Microscopic derivation of a collective bosonic Hamiltonian with the generalized density matrix method

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The collective bosonic Hamiltonian is derived from the microscopic nucleonic Hamiltonian by the generalized density matrix method. Independent parameters in the collective Hamiltonian are fixed completely, solutions are given in detail. The random phase approximation corresponds to the harmonic potential of the current approach. The full solution (very close to the exact diagonalization) is obtained over the whole region of parameters including and beyond the instability point of the random phase approximation. The method is tested in the simple Lipkin model.

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I. INTRODUCTION

The effective bosonic Hamiltonian has long been used to describe collective excitations in nuclear physics, most frequently in the form of the geometric Bohr Hamiltonian [1,2] and in the interacting boson model [3]. Broad sets of nuclear data are described with a few parameters that change smoothly across the nuclear chart. Such models provide a qualitative picture of low-lying collective motion, especially important in heavy nuclei where the full shell-model calculations are hardly feasible. To put the phenomenological theory on solid grounds, serious efforts were devoted to calculating these parameters microscopically from the underlying nucleonic Hamiltonian. But the complete microscopic theory is still missing after several decades. The original formulation [4] in terms of direct boson expansion of fermionic operators had practical problems related to convergence, see detailed review [5].

In this work it is shown that the microscopic theory based on the generalized density matrix (GDM) fixes the collective bosonic Hamiltonian completely. This method was proposed long ago [6–8] and was applied to nuclear rotation [7,9,10] and large-amplitude collective motion [11–13]. Recently the general construction of the GDM method was reexamined [14], but only one constraint was found in each even order of the anharmonic collective Hamiltonian, which seemed insufficient to fix the latter completely. In this work we show that the GDM method is actually self-sufficient: with the renormalization of collective operators, the redundant degrees of freedom in the collective Hamiltonian are removed, and the theory is left with truly independent parameters whose number is equal to the number of the constraints imposed by the GDM method. In this way, the whole procedure of calculating the collective Hamiltonian becomes clear.

Section II introduces the renormalization of collective variables and identifies the independent parameters in the collective Hamiltonian. Then we show in detail how to fix them by the GDM method in Sec. III. In Sec. IV the GDM procedure is tested in the Lipkin model with perfect agreement. Section V discusses future working directions.

II. EQUIVALENT REPRESENTATION OF BOSONIC HAMILTONIAN

In what follows, for simplicity of notations we omit all details related to the angular momentum vector coupling. This part is necessary in realistic calculations but does not contain principal difficulties. The collective bosonic Hamiltonian is first constructed as an expansion over all time-reversal invariant combinations of the collective coordinate α and collective momentum π,

$$H = \omega^2\frac{\alpha^2}{2} + \frac{\pi^2}{2} + \Lambda^{(30)}\frac{\alpha^3}{3!} + \Lambda^{(12)}\frac{\{\alpha,\pi^2\}}{4} + \Lambda^{(40)}\frac{\alpha^4}{4!} + \Lambda^{(22)}\frac{\{\alpha^2,\pi^2\}}{8} + \Lambda^{(04)}\frac{\pi^4}{4!} + \Lambda^{(50)}\frac{\alpha^5}{5!} + \cdots . \quad (1)$$

Here and below, the curly brackets denote anticommutator, $\{A, B\} = AB + BA$. Microscopic estimates of quite general type [15] show that $\Lambda^{(mn)} \sim \Omega^{-(m+n-2)/2}$, where Ω is the collectivity factor, the effective number of simple quasiparticle excitations contributing to the collective mode. The solvable Lipkin model and quadrupole plus pairing model confirm these estimates [14]. In the case of strong collectivity, $\Omega \gg 1$. In Eq. (1) all terms with the right symmetry are kept thus the expansion is complete. However, it is overcomplete. Different expansions are equivalent if they are related by canonical transformations of collective variables α and π. The number of independent parameters of H should be the number of possible combinations as in Eq. (1) minus the number of allowed transformations.

