ states in the entire chain of Zn isotopes. As to the rest of the states $I^\pi = 0^+, 2^+, 4^+, 6^+$, which are not legitimate object of study of the SU(6)-B-ERPA, their description could be classified for the most part as quantitative.

The SU(6) Boson Extended Random Phase Approximation approach contributes additionally to the repute of the "new SU(6) phenomenology" by providing microscopic foundation of IBM-1, which is mathematically rigorous, computationally sound and leads to reasonable values of the renormalized calculated parameters.

ACKNOWLEDGEMENTS

The authors express their gratitude for useful discussions to L. Aleksandrov, R. Bijker, J. Drayer, D. H. Feng, R. Gilmore, M. Guidry, F. J. W. Hahne, F. Iachello, P. V. Isaker, J. Jolie, V. M. Mikhailov, S. Pittel, V. Yu. Ponomarev, O. Scholten, F. J. Scholtz, R. D. Viollier.

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Received by Publishing Department
on February 12, 1990.

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E4-90-98

О новом подходе к микроскопическому обоснованию модели взаимодействующих бозонов. 1. Микроскопическое определение параметров МВБ и приложение к четно-четным изотопам цинка

Предложен алгебраический подход к микроскопическому обоснованию модели взаимодействующих бозонов (МВБ). При этом учтены условия, накладываемые SU(6)-динамикой. Введение коллективного пространства, как пространства, формируемого нижайшими квадрупольными фононами приближения случайных фаз, и требование выполнения SU(6)-симметрии позволяет: 1) идентифицировать коллективное подпространство как несущее пространство полностью симметричного неприводимого представления группы SU(6); 2) вывести из микроскопического гамильтониана квазичастично-фононной модели гамильтониан МВБ. Проведены расчеты параметров гамильтониана МВБ для изотопов $^{64-70}$Zn. Показано, что для описания экспериментальных спектров необходимо проводить перенормировку фононных амплитуд. Эта перенормировка связана с пренебрежением другими степенями свободы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1990

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E4-90-98

On a New Approach to the Microscopic Substantiation of the Interacting Boson Model-1. 1. Microscopic Determination of IBM-1 Hamiltonian Parameters and Application to Even-Even Zn Isotopes

An overtly Lie algebraic approach to the microscopic foundation of IBM-1 is itemized, treating on an equal footing the SU(6) governed dynamics and the accompanying SU(6) constraints. The introduction of the collective random phase apporoximation phonon operators as "preferred pairs" with subsequent enforcement of the relevant SU(6) algebra has enabled: (i) to identify the "decoupled" phonon subspace as carrier space of the totally symmetric irreducible representation of SU(6); (ii) to single out from a microscopic reference Hamiltonian the fragment with the ensuing IBM-1 sd-boson form. Using this approach, the IBM-1 parameters have been calculated for the sequence of $^{64-70}$Zn isotopes, as an example and it was shown that the required renormalization of the phonon amplitudes can be interpreted as arising due to neglected degrees of freedom.

The investigation has been performed at the Laboratory of Theoretical Physics JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1990