

Beyond mean field study of excited states: Analysis within the Lipkin modelA. P. Severyukhin,^{1,2} M. Bender,³ and P.-H. Heenen²¹*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, RU-141980 Dubna, Moscow region, Russia*²*PNTPM, CP229, Université Libre de Bruxelles, B-1050 Brussels, Belgium*³*CEA Saclay DSM/DAPNIA/SPhN, F-91191 Gif sur Yvette, France*

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We compare the generator coordinate method (GCM) and the random-phase approximation (RPA) in the framework of the exactly solvable Lipkin-Meshkov-Glick model. We show that the discretized GCM works quite well and permits to obtain results close to the exact results with a small number of discretization points.

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I. INTRODUCTION

Self-consistent mean-field methods are one of the standard microscopic approaches in nuclear structure theory [1]. At present, they are the only available microscopic method that can be systematically applied on a large scale for medium and heavy nuclei.

Despite its successes, the self-consistent mean-field method has a number of well-known limitations. From a conceptual point of view, the mean-field approach is designed to describe ground-state properties, and gives only access to the properties of very specific excited states, like collective rotational bands or high K-states. This is in contrast to the *ab initio* methods that are available for light nuclei, like the no-core shell model and the shell-model Monte Carlo, which also describe excitation spectra. A systematic way to resolve these problems is offered by symmetry restoration and configuration mixing. Several groups now develop methods going beyond a mean-field approach based on the generator coordinate method (GCM), either with nonrelativistic Skyrme [2,3] or Gogny [4] interactions, or with relativistic Lagrangians [5], see also [6,7] and references given therein. The aim is to obtain a unified description of ground states and of excited states of all nuclei, including collective correlations which cannot be included in a mean-field approach, even at the effective interaction level.

First applications have demonstrated that such a method permits to describe the energies of low-lying collective excitations and electric transition probabilities, in-band and out-of-bands. However, in many cases it has also been found that whenever states can be grouped into rotational bands, the spectra obtained with the GCM are too spread and that the excitation energies are too high. For spherical nuclei, in particular those close to doubly-magic ones, the low-energy collective spectra are only qualitatively in agreement with the data.

The origin of this problem is not obvious and it cannot be expected to be unique. A possible source of error could be the inadequacies of effective interactions to describe spectra. Another source of uncertainty comes from the choice of the variational space in which the configuration mixing is performed. It is usually constructed by introducing in the mean-field equations constraints on one or a few collective variables related to the shape of the nuclear density. Such a choice may be more appropriate to describe the properties of ground states than those of excited states, for which additional degrees of freedom might have to be included.

The random-phase approximation (RPA), or quasiparticle RPA (QRPA) when including pairing, has a reputation of working much better than the GCM for spherical nuclei. One reason is that in the limit of vanishing residual interactions, the lowest excited states in spherical nuclei might be broken-pair two-quasiparticle states. In the RPA framework, excited states are explicitly constructed as coherent superpositions of all possible two-quasiparticle states; hence, the RPA automatically contains the proper noninteracting limit for which the ground state is an HFB vacuum. In the standard GCM, by contrast, the excited states are constructed in a basis of HFB vacua which differ in one or several collective coordinates, as for example quadrupole deformation. The choice of the collective coordinates is usually such that they correspond to a superposition of decorrelated-pair two-quasiparticle and $2n$ -quasiparticle states when expressed through the Thouless theorem in terms of a single reference HFB vacuum; hence, the standard GCM might not contain the proper noninteracting limit of HFB. Including broken-pair two-quasiparticle states into the projected GCM is less a conceptual problem than a practical one, as many of the simplifications that can be used in the calculation of GCM kernels between time-reversal invariant HFB vacua are not longer valid for kernels involving explicitly quasiparticle states.

A comparison of projected GCM and QRPA in semimagic or doubly-magic nuclei for realistic cases is not a simple task, however, as it is very difficult to perform the calculations under exactly the same conditions. There are issues of convergence and consistency of the residual interaction which cause difficulties, but are not insurmountable. One more fundamental difficulty is caused by the breakdown of the HFB method to describe pairing correlations in the weak-pairing regime. The GCM has to be performed with pairing correlations, otherwise the overlap kernel between states on both sides of a level crossing at the Fermi surface vanishes, which artificially decouples regions with different deformation and causes instabilities when solving the Hill-Wheeler-Griffin equation. The problem is easily solved when enforcing pairing correlations in the generating states through the Lipkin-Nogami prescription. Such states, however, are not HFB ground states anymore, which makes it impossible to use the same procedure in the context of QRPA.