Let us count the number of transformations $(\alpha, \pi) \to (\bar\alpha, \bar\pi)$,

$$\alpha = \sum_{m\geqslant 0, n\geqslant 0} x^{(mn)}\frac{1}{2}\frac{\{\bar\alpha^m, \bar\pi^n\}}{m!n!}, \qquad \pi = \sum_{m\geqslant 0, n\geqslant 0} y^{(mn)}\frac{1}{2}\frac{\{\bar\alpha^m, \bar\pi^n\}}{m!n!}, \quad (2)$$

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which preserve the commutator algebra,

$$[\alpha, \pi] = [\bar{\alpha}, \bar{\pi}] = i. \tag{3}$$

The transformation parameters $x^{(mn)}$, $y^{(mn)}$ being of the order $\Omega^{-(m+n-1)/2}$ will not change the dependence of $\Lambda^{(mn)}$ in Eq. (1) on Ω. The constant terms, $x^{(00)}$ and $y^{(00)}$, corresponding to a trivial translation of origin are not needed as this choice is already made by selecting $\Lambda^{(10)} = \Lambda^{(01)} = 0$ in the collective Hamiltonian (1); in the case of a multipole collective mode such terms would violate rotational symmetry. In the linear terms we can set $x^{(10)} = y^{(01)} = 1$, which would correspond to a rescaling of α or π [$\Lambda^{(02)} = 1$ in Eq. (1)]. The parameters $x^{(mn)}$ and $y^{(mn)}$ vanish for odd and even n, respectively, because of the wrong time-reversal symmetry.

Using Eqs. (2) and (3) we have

$$[\alpha, \pi] = \frac{i}{2} \sum_{rsmn} x^{(mn)} y^{(r-m,s-n)} \times \frac{[m(s-n) - n(r-m)]}{m!n!(r-m)!(s-n)!} \{\bar{\alpha}^{r-1}, \bar{\pi}^{s-1}\}, \tag{4}$$

where in the coefficient of $\{\bar{\alpha}^{r-1}, \bar{\pi}^{s-1}\}$ we keep only the leading terms in $1/\Omega$, that is, terms $\sim\Omega^{-(r+s-2)/2}$. The summation runs over $r \geqslant m$ and $s \geqslant n$, and as seen from the numerator, $r \geqslant 1$ and $s \geqslant 1$. In addition, s is odd, otherwise $x^{(mn)} y^{(r-m,s-n)}$ vanishes. The starting term, $r = s = 1$, gives correctly i. The terms with $r + s \geqslant 3$ and an odd s should vanish,

$$0 = \sum_{mn} x^{(mn)} y^{(r-m,s-n)} \frac{m(s-n) - n(r-m)}{m!n!(r-m)!(s-n)!}. \tag{5}$$

These relations constrain $x^{(mn)}$ and $y^{(mn)}$ in the transformations (2).

Let us identify the independent parameters in the collective Hamiltonian (1), removing the redundant degrees of freedom related to the transformations (2). In the quadratic order, the transformations (2) do not change the harmonic terms $\frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2$; thus, there is one independent parameter ω^2. In the cubic order, the transformations (2) with nonzero $x^{(20)}$, $x^{(02)}$, and $y^{(11)}$ influence the Hamiltonian parameters $\Lambda^{(30)}$ and $\Lambda^{(12)}$ through the harmonic terms; there is one constraint (5) with $(rs) = (21)$. Thus, the renormalization of the collective variables removes the skew terms: $\Lambda^{(30)}$ and $\Lambda^{(12)}$ can be set to zero and there remains no independent parameter in this order. In the quartic order, the transformations (2) with nonzero $x^{(30)}$, $x^{(12)}$, $y^{(21)}$, and $y^{(03)}$ influence $\Lambda^{(40)}$, $\Lambda^{(22)}$, and $\Lambda^{(04)}$; and there are two constraints (5) with $(rs) = (31)$ and (13). Thus, there is one independent parameter; we can, for example, choose it to be $\Lambda^{(40)}$, and set $\Lambda^{(22)}$ and $\Lambda^{(04)}$ to zero.

This process continues to anharmonic terms of higher orders. There is one independent parameter in each even order (we can choose it to be $\Lambda^{(n0)}$ excluding all momentum-dependent high-order terms), and there are no independent parameters in odd orders. In summary, the independent parameters in the collective Hamiltonian (1) can be identified in the following form:

$$H = \frac{1}{2}\pi^2 + V(\alpha^2),$$
$$V(\alpha^2) = \omega^2 \frac{\alpha^2}{2} + \Lambda^{(40)} \frac{\alpha^4}{4!} + \Lambda^{(60)} \frac{\alpha^6}{6!} + \Lambda^{(80)} \frac{\alpha^8}{8!} + \cdots. \tag{6}$$

In Ref. [14] we have shown that the GDM method gives one constraint in each even order of anharmonicity, thus fixes all the independent parameters in Eq. (6). In this sense the collective Hamiltonian is completely determined. In the next section we rewrite the GDM equations and solutions derived in Ref. [14] in a compact form valid up to an arbitrary order.

