Reconstituting rotational band structure from deformed boson expansions: Generic treatment

E. R. Marshalek*
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556;
Institut für Theoretische Physik, Johann-Wolfgang-Goethe Universität, 6000 Frankfurt am Main, Federal Republic of Germany;
Physik Department, Technische Universität München, Theoretische Physik, 8046 Garching, Federal Republic of Germany
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The usefulness of perturbative expansions in deformed bosons has been limited by difficulties associated with zero-frequency (Goldstone) modes. A method developed earlier by Marshalek and Weneser to overcome these difficulties was restricted to the case in which the broken-symmetry generators commute. The present paper shows how to extend the method to the non-Abelian case of three-dimensional rotation of axially symmetric deformed systems. Application is made to a generic anharmonic Hamiltonian constructed from random-phase-approximation modes.

I. INTRODUCTION

Mean-field approximations applied to atomic nuclei often produce solutions with broken symmetries, implying the existence of collective bands having a rotational character.[1] Attempts to generate the band structure by means of Taylor expansions about a broken-symmetry extremum encounter well-known problems with zero-frequency (Goldstone) modes. A method for overcoming these problems in the case of two-dimensional rotation was presented by Marshalek and Weneser (MW) some time ago.[2,3] In a more recent paper,[4] the author discussed the application of this method to an exactly soluble many-body model and compared it with a new method of Bes *et al.*[5–7] The reader is referred to these papers for background, and especially to Ref. 4 for recent citations to related work. As originally formulated, the MW method is restricted to the case in which the broken symmetries constitute an Abelian group, as, for example, in the superfluid (BCS) model, in which the generators are the neutron and proton number operators.[1] The extension of this method to non-Abelian cases, however, is nontrivial, although two closely related examples exist; namely, the treatment of isospin by Ginocchio and Weneser[8] and that of high-angular-momentum states by the author.[9] These are both examples of the self-consistent cranking plus random-phase approximation (SCC + RPA) method. Although the SCC + RPA technique can indeed be continued to the low-spin limit, it becomes somewhat cumbersome.[10] Moreover, it should be possible to describe low-spin states without taking a high-spin detour. That is exactly the purpose of this paper, which outlines a viable extension of the MW method, to directly treat the low-spin band structure of nuclei with axially symmetric equilibrium deformations. It will be seen that axial symmetry poses some special problems which are absent for nonaxial systems.[11]

The extended MW method is applicable to any rotationally invariant Hamiltonian system expressible in terms of boson operators, or, equivalently, canonically conjugate coordinates and momenta, and having a classical equilibrium configuration that violates angular-momentum conservation. Its applicability to a second-quantized many-nucleon shell-model Hamiltonian is based on the fact that such a Hamiltonian can be mapped into an equivalent many-boson operator by means of the boson expansion method.[12–14] In this method, it is usual to "bosonize" all degrees of freedom of an even-even nucleus while additional odd nucleons are treated essentially as fermions. This paper is limited to purely bosonic (even-even) systems, but no difficulties are anticipated in the extension to odd systems.[14]

The aim of the MW method is to transform a given Hamiltonian, expressed as a boson expansion about the deformed equilibrium configuration, into the form of the generalized Bohr-Mottelson (BM) model of strongly deformed nuclei.[15] In this model, the Hamiltonian is represented by a power series in the body-fixed components of the angular momentum, with coefficients that create or annihilate intrinsic excitation modes, which, in general, carry angular momentum along the symmetry axis. What the MW method can achieve is a microscopic theory of low-spin rotational band structure analogous to the BM model, but without the arbitrariness inherent in a purely phenomenological model. Since the boson expansion makes the perturbational parameters explicit, the limits of applicability of the BM model can be better defined.

In the present paper, the MW method is applied to what is dubbed the *generic model,* defined as a system described by the most general bosonic polynomial Hamiltonian of a given order that can be constructed from the deformed RPA (small-oscillation) normal modes, subject to given symmetry constraints. In practice, the Hamiltonian will be truncated at quartic terms, sufficient to provide the leading-order corrections to the RPA. Although the generic model may be interpreted as the boson image of a many-fermion shell model under a generalized Holstein-Primakoff (GHP) mapping,[12–14] the actual details of the mapping will be left to a later publication. The advantage of using the generic model is that the treatment applies equally well to collective models, such as the quadrupole collective model[16,17] and the various forms of the interacting boson model (IBM),[18] and also to the rota-

tion and vibrations of a molecule. Since there appears to be no known *analytically solvable* microscopic model exhibiting rotational band structure and having an axially symmetric mean-field solution,[19] the collective models may be used instead to test the validity of the MW method. In a companion paper,[20] the method is tested on a simple version of the quadrupole collective model, and in the future it will be applied to the IBM in the deformed regime. The method has already been successfully tested for the rotation-vibration modes of a diatomic molecule,[21] but that case does not exhibit the special problems with which this paper is concerned since the vibrational quanta carry zero angular momentum along the symmetry axis.

In Sec. II the generic model is described for axially symmetric systems. In Sec. III the obstacles to the extension of the MW method to such systems are discussed. The problems which arise in naively attempting to transform the generic model into the BM representation are then elucidated by an in-depth analysis of this representation. In particular, it is shown that the BM representation involves a redundant variable, and that it can be derived from what is called a Villars representation[22] by means of a unitary transformation. From this result, a general outline of an extended MW method for axially symmetric systems may be gleaned that involves transforming from the generic model directly to the Villars representation, and from there to the BM representation via the aforementioned unitary transformation. The details are provided in Sec. IV for the Hamiltonian and for the electric quadrupole tensor, taken as representative of how to treat transition operators. Conclusions are contained in Sec. V.

II. THE GENERIC MODEL

Given a Hamiltonian H constructed entirely from certain boson operators $b_i, b_i^\dagger$, one may define a mean-field (MF) approximation as the classical equilibrium configuration obtained by replacing each boson in H by a c number, $b_i \rightarrow c_i$ and $b_i^\dagger \rightarrow c_i^*$, and then minimizing the resulting energy functional with respect to the c numbers.[3] The Hamiltonian may then be expanded about the MF solution by using the boson translation $b_i = c_i + b_i'$, $b_i^\dagger = c_i^* + b_i'^\dagger$. The MF approximation depends, of course, on the ordering of the boson operators immediately preceding the c-number replacement. For example, if the Hamiltonian is normal ordered, then the MF approximation is equivalent to averaging with respect to an oscillator coherent state. In the case that H is the GHP boson image of a many-fermion Hamiltonian, it has been shown that there exists an ordering called "c ordering," distinct from normal ordering, such that the MF approximation is equivalent to the Hartree or Hartree-Bogoliubov approximation.[3,23,24] The advantage of expanding about this kind of MF solution is that commutation rules are preserved order by order, a property which will be assumed for the generic model.

The Taylor expansion of the Hamiltonian about the MF extremum may be written in the form

$$H = E^{(0)} + H^{(2)} + H^{(3)} + H^{(4)} + \cdots , \tag{2.1}$$

where $E^{(0)}$ is a constant, the MF energy; $H^{(2)}$, the small-oscillation or RPA Hamiltonian, is a quadratic boson form; $H^{(3)}$ is a cubic odd-order and $H^{(4)}$ a quartic even-order boson polynomial. The expansion is characterized by some perturbation parameter $\Omega^{-1/2}$, so that, for example, if $E^{(0)}$ is of order Ω^2, then $H^{(2)}$ is of order Ω, $H^{(3)}$ is of order $\Omega^{1/2}$ and $H^{(4)}$ is of order 1. The term $H^{(1)}$ of order $\Omega^{3/2}$ is absent because the expansion is about an extremum point. In the case that H represents a shell-model Hamiltonian, $\Omega \sim \langle 2j+1 \rangle$, the average shell size.[14]

Since the stability of the axially symmetric MF extremum is neutral, it is always possible by means of a rotation to choose the z axis as the symmetry axis. The broken-symmetry generators are then the total-angular-momentum operators J_x and J_y, or, equivalently, $J_\pm = J_x \pm i J_y$, which then have the Taylor expansions commencing with linear boson terms:

$$J_\pm = J_\pm^{(1)} + J_\pm^{(2)} + J_\pm^{(3)} + \cdots . \tag{2.2}$$

The unbroken symmetry generator J_z in the GHP and most other boson expansions is a finite quadratic form $J_z = J_z^{(2)}$, as will be assumed in the generic model. The angular-momentum components must obey, of course, the usual SU(2) commutation rules $[J_+, J_-] = 2J_z$ and $[J_z, J_\pm] = \pm J_\pm$. Since the commutators are preserved order by order, one obtains, for example, in the first two orders,

$$[J_+^{(1)}, J_-^{(1)}] = 2J_z^{(0)} = 0 , \tag{2.3a}$$

$$[J_+^{(1)}, J_-^{(2)}] + [J_+^{(2)}, J_-^{(1)}] = 2J_z^{(1)} = 0 . \tag{2.3b}$$

In Eq. (2.3a), $J_z^{(0)}$ is the MF value, which vanishes for all components of the angular momentum for an even-even nucleus. In addition, since $J_z = J_z^{(2)}$, to any order n,

$$[J_z, J_\pm^{(n)}] = \pm J_\pm^{(n)} . \tag{2.3c}$$

Since H is rotationally invariant, for any component of angular momentum J_M one has $[H, J_M] = 0$, which must also be fulfilled order by order. In the RPA order, this becomes

$$[H^{(2)}, J_\pm^{(1)}] = 0 , \tag{2.4}$$

and in higher orders

$$\sum_{k=2}^{n} [H^{(k)}, J_\pm^{(n-k+1)}] = 0 , \tag{2.5}$$

while for any order n,

$$[H^{(n)}, J_z] = 0 . \tag{2.6}$$

The Hamiltonian of the generic model, Eq. (2.1), is constructed with the aid of the following assumptions: (i) the MF is axially symmetric; (ii) H is Hermitian; (iii) H is even under time reversal; (iv) H is rotationally invariant, i.e., Eqs. (2.4)–(2.6) apply. It is also implicitly assumed that the MF has reflection symmetry, to preclude tunneling modes that would be inconsistent with a small-oscillation ansatz. For simplicity, Goldstone modes other than the rotational ones are omitted.

A. The RPA as starting point

The diagonalized form of the RPA Hamiltonian $H^{(2)}$ is given by[25,26]

$$H^{(2)}=E^{(2)}+\sum_{\mu}\hbar\omega_{\mu}B_{\mu}^{(1)\dagger}B_{\mu}^{(1)}+\hbar^2J_{+}^{(1)}J_{-}^{(1)}/(2\mathscr{I}_0)\ , \tag{2.7}$$

where $E^{(2)}$ is a constant including the RPA correlation energy, and $B_{\mu}^{(1)},B_{\mu}^{(1)\dagger}$ are the annihilation and creation operators for the true vibrational normal modes (phonons) with nonzero frequencies ω_{μ}, which obey the boson commutation rules

$$\begin{aligned}&[B_{\mu}^{(1)},B_{\nu}^{(1)\dagger}]=\delta_{\mu,\nu}\ ,\\ &[B_{\mu}^{(1)},B_{\nu}^{(1)}]=0,\ \ [B_{\mu}^{(1)\dagger},B_{\nu}^{(1)\dagger}]=0\ .\end{aligned} \tag{2.8}$$

The last term on the right-hand side (rhs) of Eq. (2.7), which can also be written as $\hbar^2(J_x^{(1)2}+J_y^{(1)2})/(2\mathscr{I}_0)$, corresponds to a pair of Goldstone modes, one for each broken symmetry. Physically, of course, this term represents the collective rotation about an axis perpendicular to the symmetry axis. The moment of inertia $\mathscr{I}_0$ exactly coincides with the self-consistent cranking model value.[2,25,26] The normal-mode variables $J_{+}^{(1)}$ and $J_{-}^{(1)}$ commute with each other according to Eq. (2.3a), and with the $B_{\mu}^{(1)},B_{\mu}^{(1)\dagger}$ from the definition of normal modes:

$$[J_{\pm}^{(1)},B_{\mu}^{(1)}]=0\ \text{(and H.c. eq.)}\ . \tag{2.9}$$

As is well known, these variables do not suffice to form a complete set.[27] The set may be completed by adding a pair of mutually commuting angle variables $\phi_{+}^{(1)}$ and $\phi_{-}^{(1)}=\phi_{+}^{(1)\dagger}$ such that

$$\begin{aligned}&[\phi_{\pm}^{(1)},J_{\mp}^{(1)}]=i,\ \ [\phi_{\pm}^{(1)},J_{\pm}^{(1)}]=0\ ,\\ &[\phi_{\pm}^{(1)},B_{\mu}^{(1)}]=0\ \text{(and H.c. eq.)}\ .\end{aligned} \tag{2.10}$$

It will be seen later that the variables $\varphi^{(1)}$ and $\theta^{(1)}$ defined by

$$\phi_{\pm}^{(1)}=(\varphi^{(1)}\pm i\theta^{(1)})/2 \tag{2.11}$$

are the leading terms in the expansion of appropriately defined Euler angles φ and θ. From Eqs. (2.7) and (2.10), it follows that the RPA angle variables may be obtained by solving the linear inhomogeneous equation

$$[H^{(2)},\phi_{\pm}^{(1)}]=i\hbar^2J_{\pm}^{(1)}/(2\mathscr{I}_0)\ , \tag{2.12}$$

which is the Thouless-Valatin equation.[25] From Eqs. (2.10) and (2.12), the moment of inertia may be expressed in terms of a double commutator as follows:

$$\begin{aligned}\hbar^2/(2\mathscr{I}_0)&=[\phi_{+}^{(1)},[H^{(2)},\phi_{-}^{(1)}]]\\ &=[\phi_{-}^{(1)},[H^{(2)},\phi_{+}^{(1)}]]\ .\end{aligned} \tag{2.13}$$

To complete the story of the RPA, consider the angular-momentum component J_z, which is assumed to be purely quadratic in bosons, and must therefore take the form

$$J_z=\sum_{\mu}K_{\mu}B_{\mu}^{(1)\dagger}B_{\mu}^{(1)}+i\phi_{+}^{(1)}J_{-}^{(1)}-i\phi_{-}^{(1)}J_{+}^{(1)}\ . \tag{2.14}$$

The first term on the rhs follows from the fact that the RPA phonon $B_{\mu}^{(1)\dagger}$ carries K_{μ} units of angular momentum along the z axis, while the next two terms are required to satisfy Eq. (2.3c) for $n=1$.

It should be noted that for $K_{\mu}\neq 0$ each vibrational mode is doubly degenerate, with creation operators denoted by $B_{\mu}^{(1)\dagger}$ and $B_{-\mu}^{(1)\dagger}$. With the proper choice of phases, the two operators may be related by

$$B_{-\mu}^{(1)\dagger}=TB_{\mu}^{(1)\dagger}T^{-1}\ , \tag{2.15}$$

where T is the time-reversal operator. One has, of course, that $K_{-\mu}=-K_{\mu}$. In general, $\sum_{\mu}$ denotes summation over both signs.

