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# Equations of motion for a spectrum-generating algebra: Lipkin–Meshkov–Glick model

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**Abstract**

For a spectrum-generating Lie algebra, a generalized equations-of-motion scheme determines numerical values of excitation energies and algebra matrix elements. In the approach to the infinite particle number limit or, more generally, whenever the dimension of the quantum state space is very large, the equations-of-motion method may achieve results that are impractical to obtain by diagonalization of the Hamiltonian matrix. To test the method's effectiveness, we apply it to the well-known Lipkin–Meshkov–Glick (LMG) model to find its low-energy spectrum and associated generator matrix elements in the eigenenergy basis. When the dimension of the LMG representation space is $10^6$, computation time on a notebook computer is a few minutes. For a large particle number in the LMG model, the low-energy spectrum makes a quantum phase transition from a nondegenerate harmonic vibrator to a twofold degenerate harmonic oscillator. The equations-of-motion method computes critical exponents at the transition point.

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## 1. Introduction

Suppose the Hamiltonian $\hat{H}$ of some quantum system is a self-adjoint operator on a Hilbert space $\mathcal{H}$, and $\mathfrak{g}$ is a real Lie algebra of skew-adjoint operators on $\mathcal{H}$. When the commutator of the Hamiltonian with any Lie algebra operator is an operator in the enveloping algebra, $\mathrm{U}(\mathfrak{g})$, of $\mathfrak{g}$, then $\mathfrak{g}$ is said to be a spectrum-generating algebra [1, 2]. If $\{\hat{X}_1, \hat{X}_2, \ldots\}$ is a basis of a spectrum-generating algebra (SGA) $\mathfrak{g}$, then the following commutation relations are satisfied:

$$[\hat{X}_\alpha, \hat{X}_\beta] = \sum_\gamma C^\gamma_{\alpha\beta} \hat{X}_\gamma \in \mathfrak{g} \tag{1}$$

  

$$[\mathrm{i}\hat{H}, \hat{X}_\alpha] = \hat{A}_\alpha \in \mathrm{U}(\mathfrak{g}). \tag{2}$$

Such algebras characterize dynamical symmetries in physics [3]. In many cases of interest including the subject of this paper, the Hamiltonian itself is an element of $\mathrm{U}(\mathfrak{g})$.

A ubiquitous computational physics problem is to calculate the eigenvalues of the Hamiltonian on the representation space and the matrix elements of Lie algebra elements with respect to Hamiltonian's eigenvectors. The eigenvalues are the energy levels of the system and the matrix elements of other observables in the Lie algebra determine properties of the system such as transition rates.

In highly favorable situations, eigenvector equations of the Hamiltonian may be solvable due to the existence of a symmetry subalgebra, $\mathfrak{g}_0 \subset \mathfrak{g}$, of the spectrum-generating algebra, comprising operators that commute with the Hamiltonian and, for which the branching rule $\mathfrak{g} \downarrow \mathfrak{g}_0$ for the representation of interest is multiplicity free. The hydrogen atom and the $n$-dimensional harmonic oscillator are well known to be solvable due to their large symmetry algebras, $\mathfrak{o}(4)$ and $\mathfrak{u}(n)$, respectively. Other systems are said to be *exactly solvable* when there exist complete sets of commuting operators which include the Hamiltonian. Such systems, which can be solved by Bethe ansatz methods, include, for example, some magnetic systems, such as the one-dimensional Heisenberg spin chain model [4, 5]. Some other Hamiltonians are quasi-solvable or enjoy a partial dynamical symmetry [6–8]. But, for a generic Hamiltonian, the 'brute force' solution to the eigenvalue problem requires the successful completion of three steps. First choose a basis for the Hilbert space and calculate the matrix elements of any Lie algebra element with respect to this basis. The matrix elements of the Hamiltonian, when an element of the enveloping algebra, can now be computed. Second diagonalize the Hamiltonian matrix. Third make a unitary transformation to determine the matrix elements of any Lie algebra element with respect to the basis of energy eigenvectors. The brute force approach is impractical when the dimension of the Hilbert space is infinite or simply too large. Moreover, as the present investigation shows, situations arise in which accurate approximate results cannot be obtained by diagonalization when a given basis is truncated to a tractable size.

The equations-of-motion solution proceeds in a single step to solve directly for energy levels and matrix elements with respect to the energy eigenvectors. Equations (1) and (2) form the system of equations that determine these quantities.