III. GENERALIZED DENSITY MATRIX FORMALISM

Starting from the antisymmetrized fermionic Hamiltonian,

$$H = \sum_{12} \epsilon_{12} a_1^\dagger a_2 + \frac{1}{4} \sum_{1234} V_{1234} a_1^\dagger a_2^\dagger a_3 a_4, \tag{7}$$

we calculate the equations of motion for the one-body density matrix operators, $R_{12} \equiv a_2^\dagger a_1$,

$$[R_{12}, H] = [\epsilon, R]_{12} - \frac{1}{2} \sum_{345} V_{5432} a_5^\dagger a_4^\dagger a_3 a_1 + \frac{1}{2} \sum_{345} V_{1345} a_2^\dagger a_3^\dagger a_4 a_5. \tag{8}$$

Here and below the numerical indices $1, 2, \ldots$ combine all single-particle quantum numbers. On the right hand side $[\epsilon, R]_{12} = \sum_3 (\epsilon_{13} R_{32} - R_{13} \epsilon_{32})$.

It is assumed that there exists a subspace of the full spectrum of the original Hamiltonian (7), corresponding to the experimental "band" of collective states interconnected by large transition rates. We map the exact equations of motion (8) onto this collective subspace. Inside the collective subspace the dynamics of the GDM operators R_{12} is assumed to be generated by the expansion over collective operators α and π,

$$R_{12} \stackrel{\circ}{=} \sum_{m\geqslant 0, n\geqslant 0} r_{12}^{(mn)} \frac{1}{2} \frac{\{\alpha^m, \pi^n\}}{m!\,n!}, \tag{9}$$

where "$\stackrel{\circ}{=}$" means projecting onto the collective subspace. The first term $\rho \equiv r^{(00)}$ is just the usual single-particle density matrix. The terms with operators α and π generate the interaction within the band. The original fermionic Hamiltonian is mapped onto the collective subspace as

$$H \stackrel{\circ}{=} \sum_{m\geqslant 0, l\geqslant 0}^{m+2l\geqslant 2} \Lambda^{(m,2l)} \frac{1}{2} \frac{\{\alpha^m, \pi^{2l}\}}{m!(2l)!}, \tag{10}$$

where $\Lambda^{(20)} = \omega^2$, $\Lambda^{(02)} = 1$. Here we changed the numerical normalization in Eqs. (9) and (10) from $1/(2mn)$, as used in Ref. [14], to $1/2/(m!n!)$, in order to include the case of zero m or n. The relevant results for the two-body operators (the so-called "saturation principle" in Ref. [14]) can be

summarized as

$$a_4^\dagger a_3^\dagger a_2 a_1 \doteq a_4^\dagger a_1 \cdot a_3^\dagger a_2 - a_4^\dagger a_2 \cdot a_3^\dagger a_1, \tag{11}$$

that is, it factorizes into antisymmetrized products of one-body GDM operators. The term in Eq. (11) without collective variables, $\rho_{1234} = \rho_{14}\rho_{23} - \rho_{24}\rho_{13}$, is routinely used to derive the time-dependent Hartree-Fock equation. We have also calculated the equations of motion for the two-body operators $a_4^\dagger a_3^\dagger a_2 a_1$, and found that Eq. (11) is a consistent solution.

With Eqs. (9)–(11), the equation of motion (8) is mapped onto the collective subspace,

$$[R_{12}, H] \doteq [\epsilon + W\{R\}, R]_{12}, \tag{12}$$

where

$$W\{R\}_{12} \equiv \sum_{34} V_{1432} R_{34} \tag{13}$$

is the generalized self-consistent field. The substitution of Eq. (9) into Eq. (13) gives the mapping of the latter, $W\{R\} \doteq \sum_{mn} w^{(mn)} \frac{1}{2} \frac{\{\alpha^m, \pi^n\}}{m!n!}$, where $w^{(mn)} \equiv W\{r^{(mn)}\}$. On the left hand side of Eq. (12), the intermediate states (between R_{12} and H) are restricted to those of the collective subspace, assuming large transition amplitudes. Substituting Eqs. (9) and (10) into Eq. (12), comparing coefficients with the same operator structure, we come to the final set of GDM equations with different $r \geqslant 0$, $s \geqslant 0$,

$$\begin{aligned} &\sum_{0\leqslant p(\leqslant r+1), 0\leqslant 2l(\leqslant s+1)}^{p+2l\geqslant 2} \frac{2l(r+1-p)-(s+1-2l)p}{(r+1-p)!(s+1-2l)!p!(2l)!} \cdot i\Lambda^{(p,2l)} r^{(r+1-p,s+1-2l)} \\ &\quad = \frac{1}{r!s!}[\epsilon, r^{(rs)}] + \sum_{0\leqslant p(\leqslant r), 0\leqslant q(\leqslant s)} \frac{1}{(r-p)!(s-q)!p!q!}[w^{(r-p,s-q)}, r^{(pq)}]. \end{aligned} \tag{14}$$