B. Higher-order corrections to the RPA

The next task is the construction of the higher-order terms $H^{(3)},H^{(4)}$ in the Hamiltonian and $J_{\pm}^{(2)},J_{\pm}^{(3)}$ in the angular-momentum operators, using as building blocks the RPA normal modes. The most general form of $H^{(3)}$ compatible with hermiticity and invariance of H under both time reversal and arbitrary rotations is given by

$$\begin{aligned}H^{(3)}=&\tfrac{1}{2}\sum_{\mu\nu\lambda}h^{(3)}(00)_{\mu\nu\lambda}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}B_{\lambda}^{(1)}+\text{H.c.}+\left[\tfrac{1}{6}\sum_{\mu\nu\lambda}h^{(3)}(00)'_{\mu\nu\lambda}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}B_{\lambda}^{(1)\dagger}+\text{H.c.}\right]\\ &+\sum_{\mu}h^{(3)}(00)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)})+\left[J_{-}^{(1)}\sum_{\mu\nu}h^{(3)}(10)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\text{H.c.}\right]\\ &+\tfrac{1}{2}J_{-}^{(1)}\sum_{\mu\nu}h^{(3)}(10)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}-B_{-\nu}^{(1)}B_{-\mu}^{(1)})+\text{H.c.}+J_{+}^{(1)}J_{-}^{(1)}\sum_{\mu}h^{(3)}(20)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)})\\ &+J_{-}^{(1)2}\sum_{\mu}h^{(3)}(20)'_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+\text{H.c.}+\tfrac{1}{2}i[\{\phi_{+}^{(1)},J_{-}^{(1)}\}+\{\phi_{-}^{(1)},J_{+}^{(1)}\}]\sum_{\mu}h^{(3)}(11)_{\mu}(B_{\mu}^{(1)\dagger}-B_{\mu}^{(1)})\\ &+i\phi_{-}^{(1)}J_{-}^{(1)}\sum_{\mu}h^{(3)}(11)'_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})+\text{H.c.}+\left[i\phi_{-}^{(1)}\sum_{\mu\nu}h^{(3)}(01)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\text{H.c.}\right]\\ &+\tfrac{1}{2}i\phi_{-}^{(1)}\sum_{\mu\nu}h^{(3)}(01)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}+B_{-\nu}^{(1)}B_{-\mu}^{(1)})+\text{H.c.}+\phi_{+}^{(1)}\phi_{-}^{(1)}\sum_{\mu}h^{(3)}(02)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)})\\ &+\tfrac{1}{2}\phi_{-}^{(1)2}\sum_{\mu}h^{(3)}(02)'_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+\text{H.c.}\end{aligned} \tag{2.16}$$

Equation (2.16) reflects the following notation for general coefficients: In $h^{(n)}(kl)$, n denotes the order of the polynomial, k, the number of $J_{\pm}^{(1)}$ factors, and l, the number of $\phi_{\pm}^{(1)}$ factors. The coefficients may be chosen real without loss of generality. They are arbitrary in the generic model, except for certain restrictions arising from invariance requirements and exchange symmetries of indices. Taking into account J_z conservation [Eq. (2.6)] and time-reversal invariance, one obtains the following restrictions:

$$h^{(3)}(00)_{\mu\nu\lambda}=h^{(3)}(00)_{\mu\nu\lambda}\delta_{K_\mu+K_\nu-K_\lambda,0},\quad h^{(3)}(00)_{-\mu-\nu-\lambda}=h^{(3)}(00)_{\mu\nu\lambda}=h^{(3)}(00)_{\nu\mu\lambda}\ , \tag{2.17a}$$

$$h^{(3)}(00)'_{\mu\nu\lambda}=h^{(3)}(00)'_{\mu\nu\lambda}\delta_{K_\mu+K_\nu+K_\lambda,0},\quad h^{(3)}(00)'_{-\mu-\nu-\lambda}=h^{(3)}(00)'_{\mu\nu\lambda}=P(\mu\nu\lambda)h^{(3)}(00)'_{\mu\nu\lambda}\ , \tag{2.17b}$$

$$h^{(3)}(00)_{\mu}=h^{(3)}(00)_{\mu}\delta_{K_\mu,0}\ , \tag{2.17c}$$

$$h^{(3)}(10)_{\mu\nu}=h^{(3)}(10)_{\mu\nu}\delta_{K_\mu-K_\nu,1},\quad h^{(3)}(10)_{-\nu-\mu}=-h^{(3)}(10)_{\mu\nu}\ , \tag{2.17d}$$

$$h^{(3)}(10)'_{\mu\nu}=h^{(3)}(10)'_{\mu\nu}\delta_{K_\mu+K_\nu,1},\quad h^{(3)}(10)'_{\nu\mu}=h^{(3)}(10)'_{\mu\nu}\ , \tag{2.17e}$$

$$h^{(3)}(20)_{\mu}=h^{(3)}(20)_{\mu}\delta_{K_\mu,0},\quad h^{(3)}(20)'_{\mu}=h^{(3)}(20)'_{\mu}\delta_{K_\mu,2}\ , \tag{2.17f}$$

$$h^{(3)}(11)_{\mu}=h^{(3)}(11)_{\mu}\delta_{K_\mu,0},\quad h^{3}(11)'_{\mu}=h^{(3)}(11)'_{\mu}\delta_{K_\mu,2}\ , \tag{2.17g}$$

$$h^{(3)}(01)_{\mu\nu}=h^{(3)}(01)_{\mu\nu}\delta_{K_\mu-K_\nu,1},\quad h^{(3)}(01)_{-\nu-\mu}=h^{(3)}(01)_{\mu\nu}\ , \tag{2.17h}$$

$$h^{(3)}(01)'_{\mu\nu}=h^{(3)}(01)'_{\mu\nu}\delta_{K_\mu+K_\nu,1},\quad h^{(3)}(01)'_{\nu\mu}=h^{(3)}(01)'_{\mu\nu}\ , \tag{2.17i}$$

$$h^{(3)}(02)_{\mu}=h^{(3)}(02)_{\mu}\delta_{K_\mu,0},\quad h^{(3)}(02)'_{\mu}=h^{(3)}(02)'_{\mu}\delta_{K_\mu,2}\ . \tag{2.17j}$$

In Eq. (2.17b), $P(\mu\nu\lambda)$ represents an arbitrary permutation of the three indices. Equations (2.17) are used in later evaluations of various commutators. In addition to these restrictions, the rotational invariance condition (2.5) implies certain relations between coefficients of $H^{(3)}$ and those of $J_{\pm}^{(2)}$ [see Eq. (2.21) below]. The next task then is to construct the most general form of $J_{\pm}^{(2)}$.

The quadratic correction $J_{\pm}^{(2)}$ may be obtained from Eq. (2.3c) and the time-reversal property

$$TJ_{\pm}^{(n)}T^{-1}=-J_{\pm}^{(n)\dagger}=-J_{\mp}^{(n)}\ . \tag{2.18}$$

It turns out that Eq. (2.3b) is then automatically fulfilled, as may easily be checked afterwards. The most general form of $J_{\pm}^{(2)}$ is found to be

$$\begin{aligned}J_{+}^{(2)}=&J_{+}^{(1)}\sum_{\mu}j^{(2)}(10)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)})+J_{-}^{(1)}\sum_{\mu}j^{(2)}(10)'_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})\\&+i\phi_{+}^{(1)}\sum_{\mu}j^{(2)}(01)_{\mu}(B_{\mu}^{(1)\dagger}-B_{\mu}^{(1)})+i\phi_{-}^{(1)}\sum_{\mu}j^{(2)}(01)'_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})\\&+\sum_{\mu\nu}j^{(2)}(00)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\tfrac{1}{2}\sum_{\mu\nu}j^{(2)}(00)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}-B_{-\nu}^{(1)}B_{-\mu}^{(1)})\ ,\\J_{-}^{(2)}=&J_{+}^{(2)\dagger}\ ,\end{aligned} \tag{2.19}$$

where the coefficients $j^{(2)}(kl)_{\mu\ldots}$ are chosen real and the nomenclature is similar to that for the Hamiltonian coefficients. The coefficients must satisfy the following conditions:

$$j^{(2)}(10)_{\mu}=j^{(2)}(10)_{\mu}\delta_{K_\mu,0}\ , \tag{2.20a}$$

$$j^{(2)}(10)'_{\mu}=j^{(2)}(10)'_{\mu}\delta_{K_\mu,2}\ ,$$

$$j^{(2)}(01)_{\mu}=j^{(2)}(01)_{\mu}\delta_{K_\mu,0}\ , \tag{2.20b}$$

$$j^{(2)}(01)'_{\mu}=j^{(2)}(01)'_{\mu}\delta_{K_\mu,2}\ ,$$

$$j^{(2)}(00)_{\mu\nu}=j^{(2)}(00)_{\mu\nu}\delta_{K_\mu-K_\nu,1}\ , \tag{2.20c}$$

$$j^{(2)}(00)_{-\nu-\mu}=-j^{(2)}(00)_{\mu\nu}\ ,$$

$$j^{(2)}(00)'_{\mu\nu}=j^{(2)}(00)'_{\mu\nu}\delta_{K_\mu+K_\nu,1}\ , \tag{2.20d}$$

$$j^{(2)}(00)'_{\nu\mu}=j^{(2)}(00)'_{\mu\nu}\ .$$

The rotational invariance condition (2.5) for $n=3$ implies the following relations between the coefficients of $\phi_{\pm}^{(1)}$-dependent terms of $H^{(3)}$ and those of $J_{\pm}^{(2)}$:

$$\begin{aligned}&h^{(3)}(11)_{\mu}=\hbar\omega_{\mu}j^{(2)}(10)_{\mu}+\frac{\hbar^2}{2\mathcal{I}_0}j^{(2)}(01)_{\mu}\ ,\\&h^{(3)}(11)'_{\mu}=\hbar\omega_{\mu}j^{(2)}(10)'_{\mu}+\frac{\hbar^2}{2\mathcal{I}_0}j^{(2)}(01)'_{\mu}\ ,\\&h^{(3)}(02)_{\mu}=-\hbar\omega_{\mu}j^{(2)}(01)_{\mu},\quad h^{(3)}(02)'_{\mu}=-\hbar\omega_{\mu}j^{(2)}(01)'_{\mu}\ ,\\&h^{(3)}(01)_{\mu\nu}=\hbar(\omega_{\mu}-\omega_{\nu})j^{(2)}(00)_{\mu\nu}\ ,\\&h^{(3)}(01)'_{\mu\nu}=\hbar(\omega_{\mu}+\omega_{\nu})j^{(2)}(00)'_{\mu\nu}\ .\end{aligned} \tag{2.21}$$

These relations will play an important role in later developments.

Continuing in the same vein, one may construct the most general form of the quartic polynomial $H^{(4)}$ and the cubic polynomial $J_{\pm}^{(3)}$. Here one encounters a large number of different kinds of terms; for example, 34 in the case of $H^{(4)}$. Fortunately, for the purpose of evaluating the leading-order corrections to the RPA, only a small subset of these terms are actually needed. Thus, for $H^{(4)}$ it is sufficient to write

$$H^{(4)}=h^{(4)}(40)(J_+^{(1)}J_-^{(1)})^2+h^{(4)}(00)+\sum_{\mu\nu}h^{(4)}(00)_{\mu\nu}B_\mu^{(1)\dagger}B_\nu^{(1)}+\tfrac{1}{4}\sum_{\mu\nu\kappa\lambda}h^{(4)}(00)_{\mu\nu,\kappa\lambda}B_\mu^{(1)\dagger}B_\nu^{(1)\dagger}B_\kappa^{(1)}B_\lambda^{(1)}$$
$$+J_+^{(1)}J_-^{(1)}\left[h^{(4)}(20)+\sum_{\mu\nu}h^{(4)}(20)_{\mu\nu}B_\mu^{(1)\dagger}B_\nu^{(1)}\right]+\text{dispensable terms}\ , \tag{2.22}$$

where the coefficients, which are real, have the following properties:

$$\begin{aligned}&h^{(4)}(00)_{\mu\nu,\kappa\lambda}=h^{(4)}(00)_{\mu\nu,\kappa\lambda}\delta_{K_\mu+K_\nu,\,K_\kappa+K_\lambda}\ ,\\ &h^{(4)}(00)_{-\mu-\nu,\,-\kappa-\lambda}=h^{(4)}(00)_{\mu\nu,\kappa\lambda}\\ &\qquad=h^{(4)}(00)_{\nu\mu,\kappa\lambda}\\ &\qquad=h^{(4)}(00)_{\mu\nu,\lambda\kappa}\\ &\qquad=h^{(4)}(00)_{\nu\mu,\lambda\kappa}=h^{(4)}(00)_{\kappa\lambda,\mu\nu}\ ,\end{aligned} \tag{2.23a}$$

$$\begin{aligned}&h^{(4)}(00)_{\mu\nu}=h^{(4)}(00)_{\mu\nu}\delta_{K_\mu,K_\nu}\ ,\\ &h^{(4)}(00)_{-\mu-\nu}=h^{(4)}(00)_{\mu\nu}=h^{(4)}(00)_{\nu\mu}\ ,\end{aligned} \tag{2.23b}$$

$$\begin{aligned}&h^{(4)}(20)_{\mu\nu}=h^{(4)}(20)_{\mu\nu}\delta_{K_\mu,K_\nu}\ ,\\ &h^{(4)}(20)_{-\mu-\nu}=h^{(4)}(20)_{\mu\nu}=h^{(4)}(20)_{\nu\mu}\ .\end{aligned} \tag{2.23c}$$

In the case of $J_{\pm}^{(3)}$, only three terms need be explicitly considered; namely,

$$\begin{aligned}J_+^{(3)}&=J_+^{(1)}\left[j^{(3)}(10)+\sum_{\mu\nu}j^{(3)}(10)_{\mu\nu}B_\mu^{(1)\dagger}B_\nu^{(1)}\right]\\ &\quad+j^{(3)}(30)J_+^{(1)2}J_-^{(1)}+\text{dispensable terms}\ ,\\ J_-^{(3)}&=J_+^{(3)\dagger}\ .\end{aligned} \tag{2.24}$$

A term of the form

$$J_-^{(1)}\sum_{\mu\nu}j^{(3)}(10)'_{\mu\nu}B_\mu^{(1)\dagger}B_{-\nu}^{(1)}$$

also occurs on the rhs, but ultimately does not contribute to the order of interest. The (real) coefficients in (2.24) must satisfy

$$\begin{aligned}&j^{(3)}(10)_{\mu\nu}=j^{(3)}(10)_{\mu\nu}\delta_{K_\mu,K_\nu}\ ,\\ &j^{(3)}(10)_{-\mu-\nu}=j^{(3)}(10)_{\mu\nu}\ .\end{aligned} \tag{2.25}$$

It should also be mentioned that the angular-momentum conservation condition (2.5) for $n=4$, which relates certain coefficients of $J_{\pm}^{(3)}$ to those of the $\phi_{\pm}^{(1)}$-dependent terms of $H^{(4)}$, involves only the coefficients of the dispensable terms in Eqs. (2.22) and (2.24).

C. Electric quadrupole transition operators

The electric quadrupole tensor will be chosen as a typical example of how to treat transition operators in the MW formalism. In the generic model, the components of the $E2$ tensor, $\mathcal{M}(E2,M)$, may be expanded through quadratic terms as follows:

$$\mathcal{M}(E2,M)=\mathcal{M}^{(0)}(E2,M)+\mathcal{M}^{(1)}(E2,M)+\mathcal{M}^{(2)}(E2,M)+\cdots\ , \tag{2.26}$$

where the first term on the rhs is a constant of order Ω given by

$$\mathcal{M}^{(0)}(E2,M)=\left[\frac{5}{16\pi}\right]^{1/2}eQ_0\delta_{M,0}\ , \tag{2.27}$$

Q_0 being the intrinsic quadrupole moment, and the second term of order $\Omega^{1/2}$ is linear in bosons, the third term of order 1 is quadratic, etc. For the present purposes, it is sufficient to stop at quadratic terms.

In each order the $E2$ operators satisfy the time-reversal property

$$\begin{aligned}T\mathcal{M}^{(n)}(E2,M)T^{-1}&=\mathcal{M}^{(n)}(E2,M)^\dagger\\ &=(-1)^M\mathcal{M}^{(n)}(E2,-M)\ .\end{aligned} \tag{2.28}$$

These operators must satisfy the angular-momentum commutators for a rank-2 spherical tensor order by order, namely

$$[J_z,\mathcal{M}^{(n)}(E2,M)]=M\mathcal{M}^{(n)}(E2,M)\ , \tag{2.29}$$

and

$$\sum_{k=1}^{n}[J_\pm^{(n-k+1)},\mathcal{M}^{(k)}(E2,M)]=[(2\mp M)(3\pm M)]^{1/2}\mathcal{M}^{(n-1)}(E2,M\pm1)\ . \tag{2.30}$$

The general form of $\mathscr{M}^{(n)}(E2,M)$ can be deduced from Eqs. (2.28) and (2.29) alone, while (2.30) relates certain $E2$ and angular-momentum coefficients. In this way, the linear boson terms are easily found to have the forms

$$\mathscr{M}^{(1)}(E2,0)=\sum_{\mu} q_0^{(1)}(00)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)}) , \tag{2.31a}$$

$$\mathscr{M}^{(1)}(E2,1)=\sum_{\mu} q_1^{(1)}(00)_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+iq^{(1)}(01)\phi_+^{(1)} , \tag{2.31b}$$

$$\mathscr{M}^{(1)}(E2,2)=\sum_{\mu} q_2^{(1)}(00)_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)}) , \tag{2.31c}$$

where the coefficients, which are chosen real, have the following properties:

$$\begin{aligned} q_0^{(1)}(00)_{\mu}&=q_0^{(1)}(00)_{\mu}\delta_{K_{\mu},0} ,\\ q_1^{(1)}(00)_{\mu}&=q_1^{(1)}(00)_{\mu}\delta_{K_{\mu},1} ,\\ q_2^{(1)}(00)_{\mu}&=q_2^{(1)}(00)_{\mu}\delta_{K_{\mu},2} . \end{aligned} \tag{2.32}$$

The $\mathscr{M}(E2,M)$ with $M=-1,-2$ can always be found with the aid of the second equality in (2.28).