The equations-of-motion method of this paper is founded on three prior developments: a minimization technique for calculating the irreducible representations of difficult Lie algebras [9–11], the double-commutator equations-of-motion formalism [12, 13] and the Kerman–Klein equations-of-motion theory [14–16]. Thus, we refer to it as the RRKK method. Our generalization of equations-of-motion was applied recently to the five-dimensional quartic oscillator [17].

This paper applies the RRKK method to the Lipkin–Meshkov–Glick (LMG) model [18]. The Hamiltonian of the Lipkin model is a quadratic element in the enveloping algebra of $\mathfrak{su}(2)$. Our main purpose is to test the practicality of the equations-of-motion technique. We will find numerical solutions for the Lipkin model problem, even when the dimension of the representation space approaches an infinite value. For a large representation space, the Lipkin model exhibits a quantum phase transition from one harmonic oscillator vibrational phase with nondegenerate energy levels to another harmonic oscillator vibrational phase with each level twofold degenerate.

The LMG model is a tractable model that is sufficiently nontrivial to provide a useful test case for many-body approximation methods. Many researchers in nuclear physics, and, more recently, statistical and condensed matter science use the LMG model for this

purpose. For example, applying the double-commutator equations-of-motion theory to the LMG model Hamiltonian, Parikh and Rowe [19] show the limitations of the simple random phase approximation (RPA) and the improvements that can be gained by a renormalized RPA [12] in the neighborhood of the critical point. More recently, Takahara, Tohyama and Schuck test an extended RPA derived from time-dependent Hartree-Fock plus ground state correlations in the LMG model [20]. In other work, Harada studies LMG Brueckner theory [21], Abraham and Vary calculate a LMG effective interaction [22], Castaños, López-Peña and Hirsch investigate classical phase transitions using coherent states [23], Severyukhin, Bender and Heenen show a discretized generator coordinate method works effectively for the LMG model [24], and Cui, Li and Yi investigate geometric phases [25]. These are but a sampling of the many investigations using LMG reported in nuclear structure physics. Applications to other fields include Bose–Einstein condensation [26], the statistical physics of spin systems [27], the LMG thermodynamic limit [28] and quantum information theory [29–32]. The objective of several recent papers is the determination of LMG properties for large particle number.

The LMG Hamiltonian is solvable using the Bethe ansatz [33, 34]. Indeed the LMG model falls into the category of Richardson–Gaudin models for which eigenvalues are solutions to a coupled set of rational algebraic equations [35, 36]. Although these methods do not yield all results of interest, they have been shown to determine the low-energy spectra of many models for which a computation by matrix diagonalization is not possible.

A representation space $\mathcal{H}$ of a spectrum-generating algebra $\mathfrak{g}$ is an invariant subspace of any Hamiltonian in its enveloping algebra $\mathrm{U}(\mathfrak{g})$. If the representation is a direct sum of irreducible representations, say when $\mathfrak{g}$ is compact, then the general problem of finding the energies and matrix elements simplifies to the special case of an irreducible representation, an assumption we adopt.

The Lipkin Hamiltonian has some special properties which will be exploited, yet these are generally insufficient to easily find analytic solutions.

The equations of motion of the $\mathfrak{u}(n)$ SGA and the Hamiltonian eigenvalue problem on an $n$-dimensional Hilbert space are mathematically equivalent in the same way as the Heisenberg and Schrödinger formulations of quantum mechanics are equivalent. Compared to standard numerical methods for solving the $\mathfrak{u}(n)$ SGA nonlinear system, Jacobi matrix diagonalization is the superior computational tool when $n$ is not excessively large. It may also be the preferred method when one has a reasonable ordered basis in which to diagonalize so that an expansion of the eigenstates in the basis is sufficiently rapidly convergent.

The equations-of-motion method is computationally favorable compared to matrix diagonalization when the dimension of the SGA is small compared to the dimension $n$ of the representation space. For the LMG Hamiltonian, the SGA is the three-dimensional $\mathfrak{su}(2)$ algebra. The dimension $n$ of a LMG representation space of interest is much larger than three.

As computational procedures for quantum mechanical problems, equations-of-motion and matrix diagonalization are quite distinct. The most important difference is that the primary objects of the diagonalization approach are stationary states and energy eigenvalues, whereas, those of the equations-of-motion approach are dynamical quantities, such as transition matrix elements and energy differences.