Equation (14) with $(rs) = (00)$ gives the Hartree-Fock (HF) equation,

$$0 = [\epsilon + W\{\rho\}, \rho]. \tag{15}$$

It is natural to use the HF single-particle basis that diagonalizes $f\{\rho\} \equiv \epsilon + W\{\rho\}$ and ρ simultaneously, providing the orbital energies e_1 and occupation numbers n_1,

$$f_{12} = \delta_{12} e_1, \quad \rho_{12} = \delta_{12} n_1. \tag{16}$$

Later we use $e_{12} \equiv e_1 - e_2$ and $n_{12} \equiv n_1 - n_2$.

For $K = r + s \geqslant 1$ in Eq. (14), we solve a linear set of coupled equations for $r^{(rs)}|_{r+s=K}$. The formal solution can be written as

$$\begin{aligned} r^{(mn)}|_{m+n=K} = &- \sum_{r+s=K} \sum_{0\leqslant p(\leqslant r+1), 0\leqslant 2l(\leqslant s+1)}^{p+2l\geqslant 3} \frac{2l(r+1-p)-(s+1-2l)p}{(r+1)(s+1)} C_{r+1}^p C_{s+1}^{2l} \cdot i\Lambda^{(p,2l)} \cdot \eta_{(rs)}^{(mn)} : r^{(r+1-p,s+1-2l)} \\ &+ \sum_{r+s=K} \sum_{0\leqslant p(\leqslant r), 0\leqslant q(\leqslant s)}^{p+q\leqslant r+s-1} C_r^p C_s^q \cdot \eta_{(rs)}^{(mn)} : [w^{(r-p,s-q)}, r^{(pq)}], \end{aligned} \tag{17}$$

where $C_p^q = p!/[q!(p-q)!]$, and we have introduced the "weight" matrix $\eta_{(rs)}^{(mn)}$ so that $(\eta_{(rs)}^{(mn)} : r)_{12} = \eta_{(rs)12}^{(mn)} r_{12}$. The matrix η is given by

$$\eta_{(rs)}^{(mn)} = \left(D_K^{-1}\right)_{(mn)}^{(rs)}, \tag{18}$$

where D_K is a tridiagonal matrix of dimension $K+1$,

$$\begin{aligned} (D_K)_{(mn)}^{(mn)} &= -e, \\ (D_K)_{(mn)}^{(m+1,n-1)} &= i \cdot n, \\ (D_K)_{(mn)}^{(m-1,n+1)} &= -i \cdot \omega^2 m. \end{aligned} \tag{19}$$

We give as an example the first two η matrices. For $K = 1$,

$$\eta_{(rs)}^{(mn)} = \frac{1}{e^2 - \omega^2} \left(\begin{array}{c|cc} (mn)\setminus(rs) & (01) & (10) \\ \hline (01) & -e & -i \\ (10) & i\omega^2 & -e \end{array}\right), \tag{20}$$

and for $K = 2$,

$$\eta_{(rs)}^{(mn)} = \frac{1}{-e(e^2 - 4\omega^2)} \times \left(\begin{array}{c|ccc} (mn)\setminus(rs) & (02) & (11) & (20) \\ \hline (02) & e^2 - 2\omega^2 & 2ie & -2 \\ (11) & -i\omega^2 e & e^2 & ie \\ (20) & -2\omega^4 & -2i\omega^2 e & e^2 - 2\omega^2 \end{array}\right). \tag{21}$$

From Eq. (21) we read, for example, $\eta_{(02)12}^{(20)} = \{-2\omega^4\}/\{-e_{12}[(e_{12})^2 - 4\omega^2]\}$. All η matrices with an *even* K have the factor $1/e$ [see for example Eq. (21)], thus the $e_1 = e_2$ matrix elements of $r_{12}^{(mn)}$ cannot be directly calculated from the solutions (17). However, if we set $n_1 = n_2$ in Eq. (17) and simplify, the $1/e_{12}$ divergence is canceled; the resulting

expression is used to calculate $r_{12}^{(mn)}$. The $e_1 = e_2$ matrix elements of $r_{12}^{(mn)}$ are expressed in terms of lower-order quantities.