Continuing to the quadratic terms, one finds, first of all, that

$$\begin{aligned} \mathscr{M}^{(2)}(E2,0)=&q_0^{(2)}(00)+\sum_{\mu\nu} q_0^{(2)}(00)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\tfrac{1}{2}\sum_{\mu\nu} q_0^{(2)}(00)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}+B_{\nu}^{(1)}B_{\mu}^{(1)})+q_0^{(2)}(20)J_+^{(1)}J_-^{(1)}\\ &+J_-^{(1)}\sum_{\mu} q_0^{(2)}(10)_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})+\text{H.c.}+\left[i\phi_-^{(1)}\sum_{\mu} q_0^{(2)}(01)_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+\text{H.c.}\right]+q_0^{(2)}(02)\phi_+^{(1)}\phi_-^{(1)} , \end{aligned} \tag{2.33}$$

where the (real) coefficients have the following properties:

$$q_0^{(2)}(00)_{\mu\nu}=q_0^{(2)}(00)_{\mu\nu}\delta_{K_{\mu},K_{\nu}},\quad q_0^{(2)}(00)_{-\mu-\nu}=q_0^{(2)}(00)_{\mu\nu}=q_0^{(2)}(00)_{\nu\mu} , \tag{2.34a}$$

$$q_0^{(2)}(00)'_{\mu\nu}=q_0^{(2)}(00)'_{\mu\nu}\delta_{K_{\mu},-K_{\nu}},\quad q_0^{(2)}(00)'_{-\mu-\nu}=q_0^{(2)}(00)'_{\mu\nu}=q_0^{(2)}(00)_{\nu\mu} , \tag{2.34b}$$

$$q_0^{(2)}(10)_{\mu}=q_0^{(2)}(10)_{\mu}\delta_{K_{\mu},1} , \tag{2.34c}$$

$$q_0^{(2)}(01)_{\mu}=q_0^{(2)}(01)_{\mu}\delta_{K_{\mu},1} . \tag{2.34d}$$

Next, for $\mathscr{M}^{(2)}(E2,1)$, one obtains

$$\begin{aligned} \mathscr{M}^{(2)}(E2,1)=&\sum_{\mu\nu} q_1^{(2)}(00)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\tfrac{1}{2}\sum_{\mu\nu} q_1^{(2)}(00)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}+B_{-\nu}^{(1)}B_{-\mu}^{(1)})\\ &+J_+^{(1)}\sum_{\mu} q_1^{(2)}(10)_{\mu}(B_{\mu}^{(1)\dagger}-B_{\mu}^{(1)})+J_-^{(1)}\sum_{\mu} q_1^{(2)}(10)'_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})\\ &+i\phi_+^{(1)}\sum_{\mu} q_1^{(2)}(01)_{\mu}(B_{\mu}^{(1)\dagger}+B_{\mu}^{(1)})+i\phi_-^{(1)}\sum_{\mu} q_1^{(2)}(01)'_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)}) , \end{aligned} \tag{2.35}$$

with the following conditions on the coefficients:

$$q_1^{(2)}(00)_{\mu\nu}=q_1^{(2)}(00)_{\mu\nu}\delta_{K_{\mu}-K_{\nu},1},\quad q_1^{(2)}(00)_{-\mu-\nu}=q_1^{(2)}(00)_{\nu\mu} , \tag{2.36a}$$

$$q_1^{(2)}(00)'_{\mu\nu}=q_1^{(2)}(00)'_{\mu\nu}\delta_{K_{\mu}+K_{\nu},1},\quad q_1^{(2)}(00)'_{\mu\nu}=q_1^{(2)}(00)'_{\nu\mu} , \tag{2.36b}$$

$$q_1^{(2)}(10)_{\mu}=q_1^{(2)}(10)_{\mu}\delta_{K_{\mu},0},\quad q_1^{(2)}(10)'_{\mu}=q_1^{(2)}(10)'_{\mu}\delta_{K_{\mu},2} , \tag{2.36c}$$

$$q_1^{(2)}(01)_{\mu}=q_1^{(2)}(01)_{\mu}\delta_{K_{\mu},0},\quad q_1^{(2)}(01)'_{\mu}=q_1^{(2)}(01)'_{\mu}\delta_{K_{\mu},2} . \tag{2.36d}$$

Finally, for the $M=2$ component, one obtains

$$\begin{aligned} \mathscr{M}^{(2)}(E2,2)=&\sum_{\mu\nu} q_2^{(2)}(00)_{\mu\nu}B_{\mu}^{(1)\dagger}B_{\nu}^{(1)}+\tfrac{1}{2}\sum_{\mu\nu} q_2^{(2)}(00)'_{\mu\nu}(B_{\mu}^{(1)\dagger}B_{\nu}^{(1)\dagger}+B_{-\nu}^{(1)}B_{-\mu}^{(1)})+q_2^{(2)}(20)J_+^{(1)2}\\ &+J_+^{(1)}\sum_{\mu} q_2^{(2)}(10)_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})+J_-^{(1)}\sum_{\mu} q_2^{(2)}(10)'_{\mu}(B_{\mu}^{(1)\dagger}-B_{-\mu}^{(1)})\\ &+i\phi_+^{(1)}\sum_{\mu} q_2^{(2)}(01)_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+i\phi_-^{(1)}\sum_{\mu} q_2^{(2)}(01)'_{\mu}(B_{\mu}^{(1)\dagger}+B_{-\mu}^{(1)})+q_2^{(2)}(02)\phi_+^{(1)2} , \end{aligned} \tag{2.37}$$

with the following conditions on the coefficients:

$$q_2^{(2)}(00)_{\mu\nu}=q_2^{(2)}(00)_{\mu\nu}\delta_{K_\mu-K_\nu,2}\ ,$$
$$q_2^{(2)}(00)_{-\mu-\nu}=q_2^{(2)}(00)_{\nu\mu}\ , \tag{2.38a}$$
$$q_2^{(2)}(00)'_{\mu\nu}=q_2^{(2)}(00)'_{\mu\nu}\delta_{K_\mu+K_\nu,2}\ ,$$
$$q_2^{(2)}(00)'_{\mu\nu}=q_2^{(2)}(00)'_{\nu\mu}\ , \tag{2.38b}$$
$$q_2^{(2)}(10)_{\mu}=q_2^{(2)}(10)_{\mu}\delta_{K_\mu,1}\ ,$$
$$q_2^{(2)}(10)'_{\mu}=q_2^{(2)}(10)'_{\mu}\delta_{K_\mu,3}\ , \tag{2.38c}$$
$$q_2^{(2)}(01)_{\mu}=q_2^{(2)}(01)_{\mu}\delta_{K_\mu,1}\ ,$$
$$q_2^{(2)}(01)'_{\mu}=q_2^{(2)}(01)'_{\mu}\delta_{K_\mu,3}\ . \tag{2.38d}$$

To complete the discussion, the angular-momentum commutators (2.30) must be taken into account. For $n=1$, this leads to the identification

$$q^{(1)}(01)=\left[\frac{15}{18\pi}\right]^{1/2}eQ_0\ . \tag{2.39}$$

For $n=2$, with $M=0,1,2$ in succession, the following identifications are made:

$$q_0^{(2)}(01)_\mu=\sqrt{6}q_1^{(1)}(00)_\mu - \sum_\nu [j^{(2)}(00)_{\mu\nu}-j^{(2)}(00)'_{\mu\nu}]q_0^{(1)}(00)_\nu\ ,$$

$$q_0^{(2)}(02)=-\left[\frac{45}{4\pi}\right]^{1/2}eQ_0-2\sum_\mu j^{(2)}(01)_\mu q_0^{(1)}(00)_\mu\ ,$$

$$q_1^{(2)}(01)_\mu=\sqrt{6}q_0^{(1)}(00)_\mu-\left[\frac{15}{8\pi}\right]^{1/2}eQ_0j^{(2)}(10)_\mu - \sum_\nu q_1^{(1)}(00)_\nu[j^{(2)}(00)_{\nu\mu}+j^{(2)}(00)'_{\nu\mu}]\ ,$$

$$q_1^{(2)}(01)'_\mu=2q_2^{(1)}(00)_\mu-\left[\frac{15}{8\pi}\right]^{1/2}eQ_0j^{(2)}(10)'_\mu - \sum_\nu [j^{(2)}(00)_{\mu\nu}-j^{(2)}(00)'_{\mu-\nu}]q_1^{(1)}(00)_\nu\ , \tag{2.40}$$

$$q_2^{(2)}(01)_\mu=2q_1^{(1)}(00)_\mu - \sum_\nu q_2^{(1)}(00)_\nu[j^{(2)}(00)_{\nu\mu}+j^{(2)}(00)'_{\nu-\mu}]\ ,$$

$$q_2^{(2)}(01)'_\mu=\sum_\nu [j^{(2)}(00)'_{\mu-\nu}-j^{(2)}(00)_{\mu\nu}]q_2^{(1)}(00)_\nu\ ,$$

$$q_2^{(2)}(02)=-\left[\frac{15}{8\pi}\right]^{1/2}eQ_0-\sum_\mu q_2^{(1)}(00)_\mu j^{(2)}(01)'_\mu\ .$$

III. GOALS, OBSTACLES, AND SOLUTIONS

Ideally, one would like to begin with the RPA Hamiltonian $H^{(2)}$ as the zeroth order and treat the higher-order terms $H^{(3)}$, $H^{(4)}$, etc. as small perturbations. However, such a procedure could be feasible only if the Hamiltonian were truncated to the vibrational subspace;[28] any attempt to include the rotational degrees of freedom in the guise of bare Goldstone modes would lead to infrared divergences.[6] This is because the RPA variables $J_\pm^{(1)}$ have a continuous spectrum, unlike the full angular-momentum operators $J_\pm$. As a consequence, the RPA eigenstates are nonnormalizable, with each Goldstone mode contributing an infinite factor to the norm.[2] The underlying reason for this difficulty is the use of Taylor expansions indiscriminately involving all degrees of freedom.[2] Such expansions are valid, at best, in a limited region of phase space in the neighborhood of a MF minimum. While such a procedure may be satisfactory for small-amplitude vibrations, in the presence of rotational degrees of freedom the MF method does not provide a true minimum but rather a point of neutral stability. The crux of the difficulty then is that angular coordinates, which require the full range of, say, 2π, are restricted by fiat to a much smaller range, thereby precluding proper quantization of these degrees of freedom. Nevertheless, the situation is by no means hopeless; it is still possible to calculate correct results in the presence of Goldstone modes, either through the artful use of appropriate constraints and limiting procedures[5–7] or by the very different technique used in this paper, in which the Taylor expansion is exploited to uniquely reconstruct a valid Hamiltonian (and other operators) amenable to perturbation theory.

A. The goal of the MW method

Given a Hamiltonian and associated transition operators equivalent to the generic model, the goal of the MW method is to reconstitute a viable Hamiltonian and associated operators for which the generic model is a correct Taylor expansion to a given order. This reconstituted system should be unique up to arbitrary canonical transformations and it should have the form of the generalized BM model. It will be shown eventually that this goal can be achieved with the aid of formal unitary transformations.

In the generalized BM model for nuclei with axially symmetric equilibrium shapes,[15] the Hamiltonian is assumed to have the form of an angular-momentum expansion:

$$H=\sum_{mn}\mathscr{H}_{mn}\tfrac{1}{2}\{I'^m_-,I'^n_+\}\ . \tag{3.1}$$

where $I'_\pm\equiv I_1\pm iI_2$, I_k $(k=1,2,3)$ being interpreted as the components of the total angular momentum along the principal axes (PA's) of the nucleus, with the three-axis designated as the axis of symmetry. The components of **I** are usually represented as differential operators in the space of Euler angles. The operators $\mathscr{H}_{mn}$, which describe the intrinsic (nonrotational) excitations, commute with all components of **I** and with the Euler angles. In general, operators that commute with all components of the angular momentum and with the Euler angles are called *intrinsic* operators.[22] The operators $\mathscr{H}_{mn}$ in the BM model also have the special property of carrying an "intrinsic" angular momentum, denoted by J_3, along the symmetry axis, and the eigenstates of (3.1) are required to satisfy the condition $I_3=J_3$. Any scalar operator may be written in a form analogous to (3.1), while spherical ten-

sors, such as transition operators, must be expressed in a more general form involving the rotation matrices [see Eq. (3.32) below].

B. Obstacles to a naive extension of the MW method

The generic Hamiltonian defined by Eqs. (2.1), (2.7), (2.16), and (2.22) as it stands is not of the form (3.1) if the RPA modes $B_\mu^{(1)}, B_\mu^{(1)\dagger}$ are identified as the intrinsic excitations, since, first of all, the $J_\pm^{(1)}$ are not angular momentum operators, but only their leading-order approximations, and second, H contains a dependence on the angular variables $\phi_\pm^{(1)}$. In a straightforward extension of the MW method used for two-dimensional rotation, one could attempt to reconstruct a valid H of the BM form as follows. Given the boson expansions of H and the constants of motion, i.e., the angular momentum vector **J**, one may seek certain angle variables $\phi_\pm$ and intrinsic boson excitation operators $B_\mu, B_\mu^\dagger$, whose boson expansions begin with the RPA variables $\phi_\pm^{(1)}$ and $B_\mu^{(1)}, B_\mu^{(1)\dagger}$, respectively. One might proceed in the following way. First, the variables $\phi_\pm$ could be chosen as appropriate Euler angles, or functions thereof, and the Taylor expansions determined from the ansatz $\phi_\pm = \phi_\pm^{(1)} + \phi_\pm^{(2)} + \cdots$ and the requirement that $\phi_\pm$ obey the correct commutation relations with the angular momentum components order by order. Next, the expansions of intrinsic bosons can be sought in the form $B_\mu = B_\mu^{(1)} + B_\mu^{(2)} + \cdots$ (and the H.c. equation) by requiring the order-by-order fulfillment of the correct commutation relations with the components of **J** and the angle variables $\phi_\pm$. Having determined the expansions of all degrees of freedom, which, in principle, could be inverted, one would be in a position to transform H from the original variables to the final ones. That is, H would then be expressed in terms of the full-angular-momentum components and the true intrinsic variables B_μ and $B_\mu^\dagger$, but would be independent of the angle variables $\phi_\pm$ because of rotational invariance. Thus, one would expect that H would then have the BM form. While this rosy scenario will indeed eventually come to pass, there are some stumbling blocks that must first be overcome.

From physical considerations, it is clear that the intrinsic operators $\mathscr{H}_{mn}$ in Eq. (3.1) must be functions of the bosons $B_\mu, B_\mu^\dagger$ alone, which in the lowest order of the boson expansion are approximated by the RPA bosons $B_\mu^{(1)}, B_\mu^{(1)\dagger}$. Thus, it is natural to surmise that the RPA Hamiltonian (2.7) arises as the lowest-order approximation in the expansion of the following terms of a BM Hamiltonian:

$$\mathscr{H}_{00} + \tfrac{1}{2}\mathscr{H}_{11}\{I'_-, I'_+\} = \mathscr{H}_{00} + \mathscr{H}_{11}(I_1^2 + I_2^2) , \tag{3.2}$$

where

$$\begin{aligned} \mathscr{H}_{00} &= \text{const} + \sum_\mu \hbar\omega_\mu B_\mu^\dagger B_\mu + \cdots , \\ \mathscr{H}_{11} &= \hbar^2/(2\mathscr{I}_0) + \cdots , \end{aligned} \tag{3.3}$$

and the omitted terms are of higher order in Ω^{-1}. In order for this to be valid, it is necessary that the boson expansion yield $I_1^2 + I_2^2 = J_x^{(1)2} + J_y^{(1)2} + \text{higher orders}$. The higher-order contributions from the boson expansion of (3.2) would then contribute to $H^{(3)}$, $H^{(4)}$, etc. While this supposition will be justified eventually, at the present stage a basic difficulty emerges.

Since **I** denotes the total angular momentum in the BM representation and **J** the total angular momentum for the given generic (many-body) system, it would appear perfectly natural to equate the two. However, in the BM representation, all components of **I** commute with all intrinsic excitation operators by definition, and therefore should commute with all the phonons $B_\mu, B_\mu^\dagger$. But in the case of **J**, it is easy to demonstrate that at least one component cannot commute with the phonons, namely, the component J_z. From Eq. (2.14), it follows immediately that

$$[B_\mu^{(1)}, J_z] = K_\mu B_\mu^{(1)} \quad (\text{and H.c. eq.}) . \tag{3.4}$$

Since each term in the phonon expansion $B_\mu = B_\mu^{(1)} + \cdots$ would have to commute with J_z, Eq. (3.4) is sufficient to prove that J_z does not commute with the phonons. If even a single component of the angular momentum fails to commute with an operator, then that operator cannot qualify as an intrinsic one. Moreover, even if the phonons were to commute with the other laboratory components of **J** and with the Euler angles, they could not commute with the PA components of **J** as normally defined [see Eq. (3.6) below]. This can be seen explicitly for the component along the symmetry axis J_3, which in lowest order is just the phonon part of (2.14). The conclusion is that directly equating the BM angular momentum **I** with the total angular momentum **J** is inconsistent with the designation of the vibrational phonon as an intrinsic excitation operator. This difficulty is associated with the fact that the phonons carry angular momentum along the symmetry axis. In the phenomenological BM model, this problem is avoided by the introduction of an "intrinsic" angular momentum **J**, distinct from the "collective" angular momentum **I**.

The above obstacle is the most fundamental and the one most responsible for impeding progress in extending the MW method to three-dimensional rotation of axially symmetric nuclei. However, there are two other, not unrelated problems. First, in the BM model, the angular-momentum components are represented by certain differential operators in Euler-angle space. The question arises whether **J** in the generic model can also be represented in the same way. Observe, however, that **J** can be expanded in a Taylor series that involves, in part, a small-angle expansion, whereas the standard differential operators[29] cannot be so expanded. The reason is that if the usual *zyz* definition of the Euler angles is adopted, the angular-momentum components are represented by differential operators that become singular when the intermediate Euler angle vanishes. Fortunately, this problem is easily remedied by choosing an uncommon definition of the Euler angles, namely, the *xyz* definition, which leads to an expandable representation of the angular-momentum components, as will be seen later. The remaining problem is that there are, of course, three Euler angles, whereas the RPA defines the leading order of only two angular variables. The reason for this is that the third angle, representing rotations about the symmetry axis, is completely undefined. Nevertheless, such an angle is needed as a dynamic variable if a correspondence with

the BM model is to be made. It will be seen that the indeterminacy of this third Euler angle is of no physical importance.