Note that the SGA approach does not require knowledge of the basis states for the irreps concerned which, in any *a priori* defined basis, will generally be mixtures of states from the many equivalent irreps available. If the Hamiltonian is an element of the universal enveloping algebra of any spectrum-generating algebra, then its entire spectrum can be derived, at least in principle, by equations-of-motion methods in this way. Moreover, when $\hat{H} \in U(\mathfrak{g})$, an equations-of-motion solution determines absolute energies by evaluation of Hamiltonian's

expectation with respect to the ground state, cf, equation (18) for the LMG ground state energy.

Although the diagonalization method, when it can be carried out, has numerous advantages, particularly when there is an ordered symmetry-adapted basis in which the eigenstates of the Hamiltonian have reasonably rapidly convergent expansions, the equations-of-motion method has the huge advantage in general of not requiring a pre-defined basis; thus, when we seek approximate solutions to equations (1) and (2). To calculate accurately low-energy spectra, a solution to the equations of motion for the entire Hilbert space is unnecessary. It is sufficient to solve the equations in a subspace of dimension $p$ spanned by the $p$ lowest energy eigenstates of interest, where $p \ll \dim \mathcal{H}$. For example, in one calculation in this paper, $p = 6$ and $\dim \mathcal{H} = 1\,000\,000$.

By sacrificing exhaustive information about every eigenstate, most of which is of secondary or no interest, and focusing on the low-energy states, the equations-of-motion method achieves a dramatic improvement in computational speed compared to matrix diagonalization. If the dimension of the Hilbert space is so large that matrix diagonalization is a practical impossibility, equations of motion may provide a tractable method to attain usable results for eigenvalues and matrix elements.

## 2. Lipkin–Meshkov–Glick model

The complexification of the $\mathfrak{su}(2)$ algebra is spanned by $S_0, S_+, S_-$. A $\mathfrak{su}(2)$ unitary representation $\pi$ requires that $\pi(S_0) = \hat{S}_0$ is Hermitian, that the Hermitian adjoint of $\pi(S_+) = \hat{S}_+$ is $\pi(S_-) = \hat{S}_-$, that

$$\hat{S}_0 = \hat{S}_0^\dagger \tag{3}$$

$$\hat{S}_- = \hat{S}_+^\dagger, \tag{4}$$

and that the commutation relations are obeyed,

$$[\hat{S}_0, \hat{S}_+] = \hat{S}_+ \tag{5}$$

$$[\hat{S}_0, \hat{S}_-] = -\hat{S}_- \tag{6}$$

$$[\hat{S}_+, \hat{S}_-] = 2\hat{S}_0. \tag{7}$$

An $\mathfrak{su}(2)$ irreducible representation is labeled uniquely by its dimension $N + 1$, for $N = 2J = 1, 2, \ldots$. In the Lipkin model, the physical interpretation of $N$ is the number of fermions. The results of this paper do not depend on this particular physical interpretation and apply to $\mathfrak{su}(2)$ dynamical symmetry problems which can arise in other physical situations.

The LMG model Hamiltonian is the self-adjoint operator

$$\hat{H}(\alpha) = (1 - \alpha)\hat{S}_0 + \frac{\alpha}{N}\left(\hat{S}_+^2 + \hat{S}_-^2\right), \tag{8}$$

where $\alpha$ is a real number in the interval $[0, 1]$. The commutator of the Hamiltonian with the $\hat{S}_+$ operator is

$$[\hat{H}(\alpha), \hat{S}_+] = (1 - \alpha)\hat{S}_+ - \frac{2\alpha}{N}(\hat{S}_-\hat{S}_0 + \hat{S}_0\hat{S}_-). \tag{9}$$

Our parameterization by $\alpha$ of the LMG Hamiltonian differs slightly from the conventional and original choice of Lipkin, Meshkov and Glick [18], but it has the advantage of interpolating between two distinct quantum phases [37], one characterized by $\hat{H}(\alpha = 0) = \hat{S}_0$ and the other

determined by $\hat{H}(\alpha = 1) = \left(\hat{S}_+^2 + \hat{S}_-^2\right)/N$. The $\alpha = 1$ phase is invariant under the 'time-reversal' transformation, $\hat{S}_0 \to -\hat{S}_0$ and $\hat{S}_\pm \to -\hat{S}_\mp$, while the $\alpha = 0$ phase is not invariant. This difference accounts ultimately for the qualitative difference between the two excitation spectra: $\hat{H}(\alpha = 0)$ is nondegenerate, while $\hat{H}(\alpha = 1)$ is exactly twofold degenerate when $N$ is odd and asymptotically twofold degenerate when $N$ is even in the large $N$ limit.