We have performed a direct comparison of the GCM and the RPA calculation of the first 2^+ excitation in tin isotopes

which has not been very conclusive. The two main results may be summarized as followed. The experimental 2^+ energy is overestimated by the RPA, which points out to a deficiency of the effective interaction that was used (the Skyrme SLy4 parametrization). On the other hand, the 2^+ GCM energy is significantly larger than the RPA one, indicating probably a deficiency in the variational space of the GCM. However, too many differences remain between the GCM and the RPA calculations. As we discussed above, there was always some pairing for neutrons and protons in the GCM, while the proton pairing was always absent in the RPA. Several small energy terms were also not treated in a completely equivalent way in the RPA and the GCM and to make both treatments completely similar seems to be hopeless.

One therefore needs a view on the problem from another perspective. Exactly solvable models constitute a very fruitful ground for the test of and comparison between many-body methods. They also permit to explore new developments at a very limited cost. For our purpose, we need a model where collective variables similar to deformations can be introduced and where a discretized version of the GCM can be defined in a way similar to that of the realistic applications. The Lipkin-Meshkov-Glick (LMG) model, introduced in Ref. [8], has the required properties. Depending upon the strength of the interaction, two different kinds of solutions are obtained at the Hartree-Fock level [9]: “spherical” ones at low values of the strength, and “deformed” ones beyond a critical strength.

The rest of the paper will be devoted to a detailed discussion of excited states in the context of the LMG model.

II. EXCITED STATES IN THE LIPKIN-MESHKOV-GLICK MODEL

A. The model

Lipkin, Meshkov, and Glick introduced an exactly solvable model [8], usually called “Lipkin model” or “LMG model” in the literature, that has been widely used to test methods of approximation for the nuclear many-body problem.

The model consists of N fermions distributed in two N -fold degenerate shells separated by an energy ε . In their original paper, two different Hamiltonians were proposed. The one which is the most usually studied contains a monopole-monopole interaction and is given by

$$\hat{H} = \varepsilon \hat{J}_0 - \frac{1}{2} V (\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_-), \quad (1)$$

where V is the interaction strength and \hat{J}_0, \hat{J}_\pm are quasispin operators [8–10]

$$\begin{aligned} \hat{J}_0 &= \frac{1}{2} \sum_{p=1}^N (\hat{c}_{+p}^\dagger \hat{c}_{+p} - \hat{c}_{-p}^\dagger \hat{c}_{-p}), \\ \hat{J}_+ &= \sum_{p=1}^N \hat{c}_{+p}^\dagger \hat{c}_{-p}, \\ \hat{J}_- &= \hat{J}_+^\dagger \end{aligned} \quad (2)$$

with the algebra

$$[\hat{J}_+, \hat{J}_-] = 2\hat{J}_0, \quad [\hat{J}_0, \hat{J}_\pm] = \pm \hat{J}_\pm. \quad (3)$$

The operators \hat{c}_{+p}^\dagger and \hat{c}_{-p}^\dagger create a particle in the upper or lower shells, respectively, where p labels the N degenerate levels within the shells. The operator \hat{J}_0 measures half of the difference between the number of particles in the upper and the lower levels.

The exact wave functions are eigenstates of two operators, the total quasispin operator $\hat{J}^2 = \frac{1}{2}(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+) + \hat{J}_0^2$ with eigenvalue $J(J+1)$, and a signature operator $e^{i\pi \hat{J}_0}$, which, for an even number of particles, has two eigenvalues equal to ± 1 . Therefore, as discussed in detail in Ref. [8], the interaction does not mix states which have different eigenvalues of \hat{J}^2 and $e^{i\pi \hat{J}_0}$ and the Hamiltonian matrix splits into blocks, which are multiplets in J of order $2J+1$. The multiplets separate further into blocks of size of J and $J+1$ corresponding to the two values for the signature.

To understand the connection between the LMG model and realistic nuclear models, it is interesting to identify the structure of its eigenstates [11]. In the limit of vanishing interaction strength $V=0$, the exact ground state corresponds to an independent particle state with all the lower single-particle levels occupied, while the exact first excited state is given by a 1p-1h excitation on top of the ground state, the second excited state by 2p-2h excitations, etc.