The above problems are the consequence not only of axial symmetry, but also of the fact that intrinsic modes exist with $K_\mu \neq 0$. In the case of the rotation and vibration of a diatomic molecule, for example, for which the vibrational mode has $K=0$, these difficulties do not occur.[21] There are also no difficulties in extending the MW method to triaxial systems and to systems at high spin,[9] which, in general, do not have axial symmetry.

The above scheme for extending the MW method to three-dimensional rotation presupposes that, just as in the two-dimensional case, there is no need to introduce redundant variables. However, as shown next, the key to surmounting the obstacles is precisely the recognition that the BM representation involves a redundant Euler angle corresponding to a rotation about the symmetry axis, a point hidden in the fine print of Ref. 15 and historically perhaps somewhat shrouded in mystery. It will be shown that the BM representation can be related to a nonredundant description through a simple unitary transformation.

C. Connection between the BM and Villars representations

Some time ago, it was formally shown by Villars,[22] and more recently by Mikhailov[30] using a different technique, that any rotationally invariant Hamiltonian (or other such operator) may be expanded in powers of angular-momentum components along the principal axes. For a system with an axially symmetric intrinsic shape, this expansion may be written in the form

$$H=\sum_{mn} \mathring{\mathscr{H}}_{mn} \tfrac{1}{2}\{J'^{m}_{-},J'^{n}_{+}\} , \tag{3.5}$$

where the $\mathring{\mathscr{H}}_{mn}$ are intrinsic operators and $J'_{\pm}=J_1 \pm iJ_2$ are combinations of PA components of angular momentum. Since the latter are scalars, (3.5) is manifestly rotationally invariant. The relation between the spherical-vector PA and laboratory components is given, as usual, by[29]

$$J'_K=\sum_{M=-1}^{1} D^{1\dagger}_{MK}(\varphi,\theta,\psi)J_M=\sum_{M=-1}^{1} J_M D^{1\dagger}_{MK}(\varphi,\theta,\psi) \qquad (K=0,\pm 1) , \tag{3.6}$$

where the $D^1_{MK}(\varphi,\theta,\psi)$ are the matrix elements of the spin-1 irreducible representation of the rotation group, parametrized by a set of Euler angles φ,θ,ψ. According to Refs. 22 and 30, the intrinsic coefficients $\mathring{\mathscr{H}}_{mn}$ are expressible in a series involving multiple commutators of H with the $D^1_{MK}(\varphi,\theta,\psi)$, but this result will not be utilized here. It should also be mentioned that the decomposition (3.5) is hardly unique, but depends entirely on the choice of the Euler angles as functions of the nuclear degrees of freedom.

Spherical tensor operators T^L_M can be written in the form

$$T^L_M=\sum_{K=-L}^{L} \hat{T}^L_K D^L_{MK}(\varphi,\theta,\psi) , \tag{3.7}$$

where $D^L_{MK}(\varphi,\theta,\psi)$ is a rotation matrix element corresponding to the spin-L irreducible representation, and the $\hat{T}^L_K$, the PA components of the spherical tensor, are scalars, and, therefore, like H, may be expanded in powers of the angular-momentum components:

$$\hat{T}^L_K=\sum_{mn} (\mathring{t}^L_K)_{mn}\{J'^{m}_{-},J'^{n}_{+}\} , \tag{3.8}$$

where the coefficients $(\mathring{t}^L_K)_{mn}$ are intrinsic operators.

The Villars representation closely resembles the BM representation, but with one notable difference. In the former, the coefficients $\mathring{\mathscr{H}}_{mn}$ and $(\mathring{t}^L_K)_{mn}$ are truly intrinsic operators, carrying no angular momentum, whereas in the latter the corresponding coefficients do carry angular momentum along the symmetry axis. Within the Villars representation, one may proceed as follows. The Euler angle ψ describing a rotation about the symmetry axis is canonically conjugate to J_3, which may be expressed by

$$[J_3, \exp(i\psi)]=\exp(i\psi) . \tag{3.9}$$

The operators $\mathscr{H}_{mn}$ and $(t^L_K)_{mn}$, defined by

$$\mathscr{H}_{mn}=\mathring{\mathscr{H}}_{mn}\exp[i(m-n)\psi] , \tag{3.10a}$$

$$(t^L_K)_{mn}=(\mathring{t}^L_K)_{mn}\exp[i(K+m-n)\psi] , \tag{3.10b}$$

satisfy

$$[J_3,\mathscr{H}_{mn}]=(m-n)\mathscr{H}_{mn} , \tag{3.11a}$$

$$[J_3,(t^L_K)_{mn}]=(K+m-n)(t^L_K)_{mn} , \tag{3.11b}$$

since J_3 commutes with $\mathring{\mathscr{H}}_{mn}$ and $(\mathring{t}^L_K)_{mn}$. These are exactly the commutation relations obeyed by the corresponding coefficients in the BM representation, where J_3, however, is the "intrinsic" angular momentum.

With the help of Eqs. (3.10), Eqs. (3.5) and (3.8) may be written as

$$H=\sum_{mn} \mathscr{H}_{mn}\exp[i(n-m)\psi]\tfrac{1}{2}\{J'^{m}_{-},J'^{n}_{+}\} \tag{3.12}$$

and

$$\hat{T}^L_M=\sum_{mn} (t^L_K)_{mn}\exp[i(n-m-K)\psi]\tfrac{1}{2}\{J'^{m}_{-},J'^{n}_{+}\} . \tag{3.13}$$

Note that Eqs. (3.12) and (3.13), which can be rearranged in several permutations owing to the intrinsic nature of the substituted operators $\mathring{\mathscr{H}}_{mn}$ and $(\mathring{t}^L_K)_{mn}$, are, of course, just another form of the Villars representation. The coefficients $\mathscr{H}_{mn}$ and $(t^L_K)_{mn}$, however, do carry angular momentum along the symmetry axis as in the BM representation, but, on the other hand, they do not commute with $J'_{\pm}$ and therefore are not intrinsic operators with respect to **J**. Thus, this simple substitution certainly does not give the BM representation. Moreover, Eqs. (3.12) and (3.13) also carry the unesthetic ψ-dependent exponential factors. It will now be shown, however, that the Villars and BM representations are connected by a unitary transformation and thus are basically equivalent.

The key step in the transformation from the Villars to the BM representation is the prior introduction of a redundant variable $\bar{\psi}$. That is, all operators such as H and the transition operators may be regarded as defined

on an extended Hilbert space that is the direct product of the original (nuclear) Hilbert space with the space of periodic functions $e^{iK\bar{\psi}}$. To emphasize again the difference, the variable ψ is a function of the original (nuclear) degrees of freedom, whereas $\bar{\psi}$ is a dummy variable, destined, however, to assume the function of ψ. In the extended space, one may define the operator I_3 represented by

$$I_3 = -i\frac{\partial}{\partial\bar{\psi}} , \tag{3.14}$$

which is canonically conjugate to $\bar{\psi}$, i.e.,

$$[I_3, \exp(i\bar{\psi})] = \exp(i\bar{\psi}) . \tag{3.15}$$

Of course, I_3 and $\bar{\psi}$ both commute with all of the original degrees of freedom.

As intimated earlier, the reason for introducing the redundant variable is that it enables one to relate the Villars and BM representations by means of a unitary transformation defined on the extended Hilbert space. Before introducing this transformation, however, it is useful to explicitly display the angular-momentum components in terms of the Euler-angle degrees of freedom. In the immediate context, the conventional *zyz* definition would do perfectly well. On the other hand, as mentioned in Sec. III B, this definition of the Euler angles is unsuitable for the expansion procedure to be outlined later. It will be seen that the ideal definition is the *xyz* definition,[31] in which an arbitrary active rotation R is represented by

$$R = \exp(-i\varphi J_x)\exp(-i\theta J_y)\exp(-i\psi J_z) . \tag{3.16}$$

With this definition, the angle ψ has essentially the same significance as in the conventional definition, describing a rotation about the symmetry axis. For the sake of economy then, the *xyz* definition is adopted forthwith. In the space of these Euler angles, the laboratory components of **J** are represented by the differential operators

$$\begin{aligned} J_x &= -i\frac{\partial}{\partial\varphi} , \\ J_z \pm iJ_y &= -ie^{\mp i\varphi}\left[-\tan\theta\frac{\partial}{\partial\varphi} \pm i\frac{\partial}{\partial\theta} + \frac{i}{\cos\theta}J_3\right] , \end{aligned} \tag{3.17}$$

and the PA components by

$$\begin{aligned} J'_{\pm} &= J_1 \pm iJ_2 = -ie^{\mp i\psi}\left[\frac{1}{\cos\theta}\frac{\partial}{\partial\varphi} \pm i\frac{\partial}{\partial\theta} - i\tan\theta J_3\right] , \\ J_3 &= -i\frac{\partial}{\partial\psi} . \end{aligned} \tag{3.18}$$

In contrast to the standard definition of the Euler angles, there is no problem in expanding (3.17) and (3.18) about $\theta = 0$.

Consider now the following unitary transformation $\mathcal{U}$ defined on the extended Hilbert space:

$$\mathcal{U} = \exp(i\bar{\psi}J_3)\exp(-i\psi I_3) . \tag{3.19}$$

Note that the two factors do not commute, so the order is important. With the properties (3.9) and (3.15) taken into account, elementary calculations give, first of all,

$$\mathcal{U}J_3\mathcal{U}^{\dagger} = I_3 , \tag{3.20}$$

and, for an arbitrary function $f(\psi)$,

$$\mathcal{U}f(\psi)\mathcal{U}^{\dagger} = f(\psi+\bar{\psi}) . \tag{3.21}$$

This transformation has no effect on the other Euler-angle degrees of freedom:

$$\mathcal{U}g\left[\varphi, \frac{\partial}{\partial\varphi}, \theta, \frac{\partial}{\partial\theta}\right]\mathcal{U}^{\dagger} = g\left[\varphi, \frac{\partial}{\partial\varphi}, \theta, \frac{\partial}{\partial\theta}\right] , \tag{3.22}$$

for an arbitrary function g. As a consequence, the only effect of $\mathcal{U}$ on the laboratory components of **J** [Eq. (3.17)] is to replace J_3 by I_3 to give

$$\mathcal{U}J_k\mathcal{U}^{\dagger} = I_k \quad (k = x,y,z) , \tag{3.23}$$

where

$$\begin{aligned} I_x \equiv J_x &= -i\frac{\partial}{\partial\varphi} , \\ I_z \pm iI_y &\equiv -ie^{\mp i\varphi}\left[-\tan\theta\frac{\partial}{\partial\varphi} \pm i\frac{\partial}{\partial\theta} + \frac{i}{\cos\theta}I_3\right] . \end{aligned} \tag{3.24}$$

The effect on the PA components (3.18) is similar, but with an additional phase factor arising from the property (3.21) as follows:

$$\mathcal{U}J'_{\pm}\mathcal{U}^{\dagger} = e^{\mp i\psi}I'_{\pm} = I'_{\pm}e^{\mp i\psi} , \tag{3.25}$$

where

$$I'_{\pm} \equiv I_1 \pm iI_2 = -ie^{\mp i\bar{\psi}}\left[\frac{1}{\cos\theta}\frac{\partial}{\partial\varphi} \pm i\frac{\partial}{\partial\theta} - i\tan\theta I_3\right] . \tag{3.26}$$

In summary, what the transformation $\mathcal{U}$ accomplishes is replacement of the components of **J**, which depend only on the nuclear degrees of freedom, by components of a vector **I** (apart from a possible phase factor) that behaves like an angular momentum, but in which ψ and J_3 have been replaced by the redundant variables $\bar{\psi}$ and I_3, respectively. The operators $\mathcal{K}_{mn}$ and $(t_K^L)_{mn}$, which carry angular momentum along the three-axis and thereby fail to commute with all components of **J**, are easily seen to commute with all components of **I**, as compactly summarized by

$$[\mathcal{K}_{mn}, \mathbf{I}] = 0, \quad [(t_K^L)_{mn}, \mathbf{I}] = 0 . \tag{3.27}$$

Since $\mathcal{K}_{mn}$ and $(t_K^L)_{mn}$ also commute with all Euler angles, they certainly qualify as intrinsic operators with respect to **I**. Moreover, as shown by Eqs. (3.11), these operators also carry an angular momentum along the symmetry axis, with J_3 playing the role of the "intrinsic" angular momentum. In other words, these operators have all the properties necessary for the BM representation.

To clinch the case, it must be shown that the transformation (3.19), in fact, maps operators and state vectors from the Villars to the BM representation. The Hamiltonian (3.5) is easily transformed with the use of Eqs. (3.25) and (3.10) and the the fact that $\mathring{\mathcal{K}}_{mn}$, being an intrinsic operator, is invariant under $\mathcal{U}$. The result is

$$\mathcal{U} H \mathcal{U}^\dagger = \sum_{mn} \mathcal{H}_{mn} \tfrac{1}{2}\{I'^m_-, I'^n_+\} , \tag{3.28}$$

which meets all of the requirements for the BM representation of the Hamiltonian. In the same way, the PA components (3.8) of the spherical tensor are found to transform as follows:

$$\mathcal{U} \hat{T}^L_K \mathcal{U}^\dagger = e^{-iK\psi} T'^L_K = T'^L_K e^{-iK\psi} , \tag{3.29}$$

where

$$T'^L_K = \sum_{mn} (t^L_K)_{mn} \tfrac{1}{2}\{I'^m_-, I'^n_+\} . \tag{3.30}$$

In order to transform the laboratory components of the spherical tensor, it is then only necessary to note that Eq. (3.21) and the property $D^L_{MK}(\varphi,\theta,\psi) = d^L_{MK}(\varphi,\theta) e^{iK\psi}$ [see Eq. (3.49) below] imply

$$\mathcal{U} D^L_{MK}(\varphi,\theta,\psi) \mathcal{U}^\dagger = D^L_{MK}(\varphi,\theta,\bar{\psi}) e^{iK\psi} . \tag{3.31}$$

Therefore, from Eq. (3.7), one obtains the result

$$\mathcal{U} T^L_M \mathcal{U}^\dagger = \sum_{K=-L}^{L} T'^L_K D^L_{MK}(\varphi,\theta,\bar{\psi}) , \tag{3.32}$$

which meets all of the requirements for a spherical tensor in the BM representation. It should be noted that the Euler angle in the rotation matrix is no longer ψ, but rather $\bar{\psi}$.

Finally, consider the state vectors. The introduction of a redundant degree of freedom is inevitably accompanied by spurious states that must be eliminated by a suitable subsidiary condition. Prior to the transformation $\mathcal{U}$, the subspace of physical states may be chosen to satisfy the condition

$$I_3 | \; \rangle = 0 . \tag{3.33}$$

From the definition of $\mathcal{U}$ [Eq. (3.19)] it is easily found that

$$\mathcal{U} I_3 \mathcal{U}^\dagger = I_3 - J_3 . \tag{3.34}$$

Therefore, transformation of (3.33) yields

$$(I_3 - J_3) | \; \rangle' = 0 , \tag{3.35}$$

where $| \; \rangle' \equiv \mathcal{U} | \; \rangle$ are the physical states after the transformation. The condition (3.35) is a well known if somewhat mysterious feature of the BM model. It implies that the physical subspace after the transformation may be spanned by vectors of the form[32]

$$\psi^I_{MK} = D^I_{MK}(\varphi,\theta,\bar{\psi}) \chi_K , \tag{3.36}$$

where χ_K is an intrinsic wave function satisfying $J_3 \chi_K = K \chi_K$, and, of course, $I_3 D^I_{MK}(\varphi,\theta,\bar{\psi}) = K D^I_{MK}(\varphi,\theta,\bar{\psi})$. The state vectors (3.36) are easily understood. Prior to the transformation, they have the form of (3.36), but with $\bar{\psi}=0$, since there can be no dependence on the redundant variable as required by Eq. (3.33). However, the intrinsic part χ_K depends on $e^{iK\psi}$. According to Eq. (3.21), the transformation then generates an extra factor of $e^{iK\bar{\psi}}$, which gets absorbed into the final $D^I_{MK}(\varphi,\theta,\bar{\psi})$.[33] Thus, the demonstration that the transformation $\mathcal{U}$ carries the Villars into the BM representation is complete.

As a final point in this section, it is worthwhile noting that if Λ is an arbitrary intrinsic nuclear operator satisfying

$$[J_3, \Lambda] = K\Lambda , \tag{3.37}$$

then, as is easily shown from the definition of $\mathcal{U}$,

$$\mathcal{U} \Lambda \mathcal{U}^\dagger = e^{iK\bar{\psi}} \Lambda + \lambda(I_3 - J_3) , \tag{3.38}$$

where λ is a function of $I_3 - J_3$ depending on multiple commutators of ψ with Λ. Equation (3.35) shows that in the physical subspace $\lambda = 0$. That is, effectively the transformation gives $\Lambda \rightarrow e^{iK\bar{\psi}} \Lambda = \Lambda e^{iK\bar{\psi}}$. Of course, if $[\psi, \Lambda] = 0$, then λ vanishes identically. This is what happens, for example, in the cases of $\mathcal{H}_{mn}$ and $(t^L_K)_{mn}$.