Equations (3)–(7), (9) do not form an independent set. The unitarity conditions (3) and (4) plus the commutator (5) imply the commutation relation (6). Other commutators, including double and triple commutators, involving the Hamiltonian and the algebra generators are not functionally independent conditions. The commutator $[\hat{H}(\alpha), \hat{S}_-]$ is a consequence of equations (3), (4), (9), and the commutator of the LMG Hamiltonian with $\hat{S}_0$ follows from equations (3), (4), (7), (9) and the Jacobi identity.

Suppose $v_i$ is an eigenvector of the self-adjoint Hamiltonian belonging to the real eigenvalue $\epsilon_i$ for $i = 1, 2, \ldots, N+1$. Without loss of generality a set of eigenvectors $\{v_i\}$ may be chosen to form an orthonormal basis. Denote the matrix elements of the $\mathfrak{su}(2)$ operators, relative to such a basis, by $(S_\mu)_{ij} = \langle v_i | \hat{S}_\mu v_j \rangle$ for $\mu = 0, \pm$. The eigenvectors, eigenvalues and matrix elements depend on the parameter $\alpha$.

The LMG Hamiltonian has two special properties which impose restrictions on the matrix elements. Consider the standard orthonormal basis $|M\rangle$, $M = -J, -J+1, \ldots + J$, of eigenstates of $\hat{S}_0 = H(\alpha = 0)$ belonging to the eigenvalues $M$. Since the matrix of the LMG Hamiltonian with respect to the standard basis is real symmetric, it can be diagonalized by a real orthogonal matrix. Hence the matrix elements $(S_\mu)_{ij}$ with respect to the eigenenergy basis result from a real orthogonal transformation and must also be real for $\mu = 0, \pm$. The unitarity conditions (3) and (4) imply that the matrix representing $S_0$ is real symmetric, and the matrix representing $S_-$ is the transpose of the matrix representing $S_+$,

$$(S_0)_{ij} = (S_0)_{ji}, \tag{10}$$

$$(S_-)_{ij} = (S_+)_{ji}. \tag{11}$$

Another simplifying property is that the representation space is a direct sum of two invariant subspaces of the Hamiltonian, one subspace $V_o$ spanned by the standard basis vectors $|M\rangle$ for $M = -J, -J+2, -J+4, \ldots [J-1, J]$ and the other subspace $V_e$ spanned by $|M\rangle$ for $M = -J+1, -J+3, -J+5, \ldots [J-1, J]$. Each eigenvector $v_i$ is in one or the other subspace. We choose $v_1, v_3, v_5, \ldots$ to be in $V_o$ and $v_2, v_4, v_6$ to be in $V_e$. Since each subspace is invariant under the action of $\hat{S}_0$, the matrix elements of this operator connecting states in two different subspaces are zero. Similarly, $\hat{S}_+$ and $\hat{S}_-$ map $V_e$ to $V_o$ and map $V_o$ to $V_e$. These operators, therefore, have zero matrix elements connecting states in the same subspace. Thus, the matrix elements satisfy

$$(S_0)_{ij} = 0 \qquad \text{for} \quad i + j \text{ odd} \tag{12}$$

$$(S_\pm)_{ij} = 0 \qquad \text{for} \quad i + j \text{ even}. \tag{13}$$

The energies and matrix elements must satisfy the commutation relations, equations (5), (7), (9):

$$0 = \sqrt{N} f_{ij}^{(1)} = (S_+)_{ij} - \sum_k ((S_0)_{ik}(S_+)_{kj} - (S_+)_{ik}(S_0)_{kj}), \qquad \text{for} \quad i + j \text{ odd} \tag{14}$$

$$0 = \sqrt{N} f_{ij}^{(2)} = 2(S_0)_{ij} - \sum_k ((S_+)_{ik}(S_+)_{jk} - (S_+)_{ki}(S_+)_{kj}), \qquad \text{for} \quad i + j \text{ even and } i \leqslant j \tag{15}$$

$$0 = \sqrt{N} f_{ij}^{(3)} = ((\epsilon_i - \epsilon_j) - (1-\alpha))(S_+)_{ij} + \frac{2\alpha}{N} \sum_k ((S_+)_{ki}(S_0)_{kj} + (S_0)_{ik}(S_+)_{jk}), \qquad \text{for} \quad i+j \text{ odd}. \tag{16}$$