As the Hamiltonian does not mix states with different J values, the exact wave functions are linear combinations of the $2J+1$ eigenfunctions of the operator \hat{J}_0 within a multiplet of given J [8]. There is one state of each possible np - nh content in each multiplet. The non-interacting ground state has $J_0 = -N/2$, and belongs to the multiplet with maximum J , i.e., $J = N/2$. The first noninteracting excited state is a 1p-1h state which has $J_0 = -N/2 + 1$. Pure 1p-1h states are admixtures of states from the $J = N/2$ and $J = N/2 - 1$ multiplets, while pure 2p-2h states are admixtures of states within the $J = N/2, J = N/2 - 1$ and $J = N/2 - 2$ multiplets, etc., for higher np - nh excitations until $n = N$.

For small values of the interaction strength V , the mixing within the multiplets should be small and low-lying levels should have a similar structure as the noninteracting ones. By contrast, for large values of V , the eigenstates will exhibit a complicate mixing of many p-h excitations. Thus, the model exhibits a transition between shell-model-like states and collective states.

B. Mean-field approximation

In mean-field, or Hartree-Fock (HF), approximation, the many-body wave function $|\alpha, \varphi\rangle$ is given by a Slater determinant

$$|\alpha, \varphi\rangle = \prod_{p=1}^N \hat{a}_{0p}^\dagger |-\rangle, \quad (4)$$

characterized by two real degrees of freedom α and φ , that will be specified below. The particle- and hole-creation operators of the corresponding HF single particle basis are given by a unitary transformation among the operators corresponding to

the noninteracting basis [9,10]:

$$\begin{pmatrix} \hat{a}_{1p}^\dagger \\ \hat{a}_{0p}^\dagger \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha)e^{-i\varphi} \\ \sin(\alpha)e^{i\varphi} & \cos(\alpha) \end{pmatrix} \begin{pmatrix} \hat{c}_{+p}^\dagger \\ \hat{c}_{-p}^\dagger \end{pmatrix}. \quad (5)$$

The subscripts 0 and 1 denote hole and particle states, respectively. The variables α and φ vary both in the interval $[-\pi/2, \pi/2]$. They can be identified as constraints, that, due to the low dimensionality of the LMG model, map the entire space of mean-field states. New quasispin operators corresponding to the states with finite α and φ can be easily constructed, as described, for example, in Ref. [10]. An alternative manner to write the constrained HF states will be useful in the context of the GCM. Using the Thouless theorem [12], the normalized constrained HF states $|\alpha, \varphi\rangle$ can be obtained from the noninteracting ground state, that corresponds to $\alpha = \varphi = 0$, as

$$|\alpha, \varphi\rangle = \cos^N(\alpha) \exp[i\varphi \hat{J}_+] |\alpha = 0, \varphi = 0\rangle. \quad (6)$$

As pointed out by Bhaumik *et al.* [13], the constrained HF states of the LMG model can also be formulated in the language of coherent states, which allows to make use of generating functional techniques to calculate matrix elements [14].

The constrained HF ground-state energy is a function of the variables α and φ :

$$E_{gs}^{\text{HF}}(\alpha, \varphi) = -\frac{\varepsilon N}{2} \left[\cos(2\alpha) + \frac{1}{2} \chi \sin^2(2\alpha) \cos(2\varphi) \right], \quad (7)$$

where

$$\chi = \frac{(N-1)V}{\varepsilon}. \quad (8)$$

Note that, for a given value of α , the lowest HF state always corresponds to $\varphi = 0$. The eigenvalues of the single-particle Hamiltonian, usually called single-particle energies, depend on α only for any mean-field state $|\alpha, \varphi\rangle$.

One can identify the variable α as a deformation parameter. There is a phase transition at $\chi = 1$ from a spherical ($\alpha = \varphi = 0$) to a “deformed” ground state. In the latter case, the value of α is obtained by solving the equation $\chi \cos(2\alpha) = 1$. The phase transition and the properties of exact and approximated ground states in this regime were first discussed by Agassi *et al.* [15].

While the HF states remain eigenstates of \hat{J}^2 , “deformed” HF states break the signature symmetry of the exact solutions (which is often called “parity” in the literature) for any nonzero value of α . The HF states mix the np - nh states with even and odd n within a given J multiplet. As a consequence, the constrained HF states for nonzero interaction strength contain $0p$ - $0h$, $1p$ - $1h$, $2p$ - $2h$, $3p$ - $3h$, etc., states. The np - nh components with even and odd n can be separated with a projection operator [15,16]. Due to the simple structure of the LMG model with one relevant coordinate only, minimization of the energy obtained by projection after variation is equivalent to projection before variation [16].