The insight gained from the preceding analysis is that the chief obstacle discussed in Sec. III B is an artifact arising from the failure to distinguish between the Villars and BM representations. If redundant variables are to be avoided, then it is necessary to work in the Villars representation. If, in addition, the intrinsic excitation operators are chosen so as *not* to commute with J_3, then the Hamiltonian and spherical tensor operators must be written in the forms given by Eqs. (3.12) and (3.13), involving the ψ-dependent exponentials. In applications to even-even nuclei, for example, the coefficients $\mathcal{H}_{mn}$ and $(t^L_K)_{mn}$ would naturally be chosen as functions of the phonons $B_\mu, B^\dagger_\mu$. It is clear from the foregoing analysis that one cannot demand that phonons with $K_\mu \neq 0$, or functions thereof, commute with all components of **J**. However, since the noncommutation can be traced to the J_3 dependence of the operators (3.17) and (3.18), then if the phonons are assumed to satisfy

$$[J_3, B^\dagger_\mu] = K_\mu B^\dagger_\mu , \tag{3.39}$$

one can demand instead certain well-defined commutation rules that follow from Eqs. (3.17), (3.18), and (3.39). Although it is possible to work within a Villars representation including the ψ-dependent exponentials without the need for an explicit choice of ψ [aside from the stipulation (3.9)], it would be more aesthetic to be rid of these exponentials. But that is precisely what the transformation to the BM representation accomplishes. Since this representation, as is now clear, requires the introduction of a redundant degree of freedom, it is an inconvenient representation within which to formulate the MW method directly. However, a two-step approach is quite feasible, in which the MW scheme is first implemented without the redundant variable to derive a Villars representation in the form of Eqs. (3.12) and (3.13). The second step involves applying the unitary transformation $\mathcal{U}$ to pass over to the BM representation. This step is trivial to carry out, in effect amounting to setting $\psi = 0$, and making replacements $J'_\pm \rightarrow I'_\pm$ and $D^L_{MK}(\varphi,\theta,0) \rightarrow D^L_{MK}(\varphi,\theta,\bar{\psi})$. In this way, the goal of reconstructing a BM representation from the generic model can be reached. The next section is devoted to outlining a viable MW scheme for executing the first step.

D. Outline of the MW method for axially symmetric systems

With the choice of the *xyz* convention for the Euler angles, the laboratory components of **J** may be expressed in terms of the Euler angles and Hermitian canonically conjugate momenta p_φ, p_θ, and $p_\psi = J_3$ as follows:

$$J_x = p_\varphi \ , \tag{3.40a}$$

$$J_z \pm iJ_y = -\tan\theta \tfrac{1}{2}\{e^{\mp i\varphi}, p_\varphi\} \pm ie^{\mp i\varphi} p_\theta + e^{\mp i\varphi}\sec\theta J_3 \ , \tag{3.40b}$$

in accord with Eq. (3.17). The first term on the rhs of (3.40b) has been symmetrized to ensure that J_y and J_z are manifestly Hermitian. The momenta p_φ and p_θ must satisfy

$$[\varphi, p_\varphi] = [\varphi, J_x] = i \ , \tag{3.41a}$$

$$[\theta, p_\theta] = i \ , \tag{3.41b}$$

while ψ satisfies (3.9), or, equivalently, $[\psi, J_3] = i$, but, as already emphasized, ψ need not be determined explicitly. All other combinations of pairs from the set $(\varphi, \theta, \psi, p_\varphi, p_\theta, J_3)$ are required to commute.

The first step in the MW scheme is to obtain the expansions of the Euler angles and their canonically conjugate momenta, given the expansions of the laboratory components of **J**, as in the generic model. Now, Eq. (3.40a) defines the expansion of p_φ to be identical to that of J_x. The expansion of φ can then be obtained from the requirement that Eq. (3.41a) be fulfilled order by order commencing with the RPA order. Next, from the pair of Eqs. (3.40b), p_θ is easily derived in the explicit form

$$p_\theta = \frac{i}{4}\{e^{-i\varphi}, J_z - iJ_y\} - \frac{i}{4}\{e^{i\varphi}, J_z + iJ_y\} \ . \tag{3.42}$$

Having obtained the expansion of φ, that of p_θ is then fully determined, and the expansion of θ can subsequently be obtained from Eq. (3.41b). Clearly, the *xyz* representation is very convenient to work with.

In practice, it proves convenient to introduce the complex combinations of Euler angles $\phi_\pm$ defined by

$$\phi_\pm = (\varphi \pm i\theta)/2 \ , \tag{3.43}$$

and the canonically conjugate momenta $p_\pm$, given by

$$p_\pm = p_\varphi \pm i p_\theta \ , \tag{3.44}$$

and satisfying

$$[\phi_\pm, p_\mp] = i, \quad [\phi_\pm, p_\pm] = 0 \ , \tag{3.45}$$

which is equivalent to (3.41). From Eqs. (3.44), (3.40a), and (3.42), one readily finds for $p_\pm$ the expansion

$$p_\pm = p_\pm^{(1)} + p_\pm^{(2)} + p_\pm^{(3)} + \cdots \ , \tag{3.46}$$

where

$$p_\pm^{(1)} = J_\pm^{(1)}, \quad p_\pm^{(2)} = J_\pm^{(2)} \ , \tag{3.47}$$

$$p_\pm^{(3)} = J_\pm^{(3)} \pm \frac{i}{2}\{\phi_+^{(1)} + \phi_-^{(1)}, J_z\} \mp \tfrac{1}{4}(\phi_+^{(1)} + \phi_-^{(1)})^2 (J_+^{(1)} - J_-^{(1)}) \ .$$

Thus, $p_\pm$ first differs from $J_\pm$ in the cubic terms.

Once the expansions of $\phi_\pm$ and $p_\pm$ have been determined, those of B_μ and $B_\mu^\dagger$ can be obtained straightforwardly from the conditions

$$[B_\mu, \phi_\pm] = 0, \quad [B_\mu, p_\pm] = 0 \text{ (and H.c. eqs.)} \ , \tag{3.48a}$$

$$[B_\mu, B_\nu^\dagger] = \delta_{\mu\nu}, \quad [B_\mu, B_\nu] = 0 \text{ (and H.c. eq.)} \ . \tag{3.48b}$$

It should be mentioned that Eqs. (3.48a) are the main ones, with (3.48b) being weak conditions. Note also that (3.48) does not require that the phonons commute with all the components of **J**, which, as already emphasized, is impossible.

It has been seen that starting with the set of RPA variables $(\phi_\pm^{(1)}, J_\pm^{(1)}, B_\mu^{(1)}, B_\mu^{(1)\dagger})$, one may generate a new set of variables $(\phi_\pm, p_\pm, B_\mu, B_\mu^\dagger)$ that is expressed as an expansion in the RPA set. The momenta $p_\pm$ are ultimately to be eliminated in favor of the PA components of **J** with the help of Eqs. (3.44), (3.42), (3.40a), and the inverse of (3.6). In connection with Eq. (3.6), and also for treating spherical tensor operators [Eq. (3.7)], it is also useful to expand the rotation matrices, which in the *xyz* representation are given by

$$D^I_{MK}(\varphi,\theta,\psi) = \langle IK \mid \exp(i\psi J_z)\exp(i\theta J_y)\exp(i\varphi J_x) \mid IM \rangle$$
$$= e^{iK\psi}\langle IK \mid \exp(i\theta J_y)\exp(i\varphi J_x) \mid IM \rangle \ , \tag{3.49}$$

where $\mid IM \rangle$ denotes a simultaneous eigenvector of J^2 and J_z. The factor of $e^{iK\psi}$ in (3.49) is what gives rise to the ψ-dependent exponentials in the Villars representation after transformation to the final variables.

The techniques that may be used for generating the expansions of the new variables are essentially the same as in the case of two-dimensional rotation.[3,4] These consist of the *commutator* and the *formal unitary transformation* methods. The discussion thus far has been based on the first method, in which the commutator relations are solved order by order. To give a more specific example, upon expansion of $\phi_\pm$,

$$\phi_\pm = \phi_\pm^{(1)} + \phi_\pm^{(2)} + \cdots + \phi_\pm^{(n)} + \cdots \ , \tag{3.50}$$

the first of Eqs. (3.45) gives rise to the hierarchy of equations

$$[\phi_\pm^{(1)}, p_\mp^{(1)}] = i \ ,$$
$$[\phi_\pm^{(2)}, p_\mp^{(1)}] + [\phi_\pm^{(1)}, p_\mp^{(2)}] = 0, \ \ldots \ , \tag{3.51}$$
$$\sum_{k=1}^{n} [\phi_\pm^{(k)}, p_\mp^{(n-k+1)}] = 0 \ .$$

This is a sequence of recurrence relations for $\phi_\pm^{(n)}$ in terms of its lower orders, with $p_\mp^{(k)}$ given by (3.47). Since these are just linear inhomogeneous equations, they are quite straightforward to solve. Note, however, that there is an arbitrariness in the solutions. Any solution $\phi_\pm^{(n)}$ may be augmented by an arbitrary nth-order polynomial that commutes with $p_\mp^{(1)} = J_\mp^{(1)}$; in other words, a function of $J_\pm^{(1)}$, $B_\mu^{(1)}$, and $B_\mu^{(1)\dagger}$. A similar arbitrariness occurs in the solution of Eqs. (3.48) for B_μ, using the expansion

$$B_\mu = B_\mu^{(1)} + B_\mu^{(2)} + \cdots + B_\mu^{(n)} + \cdots \ , \tag{3.52}$$

where any solution for $B_\mu^{(n)}$ can be augmented by an arbitrary nth-order polynomial in $B_\mu^{(1)}$ and $B_\mu^{(1)\dagger}$. The significance of this arbitrariness is easily understood. It provides the freedom to construct the final variables in accordance with the desired form of the Hamiltonian; for example, to choose H to be diagonal (to a given accuracy in the expansion parameter Ω). This arbitrariness may also be exploited to guarantee that the phonons carry good angular momentum along the symmetry axis. This means that J_3 is required to take the form

$$J_3=\sum_\mu K_\mu B_\mu^\dagger B_\mu \ . \tag{3.53}$$

For further discussion, see Sec. IV D below.

The commutator technique, while perfectly straightforward, has the disadvantage of requiring in each order the solution of separate equations for $\phi_+^{(n)}$ and $B_\mu^{(n)}$. This can be avoided by using the formal unity transformation method, which has the added advantage of easy inversion of the expansions. The applicability of this method is based on the fact that the set of final variables $(\phi_\pm,p_\pm,B_\mu,B_\mu^\dagger)$ and the set of RPA variables $(\phi_\pm^{(1)},J_\pm^{(1)},B_\mu^{(1)},B_\mu^{(1)\dagger})$ involve the same mutual commutation relations, allowing the possibility of connecting the two sets by a canonical transformation. Specifically, the procedure is to seek a formal unitary transformation $\exp(iS)$ such that

$$\exp(iS)J_\pm^{(1)}\exp(-iS)=p_\pm^{(1)}+p_\pm^{(2)}+p_\pm^{(3)}+\cdots \ , \tag{3.54}$$

where the rhs is given by Eqs. (3.47). The generator has an expansion commencing with cubic polynomial terms:

$$S=S^{(3)}+S^{(4)}+\cdots \ . \tag{3.55}$$

With Eqs. (3.47) taken into account, Eq. (3.54) in the first two orders leads to the following linear inhomogeneous equations:

$$[iS^{(3)},J_\pm^{(1)}]=J_\pm^{(2)} \ , \tag{3.56}$$

$$[iS^{(4)},J_\pm^{(1)}]=-\tfrac{1}{2}[iS^{(3)},J_\pm^{(2)}]+J_\pm^{(3)}\pm\frac{i}{2}\{\phi_+^{(1)}+\phi_-^{(1)},J_z\}$$
$$\mp\tfrac{1}{4}(\phi_+^{(1)}+\phi_-^{(1)})^2(J_+^{(1)}-J_-^{(1)}) \ . \tag{3.57}$$

The solutions for $S^{(n)}$ are arbitrary to the extent that any solution may be augmented by an arbitrary nth-order polynomial function of $J_\pm^{(1)}$, $B_\mu^{(1)}$, and $B_\mu^{(1)\dagger}$, all of which commute with $J_\pm^{(1)}$. This arbitrariness is entirely equivalent to that occurring in the commutator approach.

Once the expansion of S has been found, the expansions of $\phi_\pm$, B_μ, and $B_\mu^\dagger$ can be generated directly by applying the unitary transformation to the corresponding RPA variables as follows:

$$\begin{aligned}&\phi_\pm=\exp(iS)\phi_\pm^{(1)}\exp(-iS)=\phi_\pm^{(1)}+[iS^{(3)},\phi_\pm^{(1)}]+\cdots \ ,\\ &B_\mu=\exp(iS)B_\mu^{(1)}\exp(-iS)\\ &\quad=B_\mu^{(1)}+[iS^{(3)},B_\mu^{(1)}]+\cdots \ \text{(and H.c. Eq.)} \ .\end{aligned} \tag{3.58}$$

Because of the unitary transformation, it follows immediately that the final variables must satisfy the same commutation relations as in the commutator method. It is then clear that Eqs. (3.58) satisfy the definition of $\phi_\pm$, B_μ, and $B_\mu^\dagger$. In practice, there is no need to generate the final degrees of freedom separately, since H and transition operators can be transformed directly using the inverse unitary transformation.

As a final point, the unitary transformation method exposes an apparent technical difficulty. On the one hand, Eq. (3.54) implies

$$\exp(iS)J_x^{(1)}\exp(-iS)=J_x^{(1)}+J_x^{(2)}+J_x^{(3)}+\cdots \ . \tag{3.59}$$

On the other hand, since $J_x^{(1)}$ has a continuous spectrum, while J_x has a discrete spectrum, no unitary transformation exists such that

$$\exp(iS)J_x^{(1)}\exp(-iS)=J_x \ .$$

This difficulty also occurs in the case of two-dimensional rotation. Nevertheless, there is no problem in finding an expansion of S satisfying (3.59). What one has is a *formal* unitary transformation that transforms $J_x^{(1)}$ not into J_x, but rather into an *expansion* of J_x. All of the expansions, including those of J_x and $\exp(iS)$, contain nonconvergent parts that arise from improperly treating the angular degrees of freedom as small quantities. The "nonexistence' of the unitary transformation shows up in the nonconvergence of the formal expansion of $\exp(iS)$. Nevertheless, the final reconstituted forms for H and transition operators are in no way improper since they are free of any small-angle expansions, as will be seen. The nonconvergent Taylor expansions are simply formal intermediate devices used to identify coefficients in a legitimate expansion. One might say that the effect of the improper parts of the formal unitary transformation is to cancel the improper parts introduced by the original boson expansion.

IV. APPLICATION OF THE MW METHOD TO THE GENERIC MODEL

In this section, the MW method outlined in Sec. III D will be applied to the generic model. The technique utilizing the formal unitary transformation is chosen for brevity. From Eqs. (3.54) and (3.58), the effect of this transformation on any operator function of the RPA variables $F(J_\pm^{(1)},\phi_\pm^{(1)},B_\mu^{(1)},B_\mu^{(1)\dagger})$ is given by

$$\begin{aligned}\widetilde{F}\equiv&\exp(iS)F(J_\pm^{(1)},\phi_\pm^{(1)},B_\mu^{(1)},B_\mu^{(1)\dagger})\\ &\times\exp(-iS)=F(p_\pm,\phi_\pm,B_\mu,B_\mu^\dagger) \ ,\end{aligned} \tag{4.1}$$

i.e., each RPA variable is replaced by its transform: $\widetilde{J}_\pm^{(1)}=p_\pm$, $\widetilde{\phi}_\pm^{(1)}=\phi_\pm$, $\widetilde{B}_\mu^{(1)}=B_\mu$, $\widetilde{B}_\mu^{(1)\dagger}=B_\mu^\dagger$, and, of course,

$$\widetilde{S}=\widetilde{S}^{(3)}+\widetilde{S}^{(4)}+\cdots=S=S^{(3)}+S^{(4)}+\cdots \ . \tag{4.2}$$

By inversion, the original operator F may be expressed in terms of the final variables as follows:

$$\begin{aligned}F=&\exp(-iS)\widetilde{F}\exp(iS)\\ =&F(p_\pm,\phi_\pm,B_\mu,B_\mu^\dagger)-[i\widetilde{S}^{(3)},F(p_\pm,\phi_\pm,B_\mu,B_\mu^\dagger)]+\cdots \ .\end{aligned} \tag{4.3}$$

In particular, the Hamiltonian expanded through quartic terms is given by

$$H=E^{(0)}+H'^{(2)}+H'^{(3)}+H'^{(4)}+\cdots\ , \tag{4.4}$$

where

$$H'^{(2)}=\tilde{H}^{(2)}\ , \tag{4.5a}$$

$$H'^{(3)}=\tilde{H}^{(3)}-[i\tilde{S}^{(3)},\tilde{H}^{(2)}]\ , \tag{4.5b}$$

$$H'^{(4)}=\tilde{H}^{(4)}-[i\tilde{S}^{(4)},\tilde{H}^{(2)}]-[i\tilde{S}^{(3)},\tilde{H}^{(3)}]+\tfrac{1}{2}[i\tilde{S}^{(3)},[i\tilde{S}^{(3)},\tilde{H}^{(2)}]]\ . \tag{4.5c}$$

The next task is to find $\tilde{S}^{(3)}$ and $\tilde{S}^{(4)}$.