Note that only energy differences occur in equation (16). The $(N+1)$-dimensional representation is required to be irreducible. Because the $\mathfrak{su}(2)$ Casimir is a multiple of the identity if and only if the representation is irreducible,

$$0 = f_{ij}^{(4)} = \sum_k \left( (S_0)_{ik}(S_0)_{kj} + \frac{1}{2}(S_+)_{ik}(S_+)_{jk} + \frac{1}{2}(S_+)_{ki}(S_+)_{kj} \right) \Big/ N(N+2) - \frac{1}{4}\delta_{ij}, \quad \text{for} \quad i+j \text{ even and } i \leqslant j. \tag{17}$$

Equations (14), (15), (17) do not form an independent set. Indeed, when the Casimir equation is satisfied merely for one diagonal entry, say $i = j = 1$, it must be satisfied for all $i, j$ on the $(N+1)$-dimensional space when the commutation relations (14) and (15) are obeyed.

Equations (14)–(17) are a system of algebraic equations of quadratic degree in the unknown energy differences $\epsilon_i - \epsilon_j$ and matrix elements $(S_0)_{ij}, (S_+)_{ij}$. There exists a solution to the system because the irreducible $\mathfrak{su}(2)$ representation exists and the self-adjoint Hamiltonian can be diagonalized. Even when the energy spectrum is nondegenerate, the solution to the system is not quite unique because there remains flexibility in phase factor choices and the energy eigenvalues are unordered.

When $\alpha = 0$, a solution is well known because the LMG Hamiltonian is $\hat{S}_0$. The excitation spectrum is the set of integers $1, 2, 3, \ldots N$, and the energy eigenvalues may be arranged in ascending order, $\epsilon_1 \leqslant \epsilon_2 \leqslant \cdots \leqslant \epsilon_{N+1}$ with $\epsilon_i = i - 1$. Since only energy differences are relevant, we are free to conventionally set the ground state energy $\epsilon_1$ equal to zero. The corresponding ordered eigenvectors $v_1, v_2, v_3, \ldots$ alternate between vectors in the subspaces $V_o$ and $V_e$. Due to continuity, there exists a neighborhood of positive $\alpha$ that maintains the eigenvalues in ascending order while the eigenvectors alternate between the two subspaces. Our calculations will show that this neighborhood extends to $\alpha = 1$.

When the Hamiltonian is in the enveloping algebra, an SGA solution provides the needed information to compute absolute energies. To find the ground state binding energy $E_{\text{gs}}$ for the LMG problem, evaluate the ground state expectation of the Hamiltonian operator, an element of the universal enveloping algebra,

$$E_{\text{gs}} = (1-\alpha)(S_0)_{11} + \frac{\alpha}{N} \sum_k ((S_+)_{1k}(S_+)_{k1} + (S_+)_{k1}(S_+)_{1k}) \,. \tag{18}$$

## 3. Approximation

The fastest way to solve the equations of motion when the Hilbert space is finite and of relatively modest dimensions is by diagonalization of the Hamiltonian matrix in a standard basis and making the corresponding unitary transformations. However, our concern in developing the RRKK equations-of-motion methods is with the solution of problems for which the space is too large for the computational facilities available and/or for which a standard basis may make truncation to a manageable subspace questionable. For example, to diagonalize the Lipkin model in a basis in which $\hat{S}_0$ is diagonal requires a basis that is considerably larger than $J/2$.

The computational benefit to the RRKK equations-of-motion scheme arises when the unknowns are limited to a small subset of the total. For our purposes, the objective is to calculate the properties of the $p$ lowest-energy states of the model. Therefore, the subset of

unknowns is restricted to just this segment of the entire spectrum. The subset of unknowns consists of the first $p-1$ excitation energies, $\epsilon_1 = 0 \leqslant \epsilon_2, \ldots, \leqslant \epsilon_p$, and the entries of the $p \times p$ block submatrices, $(S_0)_{ij}$ and $(S_+)_{ij}$ for $1 \leqslant i, j \leqslant p$, subject to the constraints of equations (10), (12), (13). When $p$ is even the total number of unknowns is $(3p^2+6p-4)/4$; for $p$ odd, the number is $(3p^2+6p-5)/4$. For example, if the dimension of the LMG representation space $\mathcal{H}$ is a million, then the total number of unknowns in this space is about a trillion; for an equations-of-motion calculation limited to the ground state and the lowest five excited states, there are thirty-five unknowns.