The signature symmetry is a discrete symmetry, in contrast to the continuous rotational symmetry broken in nuclei with a quadrupole deformation. Li *et al.* [17] have introduced a generalization of the LMG model that can be used to test

techniques for approximate angular-momentum projection, see Ref. [18] and references therein. The structure of the original LMG model is closer to parity projection in octupole-deformed nuclei [16].

The interpretation of the φ degree of freedom is less intuitive. It enters the HF states as a phase. It is explored by time-dependent HF (TDHF) states, hence a necessary ingredient of any dynamical model [19,20]. Using the variables α and φ , one can form a set of two canonically conjugate variables with which, for example, the time-dependent HF equations can be transformed to classical equations of motion [19].

C. Random phase approximation

The RPA of the LMG model was formulated for the first time in Ref. [8]. The RPA is usually constructed on top of the “spherical” HF state $|\alpha = 0, \varphi = 0\rangle$, which is the ground state for $\chi < 1$. In this regime, the RPA phonon creation operator, defined as a superposition of all possible $1p$ - $1h$ excitations, is given by

$$\hat{Q}^\dagger = \frac{1}{\sqrt{N}}(X\hat{J}_+ - Y\hat{J}_-). \quad (9)$$

One assumes that the ground state is the RPA phonon vacuum $|0\rangle$, i.e., $\hat{Q}|0\rangle = 0$. The first excited state is given by $\hat{Q}^\dagger|0\rangle$ with the normalization condition:

$$\langle 0 | [\hat{Q}, \hat{Q}^\dagger] | 0 \rangle = X^2 - Y^2 = 1. \quad (10)$$

Profiting from the simplicity of the LMG model, the authors of Ref. [8] have solved $\hat{Q}|0\rangle = 0$ exactly. The usual way is to solve the RPA equations in the space of $1p$ - $1h$ excitations by linearization. Making use of the equation-of-motion approach [21,22]:

$$\langle 0 | [\delta\hat{Q}, [\hat{H}, \hat{Q}^\dagger]] | 0 \rangle = (E - E_0) \langle 0 | [\delta\hat{Q}, \hat{Q}^\dagger] | 0 \rangle, \quad (11)$$

where E is the absolute energy of the RPA state, and E_0 the energy of the RPA ground state, one obtains the RPA equations:

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = (E - E_0) \begin{pmatrix} X \\ Y \end{pmatrix}, \quad (12)$$

where $\mathcal{A} = \varepsilon$ and $\mathcal{B} = -(N-1)V = -\varepsilon\chi$.

From these equations, the excitation energy of the first excited state of the Hamiltonian (1) within the RPA is found to be

$$E - E_0 = \varepsilon\sqrt{1 - \chi^2}. \quad (13)$$

This energy is equal to zero for $\chi = 1$, where the system undergoes a phase transition, and becomes imaginary for even larger values of χ .

The RPA is explicitly constructed as a superposition of $1p$ - $1h$ states; hence, it automatically contains the right physics of the lowest excited state in the limit $\chi \rightarrow 0$ and should be accurate in the limit of small χ .

The RPA correlation energy [9] in the ground state is given by

$$\Delta E = \frac{1}{2}(E - E_0 - \varepsilon). \quad (14)$$

D. Generator coordinate method

1. Continuous GCM

Most applications of the GCM to the LMG model are restricted to a study of the GCM ground state and test the correlations in the ground state [23]. In such cases, one can take the “deformation” α as a single generator coordinate. We are here also interested in the description of excited states and will also introduce φ as a generator coordinate.

One can write the N -particle GCM wave functions as a linear combination of the constrained HF states $|\alpha, \varphi\rangle$ (6) with an unknown weight function $f_k(\alpha, \varphi)$

$$|\Psi_k\rangle = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\varphi f_k(\alpha, \varphi) |\alpha, \varphi\rangle. \quad (15)$$

$$\begin{aligned} \langle \alpha', \varphi' | \hat{H} | \alpha, \varphi \rangle &= -\frac{\varepsilon N}{2} \langle \alpha', \varphi' | \alpha, \varphi \rangle \\ &\times \frac{\cos^2(\alpha) \cos^2(\alpha') - \sin^2(\alpha) \sin^2(\alpha') e^{2i(\varphi-\varphi')} + \chi [\sin^2(\alpha) \cos^2(\alpha') e^{2i\varphi} + \cos^2(\alpha) \sin^2(\alpha') e^{-2i\varphi}]}{[\cos(\alpha) \cos(\alpha') + \sin(\alpha) \sin(\alpha') e^{i(\varphi-\varphi')}]^2}. \end{aligned}$$