A. Solving for $\tilde{S}^{(3)}$ and $\tilde{S}^{(4)}$

Solving the linear inhomogeneous equations (3.56) and (3.57) for $S^{(3)}$ and $S^{(4)}$ is trivial, involving, apart from factors of i, partial integration of the rhs with respect to the variables $\phi_+^{(1)}$ and $\phi_-^{(1)}$. Application of Eq. (4.1) then immediately yields $\tilde{S}^{(3)}$ and $\tilde{S}^{(4)}$.[35] For $\tilde{S}^{(3)}$, the following result is obtained:

$$\begin{aligned}i\tilde{S}^{(3)}=&-\tfrac{1}{2}i[\{\phi_-,p_+\}+\{\phi_+,p_-\}]\sum_\mu j^{(2)}(10)_\mu(B_\mu^\dagger+B_\mu)-\left[i\phi_-p_-\sum_\mu j^{(2)}(10)'_\mu(B_\mu^\dagger+B_{-\mu})-\text{H.c.}\right]\\&+\phi_+\phi_-\sum_\mu j^{(2)}(01)_\mu(B_\mu^\dagger-B_\mu)+\left[\tfrac{1}{2}\phi_-^2\sum_\mu j^{(2)}(01)'_\mu(B_\mu^\dagger-B_{-\mu})-\text{H.c.}\right]\\&-i\phi_-\sum_{\mu\nu}[j^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}j^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger-B_{-\nu}B_{-\mu})]-\text{H.c.}+i\tilde{\sigma}^{(3)}(p_+,p_-,B_\mu,B_\mu^\dagger)\ ,\end{aligned} \tag{4.6}$$

where $\tilde{\sigma}^{(3)}$ is an arbitrary Hermitian cubic polynomial function of its arguments, in accordance with the discussion in Sec. III D.

In the case of $\tilde{S}^{(4)}$, only a limited subset of contributions is actually needed to evaluate the leading-order corrections to the RPA. This abbreviation is consistent with that for $H^{(4)}$ [Eq. (2.22)] and $J_\pm^{(3)}$ [Eq. (2.24)]. The point here is that only the diagonal contributions of $H'^{(4)}$ are needed, these being of the same order as the off-diagonal contributions arising from $H'^{(3)}$ in second-order perturbation theory. Among the "dispensable" terms are some $\phi_\pm$-dependent ones whose contributions to H ultimately cancel [see the discussion in connection with Eq. (4.16) below]. At any rate, the (transformed) solution of Eq. (3.57) is

$$\begin{aligned}i\tilde{S}^{(4)}=&-\tfrac{1}{2}i\{\phi_-,p_+\}\left\{j^{(3)}(10)-\tfrac{1}{2}\sum_\mu j^{(3)}(10)_{\mu\mu}\right.\\&\left.-\tfrac{1}{2}\sum_{\mu\nu}[2j^{(3)}(10)_{\mu\nu}+2j^{(2)}(10)_\mu j^{(2)}(10)_\nu+j^{(2)}(10)'_\mu j^{(2)}(10)'_\nu+j^{(2)}(10)'_{-\mu}j^{(2)}(10)'_{-\nu}](B_\mu^\dagger B_\nu+\tfrac{1}{2}\delta_{\mu\nu})\right\}\\&-\tfrac{1}{2}ij^{(3)}(30)\{\phi_-,p_-p_+^2\}-\text{H.c. of all terms}+\text{dispensable terms}+i\tilde{\sigma}^{(4)}(p_+,p_-,B_\mu,B_\mu^\dagger)\ ,\end{aligned} \tag{4.7}$$

where $\tilde{\sigma}^{(4)}$ is an arbitrary Hermitian quartic polynomial function of its arguments.

B. Treatment of the Hamiltonian

Returning to the expansion of H in terms of the variables $\phi_\pm$, $p_\pm$, B_μ, and $B_\mu^\dagger$ [Eq. (4.4)], one obtains, first of all, from Eqs. (4.5a), (4.1), and (2.7),

$$H'^{(2)}=E^{(2)}+\sum_\mu\hbar\omega_\mu B_\mu^\dagger B_\mu+\frac{\hbar^2}{2\mathcal{I}_0}p_+p_-\ . \tag{4.8}$$

From angular-momentum conservation, it follows that $H'^{(3)}$ is independent of the angle variables $\phi_\pm$. That this is indeed the case may be easily seen by calculating the commutator $[H'^{(3)},p_\pm]$. From Eq. (4.5b) and the Jacobi identity, one obtains

$$[H'^{(3)},p_\pm]=[\tilde{H}^{(3)},p_\pm]-[i\tilde{S}^{(3)},[\tilde{H}^{(2)},p_\pm]]+[\tilde{H}^{(2)},[i\tilde{S}^{(3)},p_\pm]]\ . \tag{4.9}$$

The second contribution on the rhs vanishes since the transform of the RPA conservation law (2.4) is just $[\tilde{H}^{(2)},p_\pm]=0$. Furthermore, in the last term on the rhs, the transform of Eq. (3.56), namely, $[i\tilde{S}^{(3)},p_\pm]=\tilde{J}_\pm^{(2)}$, may be substituted to give

$$[H'^{(3)},p_\pm]=[\tilde{H}^{(3)},p_\pm]+[\tilde{H}^{(2)},\tilde{J}_\pm^{(2)}]=0\ , \tag{4.10}$$

which vanishes because the result is just the transform of the higher-order angular-momentum conservation law (2.5) for $n=3$. The $\phi_\pm$ independence of $H'^{(3)}$ can also be obtained with a little more effort by direct evaluation of (4.5b), using Eqs. (2.21), which are equivalent to (2.5) for the case when $n=3$.

The considerations thus far have been independent of the arbitrary functions $\tilde{\sigma}^{(3)}$ and $\tilde{\sigma}^{(4)}$. However, the dependence of $H'^{(3)}$ on $p_\pm$, B_μ, and $B_\mu^\dagger$ is a consequence of the choice of these functions. Now, in principle, the final physical results are invariant under unitary transformations, and therefore should not depend on the choice of the arbitrary functions. As discussed earlier, the arbitrary functions allow one to shape the final form of the Hamiltonian. However, if these functions are set equal to zero,

nothing is lost, since additional unitary transformations can be performed afterwards to achieve any desired final form. Therefore, for the time being, the simple choice

$$\tilde{\sigma}^{(3)}=0, \quad \tilde{\sigma}^{(4)}=0 \tag{4.11}$$

is made. The consequences of some other possible choices are briefly discussed in Sec. IV D.

The evaluation of $H'^{(3)}$ [Eq. (4.5b)] is quite straightforward with the use of the transform of Eq. (2.16) for $\tilde{H}^{(3)}$, as well as (4.6) with $\tilde{\sigma}^{(3)}=0$ and (4.8). The somewhat tedious calculation is alleviated by not keeping track of $\phi_{\pm}$-dependent terms, since these must cancel according to Eq. (4.10). The final result is

$$\begin{aligned} H'^{(3)}=&\tfrac{1}{2}\sum_{\mu\nu\lambda} h^{(3)}(00)_{\mu\nu\lambda}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}B_{\lambda}+B^{\dagger}_{\lambda}B_{\nu}B_{\mu})+\sum_{\mu} h^{(3)}(00)_{\mu}(B^{\dagger}_{\mu}+B_{\mu}) \\ &+\tfrac{1}{6}\sum_{\mu\nu\lambda} h^{(3)}(00)'_{\mu\nu\lambda}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}B^{\dagger}_{\lambda}+B_{\lambda}B_{\nu}B_{\mu})+\left[p_{-}\sum_{\mu\nu}\Gamma^{(3)}(10)_{\mu\nu}B^{\dagger}_{\mu}B_{\nu}+\text{H.c.}\right] \\ &+\tfrac{1}{2}p_{-}\sum_{\mu\nu}\Gamma^{(3)}(10)'_{\mu\nu}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}-B_{-\nu}B_{-\mu})+\text{H.c.} \\ &+p_{+}p_{-}\sum_{\mu}\Gamma^{(3)}(20)_{\mu}(B^{\dagger}_{\mu}+B_{\mu})+\left[p^{2}_{-}\sum_{\mu}\Gamma^{(3)}(20)'_{\mu}(B^{\dagger}_{\mu}+B_{-\mu})+\text{H.c.}\right], \end{aligned} \tag{4.12}$$

where

$$\Gamma^{(3)}(10)_{\mu\nu}\equiv h^{(3)}(10)_{\mu\nu}-\frac{\hbar^2}{2\mathscr{I}_0}j^{(2)}(00)_{\mu\nu}, \tag{4.13a}$$

$$\Gamma^{(3)}(10)'_{\mu\nu}\equiv h^{(3)}(10)'_{\mu\nu}-\frac{\hbar^2}{2\mathscr{I}_0}j^{(2)}(00)'_{\mu\nu}, \tag{4.13b}$$

$$\Gamma^{(3)}(20)_{\mu}\equiv h^{(3)}(20)_{\mu}-\frac{\hbar^2}{2\mathscr{I}_0}j^{(2)}(10)_{\mu}, \tag{4.13c}$$

$$\Gamma^{(3)}(20)'_{\mu}\equiv h^{(3)}(20)'_{\mu}-\frac{\hbar^2}{2\mathscr{I}_0}j^{(2)}(10)'_{\mu}. \tag{4.13d}$$

Consider next the evaluation of $H'^{(4)}$ [Eq. (4.5c)], which carries a $\phi_{\pm}$ dependence, unlike $H'^{(3)}$. This is because H so far has been expressed in terms of $p_{\pm}$ rather than the PA components of the angular momentum. It will be shown that the introduction of the latter eliminates the explicit $\phi_{\pm}$ dependence. Although the angular dependence of $H'^{(4)}$ may be calculated by retaining all $\phi_{\pm}$-dependent terms in $\tilde{S}^{(4)}$ and the other operators entering into Eq. (4.5c), it is much less tedious to separately calculate the commutator $[H'^{(4)},p_{\pm}]$ and use (4.5c) only for the $\phi_{\pm}$-independent terms. Using the Jacobi identity, the transforms of the angular-momentum conservation equations (2.4), (2.5) ($n=3,4$), and (2.6) ($n=2$), and also the transforms of Eqs. (3.56) and (3.57), one may derive the result

$$\begin{aligned}[H'^{(4)},p_{\pm}]=&\pm\frac{i}{2}\{[H'^{(2)},\phi_{+}+\phi_{-}],\tilde{J}_z\} \\ &\mp\tfrac{1}{4}[H'^{(2)},(\phi_{+}+\phi_{-})^2](p_{+}-p_{-}), \end{aligned} \tag{4.14}$$

which may be evaluated further with the aid of Eqs. (4.8) and the transform of (2.14) to yield the explicit expression

$$\begin{aligned}[H'^{(4)},p_{\pm}]=&\pm\frac{\hbar^2}{2\mathscr{I}_0}\left[(p_{+}+p_{-})\sum_{\mu}K_{\mu}B^{\dagger}_{\mu}B_{\mu}\right. \\ &\left.+\frac{i}{4}\{\phi_{+}-\phi_{-},(p_{+}+p_{-})^2\}\right]. \end{aligned} \tag{4.15}$$

The $\phi_{\pm}$-dependent terms of $H'^{(4)}$ are then obtained by solving Eq. (4.15). The expression for $H'^{(4)}$ including only terms of interest to the given order is

$$\begin{aligned} H'^{(4)}=&E^{(4)}+\tfrac{1}{2}\sum_{\mu\nu}\Gamma^{(4)}(00)_{\mu\nu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})(B^{\dagger}_{\nu}B_{\nu}+\tfrac{1}{2})+\sum_{\mu}\Gamma^{(4)}(00)_{\mu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})+\Gamma^{(4)}(20)p_{+}p_{-}+\Gamma^{(4)}(40)p^{2}_{+}p^{2}_{-} \\ &+p_{+}p_{-}\sum_{\mu}\Gamma^{(4)}(20)_{\mu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})+\text{off-diagonal terms}+\frac{\hbar^2}{2\mathscr{I}_0}\left[\theta^2p^2_{\varphi}-2\theta p_{\varphi}\sum_{\mu}K_{\mu}B^{\dagger}_{\mu}B_{\mu}-\tfrac{1}{2}\right], \end{aligned} \tag{4.16}$$

where the last term originates from the solution of Eq. (4.15) [after the substitution of Eqs. (3.43) and (3.44) for aesthetic reasons]. In Eq. (4.16), only the diagonal terms, which are of order Ω^{-1} relative to the RPA, have been retained, whereas the off-diagonal terms, which lead to corrections of relative order Ω^{-2}, have been suppressed. In addition to the constant $E^{(4)}$, which is of no intrinsic interest in the present context, the remaining coefficients in (4.16) may be expressed in terms of the original coefficients as follows:

$$\Gamma^{(4)}(00)_{\mu\nu}\equiv\tfrac{1}{2}h^{(4)}(00)_{\mu\nu,\mu\nu}-2j^{(2)}(00)_{\mu\nu}h^{(3)}(10)_{\mu\nu}$$
$$-2j^{(2)}(00)_{\nu\mu}h^{(3)}(10)_{\nu\mu}-j^{(2)}(00)'_{\mu\nu}h^{(3)}(10)'_{\mu\nu}-j^{(2)}(00)'_{-\mu-\nu}h^{(3)}(10)'_{-\mu-\nu}$$
$$+\frac{\hbar^2}{4\mathscr{I}_0}\{4[j^{(2)}(00)_{\mu\nu}]^2+[j^{(2)}(00)'_{\mu\nu}]^2+[j^{(2)}(00)'_{-\mu-\nu}]^2\}\ , \tag{4.17a}$$

$$\Gamma^{(4)}(00)_{\mu}\equiv h^{(4)}(00)_{\mu\mu}-\tfrac{1}{2}\sum_{\nu}h^{(4)}(00)_{\mu\nu,\mu\nu}+\frac{\hbar^2}{2\mathscr{I}_0}\{2[j^{(2)}(10)_{\mu}]^2-2j^{(3)}(10)_{\mu\mu}+[j^{(2)}(10)'_{\mu}]^2+[j^{(2)}(10)'_{-\mu}]^2\}\ , \tag{4.17b}$$

$$\Gamma^{(4)}(20)\equiv h^{(4)}(20)-\tfrac{1}{2}\sum_{\mu}h^{(4)}(20)_{\mu\mu}\ , \tag{4.17c}$$

$$\Gamma^{(4)}(40)\equiv h^{(4)}(40)-\frac{\hbar^2}{\mathscr{I}_0}j^{(3)}(30)\ , \tag{4.17d}$$

$$\Gamma^{(4)}(20)_{\mu}\equiv h^{(4)}(20)_{\mu\mu}-4j^{(2)}(10)_{\mu}h^{(3)}(20)_{\mu}-4j^{(2)}(10)'_{\mu}h^{(3)}(20)'_{\mu}-4j^{(2)}(10)'_{-\mu}h^{(3)}(20)'_{-\mu}$$
$$+\frac{\hbar^2}{\mathscr{I}_0}\{2[j^{(2)}(10)_{\mu}]^2+[j^{(2)}(10)'_{\mu}]^2+[j^{(2)}(10)'_{-\mu}]^2\}\ . \tag{4.17e}$$

The next task is to replace $p_{\pm}$ in H by the PA components of angular momentum. Beginning with the identity

$$J_1^2+J_2^2+J_3^2=J_x^2+J_y^2+J_z^2\ ,$$

substituting on the rhs from Eqs. (3.40), and expanding in powers of the Euler angles, one may readily arrive at the result

$$J_1^2+J_2^2=\tfrac{1}{2}\{J'_+,J'_-\}\cong p_+p_-+\theta^2p_\varphi^2-2\theta p_\varphi J_3-\tfrac{1}{2}\ . \tag{4.18}$$