With fewer unknown excitation energies and matrix elements, fewer equations are needed to determine them. Since no attempt is made to calculate matrix elements outside the $p$-dimensional subspace, the candidates for useful equations of motion, $f^{(\sigma)}_{ij} = 0$, are limited to $1 \leqslant i, j \leqslant p$.

Each of the equations of motion, equations (14)–(17), involves an intermediate state summation from $k = 1, \ldots, \dim \mathcal{H}$. The matrix elements connecting the $p$-dimensional block to its complementary $(\dim \mathcal{H} - p)$ dimensional subspace cannot all be zero or else the $p$-dimensional block would be a proper subrepresentation, a contradiction to the assumption that the representation space $\mathcal{H}$ is irreducible. Because the approximation restricts perforce each summation to a maximum $k = p < \dim \mathcal{H}$, the intermediate state sums, in general, are not evaluated exactly. For example, in equation (14), the error in the intermediate state sum for the equation of motion $\sqrt{N} f^{(1)}_{ij}$, $1 \leqslant i, j \leqslant p$, is

$$\sum_{k=p+1}^{\dim H} ((S_0)_{ik}(S_+)_{kj} - (S_+)_{ik}(S_0)_{kj}). \tag{19}$$

If a particular summation, limited to a maximum $k = p$, introduces an unacceptably poor approximation into an equation of motion, then that equation must be eliminated from the set of determining equations. Because there are more equations of motion than unknowns, it is possible to exclude some equations and have enough remaining to determine an accurate solution in a $p - q > 0$ subspace, for some value of $q$, of the $p$-dimensional space used for the RRKK computation.

A reliable equation of motion contains an intermediate state sum involving matrix elements that are negligibly small whenever they connect states within the $p$ block to those outside it. For the RRKK method to yield accurate solutions, the following condition on matrix elements proves to be sufficient: for any $\epsilon > 0$, there exists positive integers $p > q$ such that, for $\mu = 0, \pm$,

$$|(S_\mu)_{ik}| < \frac{\epsilon}{|i-k|} \quad \text{for all} \quad 1 \leqslant i \leqslant p-q, \quad k > p \quad \text{or} \quad 1 \leqslant k \leqslant p-q, \quad i > p. \tag{20}$$

When the matrices of the Lie algebra operators in the basis which diagonalizes the Hamiltonian are approximately sparse band matrices, the above condition is satisfied. But the matrices need not be band matrices for the complete basis because the properties of the matrices within the complementary $(\dim \mathcal{H} - p)$ dimensional block are irrelevant to the approximation scheme.

To attain an accuracy consistent with the choice of $\epsilon$, the useful equations of motion, $f^{(\sigma)}_{ij} = 0$, may be limited to $1 \leqslant i, j \leqslant p - q$. When the dimension of $\mathcal{H}$ is large, the error due to a typical summation term is roughly

$$\left| \sum_{k>p} (S_\mu)_{ik}(S_\nu)_{jk} \right| \leqslant \sum_{k>p} \frac{\epsilon^2}{|k-i||k-j|} \sim \epsilon^2 \sum_{k=1}^{\infty} \frac{1}{k^2} = \epsilon^2 \pi^2/6. \tag{21}$$

The accuracy of the solution depends on $\epsilon$, and the computational speed depends on $p$, which sets the number of unknowns, and $q$, which limits the number of equations. The value of $p - q$ must yield more independent equations of motion than unknowns. Depending on the accuracy required for a particular application, there is a trade-off chosen by the researcher who must mind his $p$'s and $q$'s.

The calculations reported in the next section show that the matrices of the $\mathfrak{su}(2)$ Lie algebra elements in the basis which diagonalizes the LMG Hamiltonian are band matrices. Their largest matrix elements are located on the diagonal, and nearby superdiagonals and subdiagonals. The LMG computations demonstrate that matrix elements $(S_\mu)_{ik}$ are negligibly small for our purposes when $|i - k| \geqslant 4$.