A set of orthonormal collective wave functions are obtained by an integral transformation of f_k

$$G_k(\alpha', \varphi') = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\varphi \langle \alpha', \varphi' | \alpha, \varphi \rangle^{\frac{1}{2}} f_k(\alpha, \varphi). \quad (18)$$

The HWG integral equation can be solved exactly [9]. Thanks to the simplicity of the LMG model, the GCM with a single generator coordinate α gives already the exact solutions of the model. The GCM is build on signature-symmetry breaking constrained HF states; hence, *a priori* the GCM wave function mixes 0p-0h, 1p-1h, 2p-2h, 3p-3h, etc., states. However, one can easily see that the signature symmetry is restored by mixing of HF wave functions corresponding to $\pm\alpha$ with weights equal in modulus, which comes out automatically from Eq. (15). This situation is similar to realistic applications of the GCM when a discrete symmetry, like parity, is broken at the mean-field level but not for continuous symmetries like rotations.

2. Discretized GCM

In realistic calculations [2–5], the HWG equation is solved by discretization of the collective variables

$$|\Psi_k\rangle = \sum_{\alpha} \sum_{\varphi} f_k(\alpha, \varphi) |\alpha, \varphi\rangle. \quad (19)$$

The discretized GCM equations are obtained by replacing all integrals in Eqs. (15)–(18) by sums over discretization points. The integral equation (16) becomes a matrix equation which can be solved by diagonalization.

As our aim is to understand why the GCM overestimates excitation energies in realistic applications, we will solve the HWG equation of the LMG model by discretization. Since the continuous GCM permits to find the exact eigenstates of

Variation of the energy yields the so-called Hill-Wheeler-Griffin (HWG) equation [24], an integral equation for $f_k(\alpha, \varphi)$

$$\begin{aligned} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\varphi (\langle \alpha', \varphi' | \hat{H} | \alpha, \varphi \rangle \\ - E_k \langle \alpha', \varphi' | \alpha, \varphi \rangle) f_k(\alpha, \varphi) = 0. \end{aligned} \quad (16)$$

The two kernels entering Eq. (16) are the norm kernel

$$\langle \alpha', \varphi' | \alpha, \varphi \rangle = [\cos(\alpha) \cos(\alpha') + \sin(\alpha) \sin(\alpha') e^{i(\varphi-\varphi')}]^N, \quad (17)$$

and the Hamiltonian kernel

the LMG Hamiltonian, the number of discretization points must be small enough to avoid a trivial reproduction of the exact solution.

We have solved the LMG model for 30 and 50 particles, with a discretization on meshes symmetric around zero in α and φ and with an odd number of points. The meshes in α and φ have been limited to the region in which the collective wave function has a sizable amplitude, typically less than half the total range of variation of α . The mean-field potentials that are obtained for two values of χ , above and below the phase transition, are plotted in Fig. 1. The mean-field ground state corresponds to α and φ equal to zero when χ is smaller than 1, and to a nonzero value of α otherwise. The energy surface is very flat for small values of φ ; it is only when α is large that the energy increases rapidly with φ . Such a topography is representative of the deformation energy curve that is obtained for spherical nuclei ($\chi < 1$) and for nuclei soft as a function of deformation ($\chi > 1$).

In Fig. 2, the exact and GCM energies for the ground state and for the first two excited states are plotted as a function of the two-body interaction strength χ for a system of 30 particles. We have used α as the only generator coordinate. The GCM equations are solved with seven equidistant discretization points chosen in the region where the collective wave functions have a sizable amplitude. In realistic applications of the GCM, the overlap kernel is used to define the mesh, the requirement being that the overlap between two adjacent points is of the order of 0.8. However, in the LMG model, this kernel does not depend on the two-body interaction strength. Since we want to be as close as possible to realistic applications, where the exact solutions are not known, we have taken the same mesh for all interaction strengths. From the collective wave function obtained for a value of χ around 0.5, we have chosen points