In each order K, substituting $r^{(mn)}$ from Eq. (17) into $w_{12}^{(mn)} = \sum_{34} V_{1432} r_{34}^{(mn)}$ results in a linear set of coupled equations for the latter, from which the $e_1 \neq e_2$ matrix elements of $w_{12}^{(mn)}$ are solved in terms of lower-order quantities, which in turn gives the $e_1 \neq e_2$ matrix elements of $r_{12}^{(mn)}$ by Eq. (17). However, if $K = 2L + 1$ is odd, the determinant for $w^{(mn)}$ is zero. This can be proved as following. Summing Eq. (14) with proper weights we get

$$\begin{aligned} ix &= [W\{y\}, \rho] + [f, y] + \cdots, \\ -i\omega^2 y &= [W\{x\}, \rho] + [f, x] + \cdots, \end{aligned} \tag{22}$$

where

$$\begin{aligned} x &= \sum_{0 \leqslant t \leqslant L} \frac{\nu_t}{(2t+1)!(2L-2t)!} r^{(2t+1, 2L-2t)}, \\ y &= \sum_{0 \leqslant t \leqslant L} \frac{\mu_t}{(2t)!(2L+1-2t)!} r^{(2t, 2L+1-2t)}, \end{aligned}$$

in which μ_t and ν_t are solved from ($0 \leqslant t \leqslant L$, $\mu_{L+1} = \nu_{-1} = 0$)

$$\begin{aligned} -\frac{2L-2t}{2t+1}\omega^2 \mu_{t+1} + \mu_t &= \frac{1}{2t+1}\nu_t, \\ \omega^2 \nu_t - \frac{2t}{2L-2t+1}\nu_{t-1} &= \frac{1}{2L+1-2t}\omega^2 \mu_t. \end{aligned}$$

The "$\cdots$" in Eq. (22) are lower-order quantities. It is seen that the explicitly shown parts of Eq. (22) have the same structure as the random phase approximation (RPA) equations: $ir^{(10)} = [w^{(01)}, \rho] + [f, r^{(01)}]$ and $-i\omega^2 r^{(01)} = [w^{(10)}, \rho] + [f, r^{(10)}]$. This finishes the proof. The zero determinant means that the set of equations for $w^{(mn)}$ is linearly dependent, and there is a constraint in each order of odd K, entering as a solvability condition. These constraints are the main results of the GDM formalism, from which the parameters $\Lambda^{(pq)}$ of the collective Hamiltonian are calculated. Then $w^{(mn)}$ is solved from this zero-determinant set, with only a factor undetermined. This factor is fixed by the constraint indicated below Eq. (23).

If the GDM formalism is self-consistent, the substitution of the solutions (17) into Eq. (7) should reproduce the assumed Hamiltonian (10),

$$\begin{aligned} \Lambda^{(mn)} &= \mathrm{Tr}\,[\epsilon r^{(mn)}] \\ &\quad + \frac{1}{2} \sum_{0 \leqslant p (\leqslant m), 0 \leqslant q (\leqslant n)} C_m^p C_n^q \mathrm{Tr}[r^{(pq)} w^{(m-p, n-q)}]. \end{aligned} \tag{23}$$

In an order of odd $K = m + n$, all the parameters $\Lambda^{(mn)}$ are checked correctly. In an order of even $K = m + n$, all but one $\Lambda^{(mn)}$ are checked correctly; this one leftover degree-of-freedom/constraint is used to fix the remaining "undetermined factor" mentioned at the end of the last paragraph.

In practical applications, Eq. (6) may not be the most convenient choice for the independent parameters of the collective Hamiltonian, which means solving the equations of motion in the GDM method to infinitely high orders. Alternatively, we can pick up a certain number (labeled N) of terms in Eq. (1), putting other terms to zero; in other words, we *assume* that the original fermionic Hamiltonian (7) can be sufficiently accurately mapped onto a collective Hamiltonian with these N terms. Then in the GDM method we need to solve the equations of motion up to the $(2N)$th order, in order to get N constraints. The quality of the assumption of mapping can be checked self-consistently within the GDM method: if the assumption is good, constraints from the orders higher than $2N$ should be satisfied automatically. For the realistic nucleonic Hamiltonian, mapping onto a bosonic Hamiltonian is guaranteed by the success of old phenomenological studies. The mapped quadrupole phonon α_μ is not necessarily the RPA phonon that is "proportional" to the real quadrupole moment Q_μ; rather α_μ is such a renormalized operator (2) that the mapping onto a given form (the selected N terms) of the bosonic Hamiltonian is the "best". The possibly infinite series of the bosonic Hamiltonian expanded in the RPA phonon is "pushed"/resummed into the selected finite-N terms by the renormalization (2). The expansion of Q_μ in terms of α_μ and π_μ is obtained by substituting the solution (9) into $Q_\mu = \mathrm{Tr}[q_\mu R]$.