Since no exact solution to the equations of motion in the $p$-dimensional subspace exists, we seek approximate solutions by minimizing the nonnegative objective function,

$$F = \sum_{\sigma=1}^{4} \sum_{i,j=1}^{p} w_{ij}^{(\sigma)} \left(f_{ij}^{(\sigma)}\right)^2, \tag{22}$$

where $w_{ij}^{(\sigma)}$ is a weight factor. The domain of the objective function is the set of all unknowns in the $p$-dimensional subspace. The weight function is used to increase the importance of the more reliable equations with small $i, j$ relative to those equations near the edge of the $p$-dimensional subspace. The weight function effectively allows us to make $q$ somewhat smaller and still retain sufficient accuracy. With some exceptions we take $w_{ij}^{(\sigma)} = 1/\sqrt{ij}$ in the calculations. The exceptions take the weight function as zero for certain equations at or adjacent to the boundary:

$$w_{ij}^{(\sigma)} = 0 \begin{cases} \sigma = 1: & i + j > 2p - 2 & \text{or} & i + j \text{ even or } i = p \text{ or } j = p \\ \sigma = 2: & i + j > 2p - 2 & \text{or} & i + j \text{ odd or } i > j \\ \sigma = 3: & i + j > 2p - 3 & \text{or} & i + j \text{ even or } i = p \text{ or } j = p \\ \sigma = 4: & i \neq j & \text{or} & i = j > p - 2. \end{cases} \tag{23}$$

This choice for the weight function was discovered by numerical experimentation in the LMG model for the cases $p = 5 - 10$. We make no claim that this weighting optimizes accuracy and performance, but it gets the job done.

## 4. Results

We solve approximately the equations-of-motion system by using a modified Levenberg–Marquardt algorithm that minimizes the objective function, equation (22). The algorithm requires an initial estimate of the solution. When $\alpha = 0$ the Hamiltonian simplifies to $\hat{S}_0$ and the solution is analytic. The exact solution for $\alpha = 0$ is used as an initial estimate for $\alpha = 0.01$. The numerically determined solution for $\alpha = 0.01$ is used as the initial estimate for $\alpha = 0.02$ and so on. In this way numerical solutions are found for any positive value of $\alpha$. On a notebook computer, application of the equations-of-motion method for $p = 6$ and $\alpha$ ranging from 0 to 1 in increments of 0.01 takes a few seconds when $N < 100$.

An exact initial starting point, such as readily available in the LMG model at $\alpha = 0$, is not required for the minimization algorithm. When the matrix elements and energies at $\alpha = 0$ are shifted from their exact values to random numbers, the correct objective function minimum of zero is found invariably by the algorithm provided each shifted initial value is within a factor of 2 of the exact answer. Thus a rough estimate of matrix elements and energies is sufficient to start a successful equations-of-motion calculation.

For $5 \leqslant p \leqslant 10$ and $N \geqslant p - 1$, table 1 lists the number of unknowns and the number of equations of motion, taking into account equation (23). When $N \leqslant 3$ the equations of motion

**Table 1.** For various subspace dimensions $p$, the table provides the number of unknowns and the number of independent equations of motion.

| $p$ | Unknowns | Equations |
|---|---|---|
| 5 | 25 | 27 |
| 6 | 35 | 39 |
| 7 | 46 | 56 |
| 8 | 59 | 73 |
| 9 | 73 | 95 |
| 10 | 89 | 117 |

**Table 2.** Comparison between excitation energies computed by diagonalization and calculated from equations of motion for $\alpha = 0.3$, $\dim \mathcal{H} = 300$ and various subspace dimensions $p$.

| Diagonalization | $p = 5$ | $p = 6$ | $p = 7$ | $p = 8$ | $p = 9$ | $p = 10$ |
|---|---|---|---|---|---|---|
| 0.375 220 | 0.375 220 | 0.375 220 | 0.375 220 | 0.375 220 | 0.375 220 | 0.375 220 |
| 0.766 779 | 0.766 767 | 0.766 780 | 0.766 780 | 0.766 780 | 0.766 780 | 0.766 780 |
| 1.172 958 | 1.173 608 | 1.172 939 | 1.172 959 | 1.172 959 | 1.172 959 | 1.172 959 |
| 1.592 432 | – | 1.593 260 | 1.592 405 | 1.592 433 | 1.592 432 | 1.592 432 |
| 2.024 141 | – | – | 2.025 139 | 2.024 106 | 2.024 142 | 2.024 141 |
| 2.467 211 | – | – | – | 2.468 372 | 2.467 169 | 2.467 213 |
| 2.920 910 | – | – | – | – | 2.922 223 | 2.920 859 |
| 3.384 605 | – | – | – | – | – | 3.386 063 |