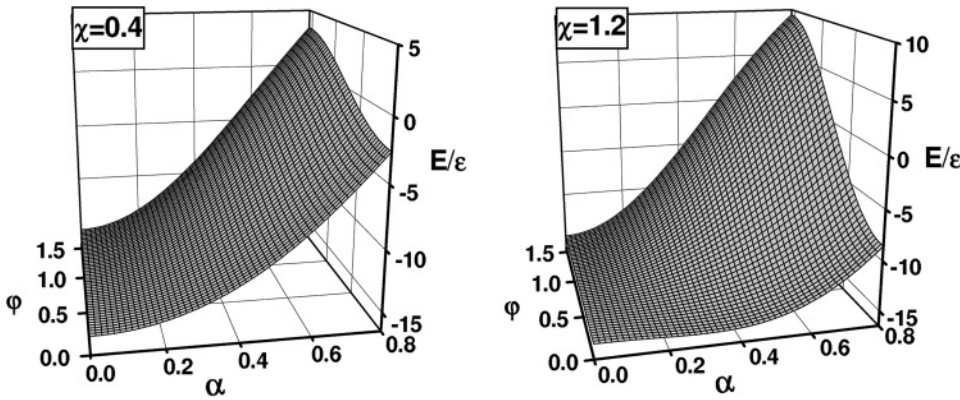


FIG. 1. Mean-field potentials for two values of the interaction strength, $\chi = 0.4$ and $\chi = 1.2$, for $N = 30$ particles.

in the interval $(-0.707, +0.707)$. Since the wave functions of the model are either even or odd with respect to α , only four discretization points are significant.

For $\chi < 1$, the HF ground-state energy does not depend on χ , as the ground state is always “spherical.” The HF excited states are then p-h states whose energy also does not vary with

χ . The correlations beyond mean-field significantly improve the HF result for the ground state and bring it very close to the exact value for all values of the interaction strength. The situation is less satisfactory for excited states: in particular, their excitation energies are far from the exact values when the interaction is switched off, while the HF method gives the exact energies. The discretized GCM becomes more accurate than HF only for χ larger than 0.25 for the second excited state and than 0.45 for the first one.

To understand this surprising result, let us analyze in more details how the continuous GCM works in the $\chi = 0$ limit. Let us first note that, while the exact ground state wave function, corresponding to α and φ equal to zero, is included in the generating functions $|\alpha, \varphi\rangle$, the first excited states corresponding to pure 1p-1h and 2p-2h excitations are not. One can easily verify that the weight functions that permit to extract the exact eigenstates are the Dirac $\delta(\alpha)$ distribution for the ground state, its first derivative for the first excited state and combination of $\delta(\alpha)$ and its derivatives for higher excitations. The collective wave functions, given by Eq. (18), are regular functions but with rather sharp peaks. One of them is located at α equal to 0 for even signature states, while the odd signature states vanish at 0. Moreover, for very small values of χ , the collective wave-functions have very small amplitudes at the most extreme mesh points, leaving only a very small number of significant discretization points.

Replacing one of the mesh points by a point close to the extrema of the wave functions of the first and second excited state for χ equal to zero, the discretized GCM results become very close to the exact values for the three first states and for low interaction strengths. For the first excited state, which has a node at the origin, this discretization is superior to the one based on the $\chi = 0.5$ ground state wave function up to $\chi = 0.75$.