IV. LIPKIN MODEL

The above GDM formalism is tested in the Lipkin model ($\sigma = \pm 1$; $l = 1, 2, \ldots, \Omega$):

$$H = \sum_{\sigma,l} \frac{\sigma}{2} a_{\sigma,l}^\dagger a_{\sigma,l} + \frac{\kappa}{2} \sum_{\sigma,l,l'} a_{\sigma,l}^\dagger a_{\sigma,l'}^\dagger a_{-\sigma,l'} a_{-\sigma,l}. \tag{24}$$

The exact solution is well known [5], using

$$J_+ = J_-^\dagger = \sum_l a_{+1,l}^\dagger a_{-1,l}, \quad J_z = \frac{1}{2} \sum_{\sigma,l} \sigma a_{\sigma,l}^\dagger a_{\sigma,l}, \tag{25}$$

$$J_+ = A^\dagger \sqrt{2J - A^\dagger A}, \quad J_z = -J + A^\dagger A, \quad 2J = \Omega, \tag{26}$$

$$A = \frac{1}{\sqrt{2}}(iu\alpha + v\pi), \quad A^\dagger = \frac{1}{\sqrt{2}}(-iu\alpha + v\pi), \tag{27}$$

$$u \approx \sqrt{1 + 2\kappa J}, \quad v = -\frac{1}{u}, \tag{28}$$

the Hamiltonian (24) is written in the form (10) with only three nonzero terms,

$$\begin{aligned} \omega^2 &= 1 - (\kappa\Omega)^2, \\ \Lambda^{(40)} &= 6\kappa(1 + \kappa\Omega)^2, \\ \Lambda^{(04)} &= \frac{-6\kappa}{(1 + \kappa\Omega)^2}. \end{aligned} \tag{29}$$

Equations (29) are accurate in the leading order of $1/\Omega$. In the mapping, the Hamiltonian (24) is first written in terms of the quasi-spin operators J_z and $J_\pm$ by Eq. (25), then of the boson operators $A^\dagger$ and A by the Holstein-Primakoff transformation (26). The canonical transformation (27) introduces the collective coordinate α and momentum π, whose scales are fixed by Eq. (28), so that $\Lambda^{(02)} = 1$.

Now we apply the GDM formalism to the Hamiltonian (24). By going up to the sixth order in equations of motion, we get three constraints to fix ω^2, $\Lambda^{(40)}$, and $\Lambda^{(04)}$, and they agree with the exact results (29). Hence the GDM method solves the Lipkin model completely in the leading order of $1/\Omega$.

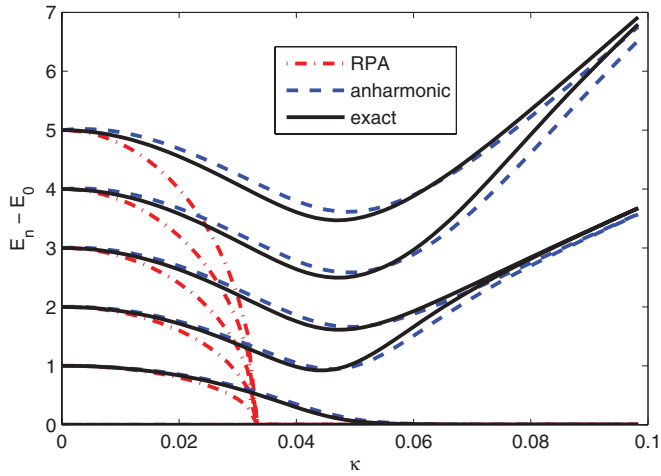

FIG. 1. (Color online) The excitation energies $E_n - E_0$ of the first five excited states as a function of κ in the model (24) with $\Omega = 30$. The red dashed-dotted lines are the RPA results (diagonalizing the harmonic Hamiltonian $\frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2$). The blue dashed lines are obtained by diagonalizing $\frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2 + \frac{\Lambda^{(40)}}{4!}\alpha^4$ in the infinite phonon space $\{|0 \leqslant n < +\infty\rangle\}$, where ω^2 and $\Lambda^{(40)}$ are given by Eq. (29). The black solid lines show the exact results by diagonalizing the original fermionic Hamiltonian (24) directly.