This result is valid through quartic terms. After multiplying Eq. (4.18) across by $\hbar^2/(2\mathscr{I}_0)$, it is seen that the rhs accounts for the rotational term in $H'^{(2)}$ [Eq. (4.8)] and also for the last Euler-angle-dependent term in $H'^{(4)}$ [Eq. (4.16)]. That is, these two contributions to H may be replaced to the given order by the single contribution

$$\frac{\hbar^2}{2\mathscr{I}_0}(J_1^2+J_2^2)\ ,$$

provided that the identification of J_3 given by Eq. (3.53) is valid, as is shown to be the case in Sec. IV C. This replacement then removes the angle dependence in $H'^{(4)}$. In general, as mentioned earlier, $p_{\pm}$ can be related to the laboratory components of J using Eqs. (3.40a) and (3.42), and subsequently to the PA components through the inverse of Eqs. (3.6). It is then not difficult to show that

$$p_{\pm}\cong\exp(\pm i\psi)J'_{\pm}+\text{cubic terms}$$
$$=J'_{\pm}\exp(\pm i\psi)+(\text{cubic terms})'\ , \tag{4.19}$$

where the $\exp(\pm i\psi)$ dependence arises from the rotation matrix in Eq. (3.6). Since H is expanded only through quartic terms, substitution of (4.19) in $H'^{(3)}$ and $H'^{(4)}$ does not require the use of the cubic terms, i.e., effectively one makes the replacement $p_{\pm}\rightarrow\exp(\pm i\psi)J'_{\pm}\cong J'_{\pm}\exp(\pm i\psi)$.[36,37] With the elimination of $p_{\pm}$ in favor of the PA components of J, H may finally be written as the expansion

$$H=E^{(0)}+H''^{(2)}+H''^{(3)}+H''^{(4)}+\cdots\ , \tag{4.20}$$

where

$$H''^{(2)}=E^{(2)}+\sum_{\mu}\hbar\omega_{\mu}B_{\mu}^{\dagger}B_{\mu}+\frac{\hbar^2}{2\mathscr{I}_0}(J_1^2+J_2^2)\ , \tag{4.21a}$$

$$H''^{(3)}=\tfrac{1}{2}\sum_{\mu\nu\lambda}h^{(3)}(00)_{\mu\nu\lambda}(B_{\mu}^{\dagger}B_{\nu}^{\dagger}B_{\lambda}+B_{\lambda}^{\dagger}B_{\nu}B_{\mu})+\sum_{\mu}h^{(3)}(00)_{\mu}(B_{\mu}^{\dagger}+B_{\mu})+\tfrac{1}{6}\sum_{\mu\nu\lambda}h^{(3)}(00)'_{\mu\nu\lambda}(B_{\mu}^{\dagger}B_{\nu}^{\dagger}B_{\lambda}^{\dagger}+B_{\lambda}B_{\nu}B_{\mu})$$
$$+J'_-e^{-i\psi}\sum_{\mu\nu}[\Gamma^{(3)}(10)_{\mu\nu}B_{\mu}^{\dagger}B_{\nu}+\tfrac{1}{2}\Gamma^{(3)}(10)'_{\mu\nu}(B_{\mu}^{\dagger}B_{\nu}^{\dagger}-B_{-\nu}B_{-\mu})]+\text{H.c.}$$
$$+(J_1^2+J_2^2)\sum_{\mu}\Gamma^{(3)}(20)_{\mu}(B_{\mu}^{\dagger}+B_{\mu})+J'^2_-e^{-2i\psi}\sum_{\mu}\Gamma^{(3)}(20)'_{\mu}(B_{\mu}^{\dagger}+B_{-\mu})+\text{H.c.}\ , \tag{4.21b}$$

$$H''^{(4)}=E^{(4)}+\tfrac{1}{2}\sum_{\mu\nu}\Gamma^{(4)}(00)_{\mu\nu}(B_{\mu}^{\dagger}B_{\mu}+\tfrac{1}{2})(B_{\nu}^{\dagger}B_{\nu}+\tfrac{1}{2})+\sum_{\mu}\Gamma^{(4)}(00)_{\mu}(B_{\mu}^{\dagger}B_{\mu}+\tfrac{1}{2})$$
$$+\Gamma^{(4)}(20)(J_1^2+J_2^2)+\Gamma^{(4)}(40)(J_1^2+J_2^2)^2+(J_1^2+J_2^2)\sum_{\mu}\Gamma^{(4)}(20)_{\mu}(B_{\mu}^{\dagger}B_{\mu}+\tfrac{1}{2})+\text{off-diagonal terms}\ . \tag{4.21c}$$

The Hamiltonian to the given order is now in the form of the Villars representation (3.12).

The final step in the reconstruction of the Hamiltonian is the application of the unitary transformation (3.19) in order to pass over to the BM representation. Thus, in accordance with the discussion in Sec. III C, the transition from the Villars representation given by Eqs. (4.20) and (4.21) to the BM representation is immediate:

$$H_{\rm BM}=\mathscr{U}H\mathscr{U}^{\dagger}=E^{(0)}+H^{(2)}_{\rm BM}+H^{(3)}_{\rm BM}+H^{(4)}_{\rm BM}+\cdots\ , \tag{4.22}$$

where

$$H^{(2)}_{\rm BM}=E^{(2)}+\sum_{\mu}\hbar\omega_{\mu}B^{\dagger}_{\mu}B_{\mu}+\frac{\hbar^2}{2\mathscr{I}_0}(I_1^2+I_2^2)\ , \tag{4.23a}$$

$$\begin{aligned}H^{(3)}_{\rm BM}=&\tfrac{1}{2}\sum_{\mu\nu\lambda}h^{(3)}(00)_{\mu\nu\lambda}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}B_{\lambda}+B^{\dagger}_{\lambda}B_{\nu}B_{\mu})+\sum_{\mu}h^{(3)}(00)_{\mu}(B^{\dagger}_{\mu}+B_{\mu})+\tfrac{1}{6}\sum_{\mu\nu\lambda}h^{(3)}(00)'_{\mu\nu\lambda}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}B^{\dagger}_{\lambda}+B_{\lambda}B_{\nu}B_{\mu})\\&+I'_{-}\sum_{\mu\nu}[\Gamma^{(3)}(10)_{\mu\nu}B^{\dagger}_{\mu}B_{\nu}+\tfrac{1}{2}\Gamma^{(3)}(10)'_{\mu\nu}(B^{\dagger}_{\mu}B^{\dagger}_{\nu}-B_{-\nu}B_{-\mu})]+\text{H.c.}+(I_1^2+I_2^2)\sum_{\mu}\Gamma^{(3)}(20)_{\mu}(B^{\dagger}_{\mu}+B_{\mu})\\&+I'^{2}_{-}\sum_{\mu}\Gamma^{(3)}(20)'_{\mu}(B^{\dagger}_{\mu}+B_{-\mu})+\text{H.c.}\ ,\end{aligned} \tag{4.23b}$$

$$\begin{aligned}H^{(4)}_{\rm BM}=&E^{(4)}+\tfrac{1}{2}\sum_{\mu\nu}\Gamma^{(4)}(00)_{\mu\nu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})(B^{\dagger}_{\nu}B_{\nu}+\tfrac{1}{2})+\sum_{\mu}\Gamma^{(4)}(00)_{\mu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})\\&+\Gamma^{(4)}(20)(I_1^2+I_2^2)+\Gamma^{(4)}(40)(I_1^2+I_2^2)^2+(I_1^2+I_2^2)\sum_{\mu}\Gamma^{(4)}(20)_{\mu}(B^{\dagger}_{\mu}B_{\mu}+\tfrac{1}{2})+\text{off-diagonal terms}\ .\end{aligned} \tag{4.23c}$$

Further discussion of the perturbative treatment of the Hamiltonian is deferred to Sec. IV D.

C. Diagonalization of J_3

In this subsection it is shown that the condition $J_3=\sum_{\mu}K_{\mu}B^{\dagger}_{\mu}B_{\mu}$ [Eq. (3.53)] can always be satisfied, at least to the order of interest. From Eq. (3.6), J_3 is given by

$$J_3=\sum_{M=-1}^{1}D^{1\dagger}_{M0}(\varphi,\theta,\psi)J_M=\sin\theta J_x-\sin\varphi\cos\theta J_y+\cos\varphi\cos\theta J_z\ , \tag{4.24}$$

where the second form on the rhs can easily be obtained by solving the pair of Eqs. (3.40b) for J_3. Upon expanding J_3 through quartic terms, one obtains

$$J_3=J_3^{(2)}+J_3^{(3)}+J_3^{(4)}+\cdots\ , \tag{4.25}$$

where

$$J_3^{(2)}=J_z-i\phi_+^{(1)}J_-^{(1)}+i\phi_-^{(1)}J_+^{(1)}=\sum_{\mu}K_{\mu}B^{(1)\dagger}_{\mu}B^{(1)}_{\mu}\ , \tag{4.26a}$$

$$J_3^{(3)}=-i(\phi_+p_--\phi_-p_+)^{(3)}\ , \tag{4.26b}$$

$$\begin{aligned}J_3^{(4)}=&-i(\phi_+p_--\phi_-p_+)^{(4)}+\tfrac{1}{2}\{\phi_+^{(1)2}+\phi_-^{(1)2},J_z\}\\&+\tfrac{1}{3}i(\phi_+^{(1)3}J_+^{(1)}-\phi_-^{(1)3}J_-^{(1)})\\&+\tfrac{1}{4}i\phi_+^{(1)2}\{\phi_-^{(1)},J_+^{(1)}\}+\text{H.c.}\\&+\tfrac{1}{4}i\{\phi_-^{(1)3},J_+^{(1)}\}+\text{H.c.}\ ,\end{aligned} \tag{4.26c}$$

and the notation $(\phi_+p_--\phi_-p_+)^{(n)}$ stands for the nth-order polynomial in the expansion of $\phi_+p_--\phi_-p_+$.

Next, consider the expansion of $\mathscr{J}_3\equiv\sum_{\mu}K_{\mu}B^{\dagger}_{\mu}B_{\mu}$. From Eqs. (2.14), (4.1), and (4.26a), one obtains

$$\begin{aligned}\mathscr{J}_3\equiv&\sum_{\mu}K_{\mu}B^{\dagger}_{\mu}B_{\mu}\\=&\exp(iS)\sum_{\mu}K_{\mu}B^{(1)\dagger}_{\mu}B^{(1)}_{\mu}\exp(-iS)\\=&\exp(iS)(J_z-i\phi_+^{(1)}J_-^{(1)}+i\phi_-^{(1)}J_+^{(1)})\exp(-iS)\\=&\exp(iS)J_z\exp(-iS)-i(\phi_+p_--\phi_-p_+)\ .\end{aligned} \tag{4.27}$$

This result can be expanded through quartic terms as follows:

$$\mathscr{J}_3=\mathscr{J}_3^{(2)}+\mathscr{J}_3^{(3)}+\mathscr{J}_3^{(4)}+\cdots\ , \tag{4.28}$$

where

$$\mathscr{J}_3^{(2)}=\sum_{\mu}K_{\mu}B^{(1)\dagger}_{\mu}B^{(1)}_{\mu}\ , \tag{4.29a}$$

$$\mathscr{J}_3^{(3)}=-i(\phi_+p_--\phi_-p_+)^{(3)}-[J_z,iS^{(3)}]\ , \tag{4.29b}$$

$$\begin{aligned}\mathscr{J}_3^{(4)}=&-i(\phi_+p_--\phi_-p_+)^{(4)}-[J_z,iS^{(4)}]\\&+\tfrac{1}{2}[[J_z,iS^{(3)}],iS^{(3)}]\ .\end{aligned} \tag{4.29c}$$

Comparison of Eqs. (4.26a) and (4.29a) shows that Eq. (3.53), i.e., the condition $J_3=\mathscr{J}_3$, is fulfilled through quadratic terms. It is also fulfilled through cubic terms, provided that

$$[J_z,iS^{(3)}]=0\ , \tag{4.30a}$$

as is seen from Eqs. (4.26b) and (4.29b). It follows from the inverse transform of Eq. (4.6) that (4.30a) is satisfied by all of the angle-dependent contributions to $S^{(3)}$, and therefore (4.30a) is equivalent to

$$[J_z,i\sigma^{(3)}]=0\ , \tag{4.30b}$$

where $\sigma^{(3)}\equiv\tilde{\tilde{\sigma}}^{(3)}$. This condition is fulfilled not only for $\sigma^{(3)}=0$, but also for any physically useful choice such as discussed in Sec. IV D below.

Continuing to the next order, and assuming that (4.30) is satisfied, one sees that (4.29c) reduces to

$$\mathscr{J}_3^{(4)} = -i(\phi_+ p_- - \phi_- p_+)^{(4)} - [J_z, iS^{(4)}] \ . \tag{4.31}$$

Although the commutator in (4.31) receives no contributions stemming from the terms explicitly given in Eq. (4.7), there are nonvanishing contributions from some of the "dispensable terms," namely those that give rise to the last angle-dependent term in $H'^{(4)}$ [Eq. (4.16)]. The commutator $[J_z, iS^{(4)}]$ can be obtained by first solving fully for $iS^{(4)}$, or, alternatively, by calculating the double commutator $[[J_z, iS^{(4)}], J_\pm^{(1)}]$ from Eq. (3.57), using the Jacobi identity, and then "integrating" with respect to $\phi_\pm^{(1)}$. Either way gives the result

$$\begin{aligned}[J_z, iS^{(4)}] = &-\tfrac{1}{2}\{\phi_+^{(1)2} + \phi_-^{(1)2}, J_z\} - \tfrac{1}{3} i(\phi_+^{(1)3} J_+^{(1)} - \phi_-^{(1)3} J_-^{(1)}) \\ &- [\tfrac{1}{4} i \phi_+^{(1)2} \{\phi_-^{(1)}, J_+^{(1)}\} + \text{H.c.}] - [\tfrac{1}{4} i \{\phi_-^{(1)3}, J_+^{(1)}\} + \text{H.c.}] + [J_z, i\sigma^{(4)}] \ .\end{aligned} \tag{4.32}$$

Comparison of (4.26c) with (4.31), taking (4.32) into account, shows that

$$J_3^{(4)} = \mathscr{J}_3^{(4)} + [J_z, i\sigma^{(4)}] \ . \tag{4.33}$$

Again, for any physically useful choice of $\sigma^{(4)}$, the condition

$$[J_z, i\sigma^{(4)}] = 0 \tag{4.34}$$

is satisfied. Since to the order of interest in this paper the choice of $\sigma^{(4)}$ is irrelevant, one can always take $\sigma^{(4)} = 0$.

The conclusion then is that for any physically sensible choice of S, the condition $J_3 = \mathscr{J}_3$, i.e., Eq. (3.53), is satisfied. Although this has been demonstrated through quartic terms, it is surmised to hold to all orders.

D. On the choice of the arbitrary functions $\sigma^{(3)}$ and $\sigma^{(4)}$

The final BM form of the reconstituted Hamiltonian given by Eqs. (4.22) and (4.23) contains a variety of terms analogous to those found in the purely phenomenological model.[15] The leading-order Hamiltonian $H_{\text{BM}}^{(2)}$ stems directly from the RPA, and identifies the zero-order eigenstates which provide a basis for a perturbative treatment of the higher-order coupling terms as products of rotational and RPA vibrational states. In particular, $H_{\text{BM}}^{(3)}$ contains anharmonic vibrational corrections to the intrinsic excitation modes as well as couplings of the rotational and intrinsic modes. The couplings linear in $I'_\pm$, which change the quantum number K by one unit, are analogous to what is usually referred to as the "Coriolis" interaction, but the matrix elements may be quite different from the usual angular-momentum matrix elements. Indeed, Eqs. (4.13a) and (4.13b) suggest that only part of the contribution to such matrix elements comes from the angular momentum, although this is not a rigorous argument. The remaining coupling terms quadratic in angular momentum resemble what is usually called the rotation-vibration interaction (centrifugal stretching), with the terms involving $I_1^2 + I_2^2$ corresponding to mixing with $K = 0$ modes ("β vibrations"), and those involving $I_\pm'^2$ corresponding to mixing with $K = 2$ modes ("γ vibrations"). In second-order perturbation theory, these couplings give rise to contributions of order 1 to the eigenvalues, since all terms of $H_{\text{BM}}^{(3)}$ are of order $\Omega^{1/2}$, thus contributing a factor of order Ω to numerators, while the RPA energy denominators are also of order Ω. However, in an *ab initio* microscopic treatment, one finds that among the diagonal terms of $H_{\text{BM}}^{(4)}$, which are also of order 1, those proportional to powers of $I_1^2 + I_2^2$ physically also involve Coriolis-like and centrifugal stretching effects. In other words, these effects to the given order are smeared between $H_{\text{BM}}^{(3)}$ and $H_{\text{BM}}^{(4)}$. In the case that there are no small energy denominators, nondegenerate perturbation theory may be used, which is equivalent to performing a unitary transformation that removes terms of $H_{\text{BM}}^{(3)}$. The physical effects to the given order then all appear as renormalizations of the diagonal quartic terms of the Hamiltonian, the off-diagonal terms contributing to the next higher order (Ω^{-1}). The same unitary transformation also renormalizes transition operators, thereby taking into account the effect of the couplings on transitions.[15] Alternatively, a unitary transformation could be performed to remove *diagonal* terms of $H_{\text{BM}}^{(4)}$. The advantage is that this procedure would concentrate all of the effects of centrifugal stretching and the Coriolis force to the given order in a renormalized $H_{\text{BM}}^{(3)}$, rather than having these effects distributed between the two terms in an arbitrary manner. Such an approach would be especially useful if one wishes to compare the matrix elements with those of some phenomenological model. It could be useful if some of the couplings have small energy denominators so that degenerate perturbation theory has to be employed.