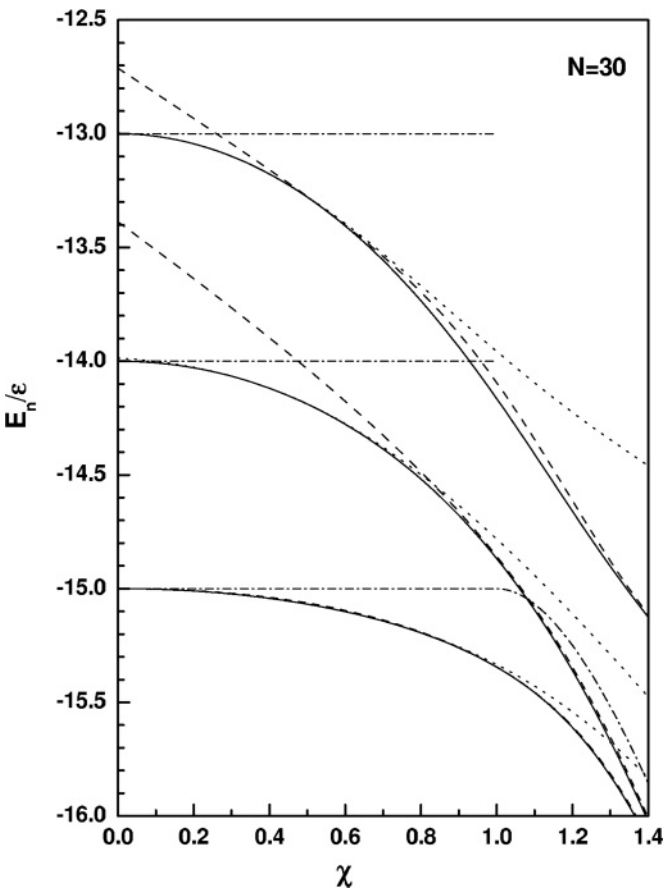


FIG. 2. Comparison between the exact and GCM energies of the first three states of the LMG model for 30 particles. The solid lines are the exact result, while the dashed and dotted lines represent the GCM solutions obtained with the two different meshes (see text) with seven points in α . The HF results are indicated by a dash-dotted line.

3. The role of the second generator coordinate

The influence of a second generator coordinate is shown in Fig. 3, where are plotted the energies of the first three states of a system with 50 particles. The calculations are performed with seven and nine points in α , and one or three points in φ . For the mesh in α we choose equidistant points in the interval

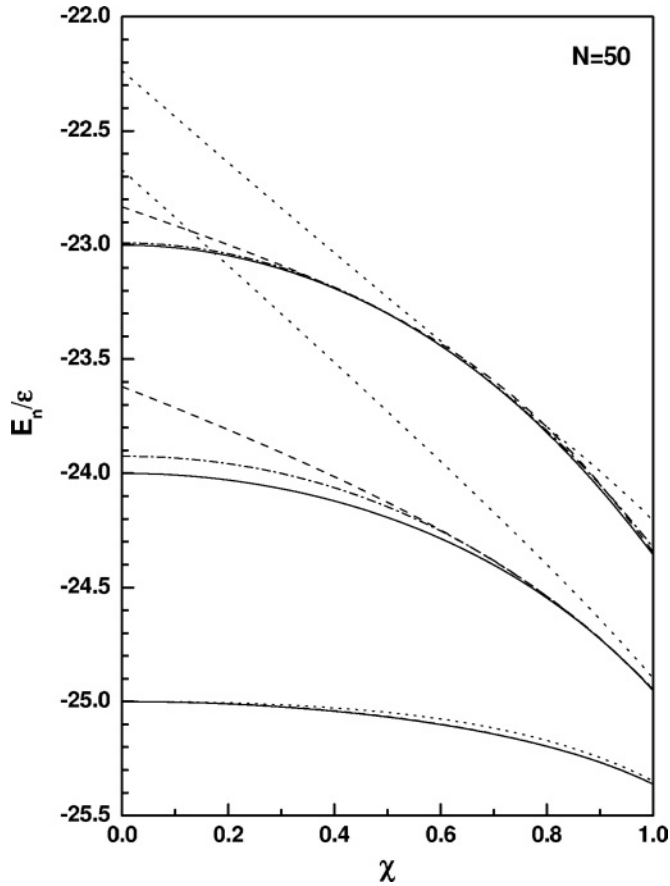


FIG. 3. Comparison between the exact and GCM energies of the first three states of the LMG model for a system with $N = 50$. Two generator coordinates, α and φ are used in the GCM. The exact result are represented by solid lines. The dotted and dashed lines are GCM results with seven and nine points in α ; the dash-dotted lines are results of calculations with seven points in α and three points in φ .

$(-0.660, +0.660)$. Since the mesh in φ is symmetric and $\varphi = 0$ is always a mesh point, there is in practice one active point in φ . All discretizations give accurate results for the ground state. With a mesh in α only, the energies of the first excited state are inaccurate, for all interaction strengths with seven points, and below χ equal to 0.4 for a nine point discretization. The second excited state is slightly better described although the accuracy is still limited for small interaction strengths. Adding points in φ to the calculation with seven points in α corrects the behavior near the origin and leads to very accurate results for the ground state and the second excited state. The energy of the first excited state is also improved although there still remains a small discrepancy for small interaction strengths. The combination of nine points in α and three points in φ leads to results indistinguishable from the exact ones.

4. Comparison between the GCM and the RPA

The RPA permits to determine excited states as well as correlation energies in the ground state. The correlations that are given by Eq. (14) are very accurate and make the RPA

ground state energies very close to the exact values up to interaction strength equal to 0.9. Beyond this value, the GCM with seven discretization points is more accurate than the RPA.