In Fig. 1, a numerical example is performed for $\Omega = 30$. As one can see, the first few excited states of the anharmonic Hamiltonian agree very well with the exact results, while the RPA fails very soon as κ increases to the critical point. For realistic medium and heavy even-even nuclei, only in the vicinity of magic numbers the low-lying collective excitations can be sufficiently described by the QRPA; in very many cases, including the soft-spherical, γ-unstable, and rotational dynamics, the collective modes lie beyond the critical point of RPA, so that the higher-order anharmonicities in the collective Hamiltonian are indispensable.

In Fig. 1, as conventionally done, the bosonic Hamiltonian (29) is diagonalized in the infinite phonon space $\{|0 \leqslant n < +\infty\rangle\}$ ($|n\rangle$ is the state with n phonons, $A^\dagger A|n\rangle = n|n\rangle$), dropping the "divergent" $\Lambda^{(04)} < 0$ term. However, as discussed in Ref. [14], the Hamiltonian (29) should be diagonalized in the finite physical space, which is known in the Lipkin model to be $\{|0 \leqslant n \leqslant \Omega\rangle\}$. Acting $A^\dagger$ more than Ω times on the ground state runs out of valence particles thus gives zero. Within the finite physical space, the $\Lambda^{(04)} < 0$ term does not generate divergences and should be kept. In order to identify the errors of the "anharmonic" curve in Fig. 1, we plot the errors of the excitation energies for the first four excited states in a set of calculations in Fig. 2. The overlap of curves 1 and 2 means that convergence is reached for the first few excitation energies in the finite physical space $\{|0 \leqslant n \leqslant \Omega\rangle\}$. Going from curve 2 to curve 3, we remove the error owing to the inaccuracy of the harmonic potential ω^2 in the next-to-leading order in $1/\Omega$: We replace ω^2 in Eq. (29) by $\omega^2 = 1 - \kappa^2\Omega(\Omega + 2)$, which is correct not only in the leading order but also in the next-to-leading order of $1/\Omega$. Finally in curve 4 the "divergent" term $\Lambda^{(04)} < 0$ is included. We see that curve 4 is a much better calculation than curve 1. The little "kink" on curve 4 near $\kappa = 0.05$ coincides with the phase transition of the system, where the spectrum becomes double-degenerate inside a