It has been seen that the choice of arbitrary functions $\tilde{\sigma}^{(3)} = \tilde{\sigma}^{(4)} = 0$ gives rise to a variety of anharmonic and band-mixing corrections, which are distributed between the off-diagonal cubic and the diagonal quartic polynomial terms of the Hamiltonian, and that these corrections may be treated by perturbative unitary transformations subsequent to completion of the reconstruction of H_{BM}. As an alternative at an earlier stage, one may choose nonvanishing values of $\tilde{\sigma}^{(3)}$ and $\tilde{\sigma}^{(4)}$ with the aim of obtaining the desired final form of the Hamiltonian immediately upon passing over to the BM representation. For example, if the goal is to diagonalize the Hamiltonian, then $\tilde{S}^{(3)}$ may be chosen to satisfy

$$[i\tilde{S}^{(3)}, \tilde{H}^{(2)}] = \tilde{H}^{(3)} \ , \tag{4.35}$$

so as to entirely remove cubic polynomial terms. Since the terms explicitly given by Eq. (4.6) already remove all the $\phi_\pm$-dependent terms, $\tilde{\sigma}^{(3)}$ should be chosen to remove the additional terms given by the rhs of Eq. (4.12). This is accomplished by taking[38]

$$i\tilde{\sigma}^{(3)}=-\tfrac{1}{2}\sum_{\mu\nu\lambda}\frac{h^{(3)}(00)_{\mu\nu\lambda}}{\hbar\omega_\mu+\hbar\omega_\nu-\hbar\omega_\lambda}(B^\dagger_\mu B^\dagger_\nu B_\lambda-\text{H.c.})-\sum_\mu\frac{h^{(3)}(00)_\mu}{\hbar\omega_\mu}(B^\dagger_\mu-B_\mu)-\tfrac{1}{6}\sum_{\mu\nu\lambda}\frac{h^{(3)}(00)'_{\mu\nu\lambda}}{\hbar\omega_\mu+\hbar\omega_\nu+\hbar\omega_\lambda}(B^\dagger_\mu B^\dagger_\nu B^\dagger_\lambda-\text{H.c.})$$
$$-p_-\sum_{\mu\nu}\left[\frac{\Gamma^{(3)}(10)_{\mu\nu}}{\hbar\omega_\mu-\hbar\omega_\nu}B^\dagger_\mu B_\nu+\frac{1}{2}\frac{\Gamma^{(3)}(10)'_{\mu\nu}}{\hbar\omega_\mu+\hbar\omega_\nu}(B^\dagger_\mu B^\dagger_\nu+B_{-\nu}B_{-\mu})\right]-\text{H.c.}$$
$$-p_+p_-\sum_\mu\frac{\Gamma^{(3)}(20)_\mu}{\hbar\omega_\mu}(B^\dagger_\mu-B_\mu)-\left[p^2_-\sum_\mu\frac{\Gamma^{(3)}(20)'_\mu}{\hbar\omega_\mu}(B^\dagger_\mu-B_{-\mu})-\text{H.c.}\right]. \tag{4.36}$$

The connection with perturbation theory is obvious. While the transformation completely eliminates $H'^{(3)}$, its double commutator with H generates quartic polynomial and higher-order terms. To the order of interest, only the diagonal quartic contributions, which renormalize the terms of $H'^{(4)}$ given in Eq. (4.16), are needed. The choice of $\tilde{\sigma}^{(4)}$ is irrelevant to this order. However, if the total elimination of the off-diagonal quartic terms is also desired, which is of consequence to the next higher order, than an appropriate choice of $\tilde{\sigma}^{(4)}$ can also be made.

Any final form of $H_{\rm BM}$ that can be attained by means of unitary transformations within the BM framework can also be attained through appropriate choices of the arbitrary functions $\tilde{\sigma}^{(n)}$. In general, the approach used is largely a matter of taste, although the manipulations are a little easier using the canonical variables $p_\pm$ than the angular momentum components $I'_\pm$, but at the expense of having to carry along the contributions from the $\tilde{\sigma}^{(n)}$ throughout. It should be kept in mind that whatever the choice the concomitant transformation of the transition operators preserves the physical amplitudes.

The foregoing discussion suggests the possibility of reducing the Hamiltonian by means of successive unitary transformations to the following diagonal form:

$$H_{\rm BM}=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{\mu_1,\ldots,\mu_n}h(m)_{\mu_1,\ldots,\mu_n}(\hat{I}^2-I_3^2)^m\times\prod_{\mu=\mu_1}^{\mu_n}(\hat{N}_\mu+\tfrac{1}{2}), \tag{4.37}$$

where $\hat{N}_\mu\equiv B^\dagger_\mu B_\mu$, and the replacement $I_1^2+I_2^2=\hat{I}^2-I_3^2$ was used. The energies could then be read off immediately by replacing the operators by their eigenvalues as follows: $\hat{N}_\mu\to n_\mu$, and $\hat{I}^2-I_3^2\to I(I+1)-K^2$. The numerical coefficients $h(m)_{\mu_1,\ldots,\mu_n}$, as generated by the unitary transformation method outlined above, would appear as $1/\Omega$ expansions. The Hamiltonian (4.37) may be regarded as a quantal analog of the classical Birkhoff-Gustavson (BG) normal form,[39] but extended to include rotational as well as vibrational motion. However, since the angular momentum operators in the Schwinger representation[40,41] are expressed in terms of boson creation and annihilation operators, it should be possible to rewrite (4.37) as an ordinary BG normal form. It is well known that the BG expansion usually diverges, although it may still be useful as an asymptotic expansion. There has recently been considerable interest in quantization of BG expansions in connection with summation of series using Padé approximation.[42] However, the practical application of these methods to systems with many degrees of freedom may be problematic.

E. Treatment of transition operators—$E2$ operators

In this section the MW method is applied in detail to the electric quadrupole ($E2$) tensor as a typical example of the treatment of transition operators. In general, boson expansion provides a local Taylor-series representation of a spherical tensor T^L_M, while the aim is to reconstruct this tensor in the "global" form defined by Eqs. (3.7) and (3.13) in the case of the Villars representation, or Eqs. (3.30) and (3.32) in the case of the BM representation. This can be done in a straightforward fashion by observing that since

$$\lim_{\varphi\to0,\ \theta\to0}D^L_{MK}(\varphi,\theta,\psi)=e^{iK\psi}\delta_{MK}, \tag{4.38}$$

which follows immediately from the definition of the rotation matrix (3.49), then, from Eq. (3.7),

$$\lim_{\phi_\pm\to0}T^L_M=\lim_{\varphi\to0,\ \theta\to0}T^L_M=\hat{T}^L_M e^{iM\psi}. \tag{4.39}$$

This permits one to find the intrinsic components in the Villars representation by simply allowing the Euler angles to vanish in the expansions of the laboratory components and then multiplying by $\exp(-iM\psi)$. According to Eqs. (3.32), (3.30), and (3.13), the intrinsic components in the BM representation T'^L_K can be obtained through the replacements $\psi\to0$, $J'_\pm\to I'_\pm$ in $\hat{T}^L_K$. Equations (3.7) or (3.32) then provide the fully reconstructed operators. As a check, the $D^L_{MK}(\varphi,\theta,0)$ dependence in these operators may be expanded in powers of $\phi_\pm$ afterwards to regenerate the original expansions of the spherical tensor components, but this is not necessary. The procedure just outlined will now be applied to the $E2$ tensor described in Sec. II C.

The first step is to perform the transformation (4.3) from the RPA variables $\phi^{(1)}_\pm, J^{(1)}_\pm, B^{(1)}_\mu, B^{(1)\dagger}_\mu$, to the variables $\phi_\pm, p_\pm, B_\mu, B^\dagger_\mu$. Consistent with the truncation of the Hamiltonian, transition operators need only be expanded through quadratic terms. One therefore has

$$\mathcal{M}(E2,M)=\mathcal{M}^{(0)}(E2,M)+\tilde{\mathcal{M}}^{(1)}(E2,M)+\tilde{\mathcal{M}}^{(2)}(E2,M)-[i\tilde{S}^{(3)},\tilde{\mathcal{M}}^{(1)}(E2,M)]+\cdots, \tag{4.40}$$

where $\mathcal{M}^{(0)}(E2,M)$ is a constant given by Eq. (2.27). Equations (4.40) are readily evaluated with the aid of Eqs. (2.31)–(2.40) and (4.6), with the choice (4.11) for the arbitrary functions. The following results are then obtained through quartic terms:

$$\mathcal{M}(E2,0)=\left[\frac{5}{16\pi}\right]^{1/2}eQ_0+\sum_\mu q_0^{(1)}(00)_\mu(B_\mu^\dagger+B_\mu)+q_0^{(2)}(00)+\sum_{\mu\nu}q_0^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu$$
$$+\tfrac{1}{2}\sum_{\mu\nu}q_0^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_\nu B_\mu)+q_0^{(2)}(20)p_+p_-+\left[p_-\sum_\mu q_0^{(2)}(10)_\mu(B_\mu^\dagger-B_{-\mu})+\text{H.c.}\right]-\left[\frac{45}{4\pi}\right]^{1/2}eQ_0\phi_+\phi_-$$
$$+i\sqrt{6}\phi_-\sum_\mu q_1^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})+\text{H.c.}\ , \tag{4.41a}$$

$$\mathcal{M}(E2,1)=\sum_\mu q_1^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})+i\left[\frac{15}{8\pi}\right]^{1/2}eQ_0\phi_+ +\sum_{\mu\nu}q_1^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}\sum_{\mu\nu}q_1^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_{-\nu}B_{-\mu})$$
$$+p_+\sum_\mu q_1^{(2)}(10)_\mu(B_\mu^\dagger-B_\mu)+p_-\sum_\mu q_1^{(2)}(10)'_\mu(B_\mu^\dagger-B_{-\mu})$$
$$+i\sqrt{6}\phi_+\sum_\mu q_0^{(1)}(00)_\mu(B_\mu^\dagger+B_\mu)+2i\phi_-\sum_\mu q_2^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})\ , \tag{4.41b}$$

$$\mathcal{M}(E2,2)=\sum_\mu q_2^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})+\sum_{\mu\nu}q_2^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}\sum_{\mu\nu}q_2^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_{-\nu}B_{-\mu})+q_2^{(2)}(20)p_+^2$$
$$+p_+\sum_\mu q_2^{(2)}(10)_\mu(B_\mu^\dagger-B_{-\mu})+p_-\sum_\mu q_2^{(2)}(10)'_\mu(B_\mu^\dagger-B_{-\mu})$$
$$-\left[\frac{15}{8\pi}\right]^{1/2}eQ_0\phi_+^2+2i\phi_+\sum_\mu q_1^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})\ . \tag{4.41c}$$

It should be noted that in Eqs. (4.41) the coefficients of the $\phi_\pm$-dependent terms were obtained with the aid of the relations (2.40).

The intrinsic components in the Villars representation may be obtained straightforwardly from Eqs. (4.41) by applying (4.39) to $\mathcal{M}(E2,M)$ and then replacing $p_\pm$ by the PA components of angular momentum, using Eq. (4.19). Finally, from the $\hat{\mathcal{M}}(E2,M)$ the intrinsic components $\mathcal{M}'(E2,M)$ in the BM representation are obtained, as already indicated, by making the replacements $\psi\to 0$ and $J'_\pm\to I'_\pm$, the results for which through second order are

$$\mathcal{M}'(E2,0)=\left[\frac{5}{16\pi}\right]^{1/2}eQ_0+\sum_\mu q_0^{(1)}(00)_\mu(B_\mu^\dagger+B_\mu)+q_0^{(2)}(00)+\sum_{\mu\nu}[q_0^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}q_0^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_\nu B_\mu)]$$
$$+q_0^{(2)}(20)(I_1^2+I_2^2)+\left[I'_-\sum_\mu q_0^{(2)}(10)_\mu(B_\mu^\dagger-B_{-\mu})+\text{H.c.}\right]\ , \tag{4.42a}$$

$$\mathcal{M}'(E2,1)=\sum_\mu q_1^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})+\sum_{\mu\nu}q_1^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}\sum_{\mu\nu}q_1^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_{-\nu}B_{-\mu})$$
$$+I'_+\sum_\mu q_1^{(2)}(10)_\mu(B_\mu^\dagger-B_\mu)+I'_-\sum_\mu q_1^{(2)}(10)'_\mu(B_\mu^\dagger-B_{-\mu})\ , \tag{4.42b}$$

$$\mathcal{M}'(E2,2)=\sum_\mu q_2^{(1)}(00)_\mu(B_\mu^\dagger+B_{-\mu})+\sum_{\mu\nu}q_2^{(2)}(00)_{\mu\nu}B_\mu^\dagger B_\nu+\tfrac{1}{2}\sum_{\mu\nu}q_2^{(2)}(00)'_{\mu\nu}(B_\mu^\dagger B_\nu^\dagger+B_{-\nu}B_{-\mu})+q_2^{(2)}(20)I_+'^2$$
$$+I'_+\sum_\mu q_2^{(2)}(10)_\mu(B_\mu^\dagger-B_{-\mu})+I'_-\sum_\mu q_2^{(2)}(10)'_\mu(B_\mu^\dagger-B_{-\mu})\ . \tag{4.42c}$$

The remaining $\mathcal{M}'(E2,K)$ can be obtained from the relation $\mathcal{M}'(E2,-K)=(-1)^K\mathcal{M}'(E2,K)^\dagger$. This completes the demonstration of how to treat transition operators in the MW formalism. Two comments, however, are in order.

First, it should be kept in mind that the expressions are still expansions in a small parameter. Thus, for example, in Eq. (4.42a), the first constant term on the rhs, related to the static quadrupole moment, is of order Ω, the linear term is of order $\Omega^{1/2}$, and the remaining quadratic terms, including the correction to the static quadrupole moment $q_0^{(2)}(00)$, are of order 1. Second, the effect of making a nonzero choice of $\sigma^{(3)}$ as discussed in Sec. IV C is to renormalize the coefficients in Eqs. (4.42). In particular, if the Hamiltonian is diagonalized to the order of interest, then the effects of band mixing are entirely incorporated

in the transition operators. These effects may then be read off by inspection of the transition operators. Further details may be found in Ref. 15.

V. SUMMARY AND CONCLUSIONS

Finite systems with broken continuous symmetries are represented in two distinct ways. First, there are *local representations,* which are Taylor series expansions involving all degrees of freedom about a mean-field solution with broken symmetry. Expansions in deformed bosons about a deformed Hartree-Fock solution are examples. Although such representations are easy to generate, they have well-known problems associated with zero-frequency (Goldstone) modes that render them unsuitable for direct application to the band structures associated with the broken symmetries. On the other hand, there are *global representations,* such as the Villars[22] and Bohr-Mottelson[15] (BM) representations, which are also expansions, but of a type that preserve the constants of motion and associated cyclic variables. Although such representations are naturally fitted for the description of band structure, they are in general quite difficult to derive. The MW method makes it possible to pass from a local to a global representation in an elementary way by means of formal unitary transformations.

While much of the previous work using the MW method has been limited to cases involving Abelian groups of broken symmetry, the present paper has demonstrated that the method is applicable also to the rotation group. Specifically, the application has been to the problem of low-spin rotation of strongly deformed systems with axially symmetric equilibrium shapes. In order that the outlines of the method be as clear as possible, the manipulations were carried out for a generic boson Hamiltonian and associated transition operators. Consequently, the results are manifestly independent of the choice of internucleon interactions, and one avoids the (in the present context irrelevant) clutter that would result from a microscopic boson expansion. It should also be apparent that the method has a broad range of application, including microscopic systems treated by means of boson mappings, phenomenological boson models such as the old Bohr-Mottelson quadrupole collective model and the newer IBM's, and even molecular systems.

In the course of the discussion, it has been shown that some ostensible obstacles to the application of the MW method disappear if due note is taken of the redundant degree of freedom in the BM representation. In this connection, a novel treatment was given of the relation between the Villars and BM representations, which, it is hoped, will dispel some of the mysteries surrounding the latter. Since difficulties associated with this redundant degree of freedom have apparently also been a source of irritation in molecular physics,[43] the unitary transformation method used here might be of some interest in that area.

As for future work, a planned sequel to this paper will discuss the application of the MW method to an exactly soluble model, namely, the quadrupole collective model, in lieu of a suitable exactly soluble microscopic model. Also planned are applications to various versions of the IBM's, of which those involving extra bosons, such as the g boson, might benefit from the present treatment. Another area of application is presented by odd nuclei, for which the MW method can be readily extended. An interesting question here is whether the method can illuminate the infamous "Coriolis attenuation" problem,[44] for which, of course, a fully microscopic treatment is needed.

Finally, it should be acknowledged that the problem of describing nuclear rotational band structure could also be attacked with a variety of elegant techniques, most of which were referred to in Ref. 4. Among the older methods overlooked there, however, is the *ideal collective coordinate method,*[45] which was used to derive the Villars expansion for two-dimensional rotators, and, undoubtedly, could be extended to three dimensions. Among the latest methods, the nuclear Born-Oppenheimer approximation looks promising.[46] The reader's attention is also called to two recent review particles discussing the roton approach[47] and the generalized density matrix method.[48] These are all methods that circumvent Goldstone modes.

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*Permanent address: Department of Physics, University of Notre Dame, Notre Dame, IN 46556.

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[34]There is no need to determine the Euler angle ψ explicitly; Eq. (3.9), or, equivalently, $[\psi,J_3]=i$, is sufficient.

[35]Equivalently, the transformation (4.1) may be first performed on Eqs. (3.56) and (3.57), which can be solved directly to yield $\tilde{S}^{(3)}$ and $\tilde{S}^{(4)}$.

[36]This does not mean that $\exp(\pm i\psi)$ commutes with $J'_{\pm}$, but merely that the commutator is of higher order than the one of interest.

[37]With the full evaluation of the cubic terms in Eq. (4.19), one may show that through quartic terms $p_+p_- \cong J_1^2+J_2^2 -\theta^2 p_\varphi^2+2\theta p_\varphi J_3+\frac{1}{2}$, but the work is a bit tedious.

[38]Lest the notation prove deceptive, it should be pointed out that the nonvanishing choice of $\tilde{\sigma}^{(3)}$ leads to a renormalization of $\phi_{\pm}$, B_μ, and $B_\mu^\dagger$ relative to the case of $\tilde{\sigma}^{(3)}=0$.

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