The GCM and RPA results for the excitation energies of the first two excited states are compared to the exact values in Fig. 4. It is the accuracy of this energy difference which is the most interesting in usual applications of the GCM. The use of a mesh adjusted for an intermediate interaction strength ($\chi = 0.5$) and on the ground state gives values for the energies of the second excited state close to the exact ones when the interaction strength is large but it fails for weak interactions. The situation is even worse for the first excited state which does not have the same symmetry as the ground state. In this case, results are close to the exact ones only beyond χ equal to 0.75, the error being as large as 60% for χ close to zero. The results are by far better when the mesh is adapted for low- χ values, as discussed above. Then, even for a small number of mesh points, the exact results for both excited states are correctly reproduced by a discretized GCM calculation. The RPA results have a very different behavior. They reproduce the exact results quite well for small interaction strengths. The first excited state becomes inaccurate above χ equal to 0.7;

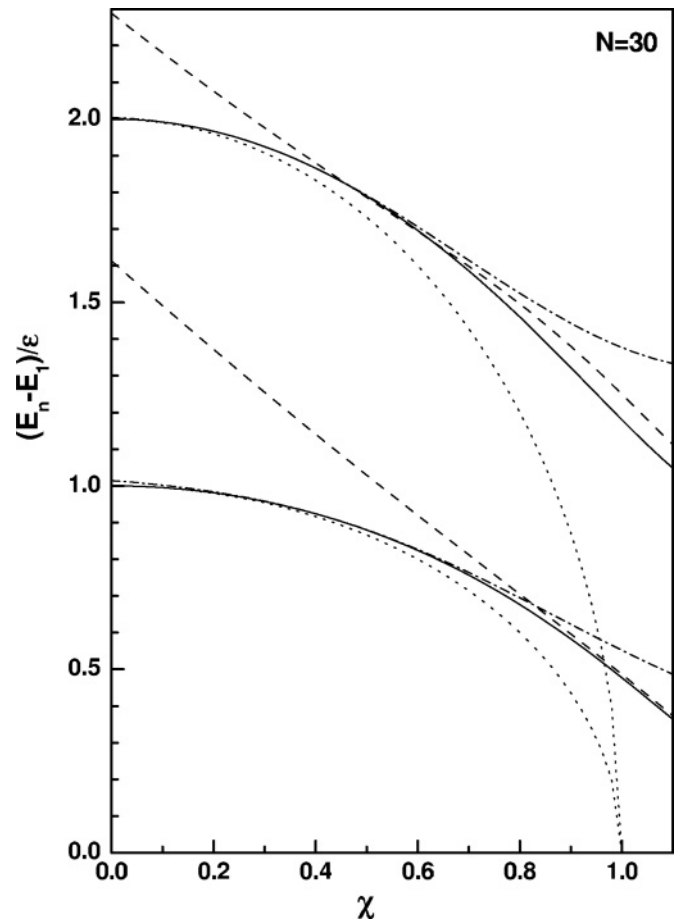


FIG. 4. Excitation energies of the first two excited states as a function of the interaction strength χ . Exact results are given by solid lines, the RPA results by dotted lines. The dashed and dash-dotted lines correspond to GCM calculations with the same choices of points as in Fig. 2.

the second one deteriorates more quickly and is worse than the blind GCM discretization above χ around 0.5.

III. CONCLUSIONS

In this paper, we have analyzed the quality of GCM and RPA to describe excited states within the LMG model. To the best of our knowledge, we have analyzed for the first time the application of the discretized GCM to the LMG model. To summarize our results, one can say first that the discretized version of the GCM works remarkably well and permits to reproduce the exact results with a very limited number of points. Of course, the dimension of the LMG model is very limited but nearly exact results are obtained for the three first states using only approximately 1% of the total number of independent vectors of the LMG space. A second result is that correlations in the ground state are better described than correlations in excited state. We have also seen that results are closer for the second excited state which has the same

symmetry as the ground state than for the first one. The fact that an appropriate choice of a small number of discretization points permits to obtain excellent results, better than the RPA, seems to be an artefact of the LMG model, hard to transpose on realistic cases. On the other hand, it seems encouraging that the excited states are well described by the GCM when the collectivity due to the generator coordinate is large. Finally, the introduction of a second generator coordinate, with which one can form a coordinate conjugate to the first one, also improves the GCM results and seem to make them more independent on the way the discretization is performed.

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