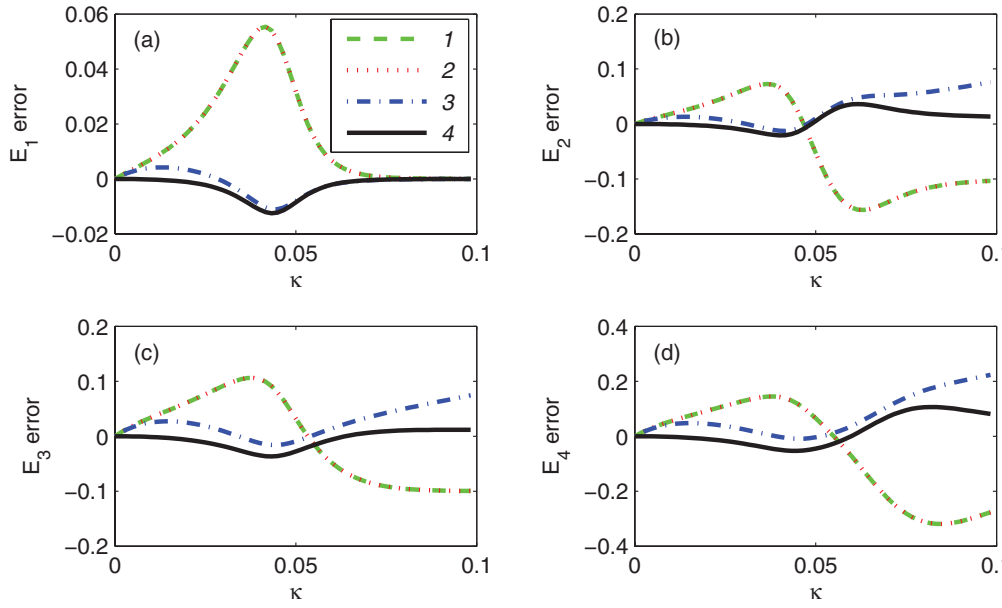

FIG. 2. (Color online) The errors of the first four excitation energies $E - E_{\text{exact}}$ as a function of κ in a set of calculations. (a), (b), (c), and (d) are for the first, second, third, and fourth excitation energy, respectively. Four lines on each panel are obtained by diagonalizing different collective Hamiltonian in different phonon space. Curve 1 (green dashed line): $H = \frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2 + \frac{\Lambda^{(40)}}{4!}\alpha^4$ in $\{|0 \leqslant n < +\infty\rangle\}$. Curve 2 (red dotted line): $H = \frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2 + \frac{\Lambda^{(40)}}{4!}\alpha^4$ in $\{|0 \leqslant n \leqslant \Omega\rangle\}$. Curve 3 (blue dashed-dotted line): $H = \frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2 + \frac{\Lambda^{(40)}}{4!}\alpha^4$ in $\{|0 \leqslant n \leqslant \Omega\rangle\}$, but with $\omega^2 = 1 - \kappa^2\Omega(\Omega + 2)$ replacing that in Eq. (29). Curve 4 (black solid line): $H = \frac{\omega^2}{2}\alpha^2 + \frac{1}{2}\pi^2 + \frac{\Lambda^{(40)}}{4!}\alpha^4 + \frac{\Lambda^{(04)}}{4!}\pi^4$ in $\{|0 \leqslant n \leqslant \Omega\rangle\}$, also with $\omega^2 = 1 - \kappa^2\Omega(\Omega + 2)$. Curves 1 and 2 closely overlap and are indistinguishable on the figure.

well-developed (large enough $\omega^2 < 0$) double-well potential (see Fig. 1).

The *microscopically* calculated "divergent" terms should always be kept in the bosonic Hamiltonian when diagonalizing. Within the *finite* physical space, they mix nearby states without causing divergences. Because we are considering large amplitude (α^2) vibrations, the effect of the $\Lambda^{(04)}\pi^4 < 0$ term in the Lipkin model is small. "Divergent" terms with α will have a bigger effect; also they may influence transition rates more than energies. In general, the exact finite physical space, bounded approximately by the collectivity factor Ω, is unknown. However, Ω can be estimated by the number of effectively nonvanishing one-particle–one-hole excitations in $r_{12}^{(10)}$ and $r_{12}^{(01)}$. Changing slightly the boundary of the physical space, the lowest several states would not change much, as they were composed mainly of the states with the smallest phonon numbers and therefore insensitive to the boundary. In this way the physical effects of the microscopically calculated "divergent" terms can be included.

From Fig. 2 we see that the next-to-leading order terms in $1/\Omega$ of the RPA frequency ω^2 could be important. In realistic nuclei, the critical point $\omega^2 \approx 0$ could be reached at a relatively small Ω. For example, $^{100}_{46}$Pd at the critical point [16] has only eight valence particles (although pairing increases collectivity). Within the GDM method, we should calculate the next-to-leading order terms in $1/\Omega$ in the RPA equations. Firstly, Eq. (11), which is equivalent to $N[a_4^\dagger a_3^\dagger a_2 a_1] \doteq N[a_4^\dagger a_1]N[a_3^\dagger a_2] - N[a_4^\dagger a_2]N[a_3^\dagger a_1]$ by Wick theorem ($N[\cdots]$ is normal ordering with respect to the HF ground state), should be replaced by $2N[a_4^\dagger a_3^\dagger a_2 a_1] \doteq N[a_4^\dagger a_1]N[a_3^\dagger a_2] - N[a_4^\dagger a_2]N[a_3^\dagger a_1] + N[a_3^\dagger a_2]N[a_4^\dagger a_1] - N[a_3^\dagger a_1]N[a_4^\dagger a_2]$, because of the apparent antisymmetry. Secondly, terms in Eq. (11) that are not factorizable into products of one-body GDM operators should be taken into account, probably by calculating the equations of motion of $a_4^\dagger a_3^\dagger a_2 a_1$.

V. CONCLUSION

In summary, we presented the detailed procedure of microscopic calculations of the collective bosonic Hamiltonian by the GDM method. The correct rotational symmetry and effects of pairing for realistic nuclear systems were not discussed here but they are included in the whole scheme in a straightforward manner, see Secs. VI and VII of Ref. [14]. The most interesting realistic problems include the microscopic description of soft nuclei with large vibrational amplitude and therefore strong anharmonicity that leads to various group structures of the dynamics and possible shape instability and coexistence. Another type of problems concerns the coupling between various collective modes, an interesting example of recent experimental observation of clear quadrupole-octupole correlation in Xe isotopes can be found in Ref. [17]. We can also mention that the noncollective states not included in the band form an environment that can be accounted for at least in average using the statistical approach based on the ideas of quantum chaos and complexity. The work along these lines is in progress.

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