may be solved easily without any approximations in the space $\mathcal{H}$, i.e., $p = \dim \mathcal{H} = \mathrm{N} + 1$; in such trivial cases, the summations are evaluated exactly and the weight function $w_{ij}^{(\sigma)} = 1$. When $p \leqslant 4$ and $N > 3$, the weight function of equation (23) yields fewer independent equations than unknowns and solutions to the equations of motion are undetermined.

For $\alpha = 0.3$ and $N = 2J = 299$, table 2 lists the low-energy excitation spectrum calculated by diagonalization and, for several subspace dimensions $p$, by the equations-of-motion method. The value of the objective function $F$ for the calculations in this table is always smaller than $1.4 \times 10^{-8}$. The computation time is greatest for $p = 10$ and, on a notebook computer, is 35 s. Accurate to the seven significant digits shown in the table, energies determined via diagonalization provide reference values. The RRKK lowest $(p-4)$ excitation energies are accurate to better than two parts in a million. Up to the $(p-3)$ level, the accuracy is no less than 3 parts in $10^5$; the $(p-2)$ excitation energy is correct to 4 parts in ten thousand. Due to the zeros of the weight function, the highest $(p-1)$ excitation energy is undetermined by the equations of motion and is not listed in the table. Thus the numerical accuracy of the low-lying excitation energies computed via equations of motion improves as the subspace dimension $p$ increases.

Tables 3 and 4 show the values of the matrix elements of $(S_0)_{ij}$ and $(S_+)_{ij}$ involving low-energy states calculated by unitary transformation following diagonalization and by equations of motion for $\alpha = 0.3$. The RRKK calculations give improved results as $p$ increases. The accuracy of the matrix elements is comparable to that of the excitation energies. Both $(S_0)_{ij}$ and $(S_+)_{ij}$ are nearly sparse band matrices. Since the dominant matrix elements are confined to the main diagonal and the second diagonal above and below the main diagonal, the matrix $(S_0)_{ij}$ is approximately pentadiagonal. The matrix $(S_+)_{ij}$ is approximately tridiagonal.

For $\alpha = 0.7$ and $\dim \mathcal{H} = 300$, the character of the solution changes from the $\alpha = 0.3$ results. The low-energy levels are twofold degenerate to an accuracy of one part in $10^8$.

**Table 3.** Matrix elements of $S_0$ calculated from the equations of motion for $\alpha = 0.3$, $\dim \mathcal{H} = 300$ and subspace dimensions $p = 6, 8, 10$ are compared to diagonalized values.

| Dimension | $(S_0)_{11}$ | $(S_0)_{13}$ | $(S_0)_{15}$ | $(S_0)_{22}$ | $(S_0)_{24}$ | $(S_0)_{33}$ | $(S_0)_{35}$ | $(S_0)_{44}$ |
|---|---|---|---|---|---|---|---|---|
| $p = 6$ | −149.0611 | −1.111 450 | 0.020 7250 | −147.2509 | −1.849 612 | −145.5580 | −2.523 849 | −143.9587 |
| $p = 8$ | −149.0611 | −1.111 450 | 0.020 7384 | −147.2509 | −1.849 628 | −145.5580 | −2.523 951 | −143.9537 |
| $p = 10$ | −149.0611 | −1.111 450 | 0.020 7384 | −147.2509 | −1.849 628 | −145.5580 | −2.523 950 | −143.9537 |
| Diag. | −149.0611 | −1.111 450 | 0.020 7385 | −147.2509 | −1.849 629 | −145.5581 | −2.523 951 | −143.9537 |

**Table 4.** Matrix elements of $S_+$ calculated from the equations of motion for $\alpha = 0.3$, $\dim \mathcal{H} = 300$ and subspace dimensions $p = 6, 8, 10$ are compared to diagonalized values.

| Dimension | $(S_+)_{12}$ | $(S_+)_{21}$ | $(S_+)_{23}$ | $(S_+)_{32}$ | $(S_+)_{14}$ | $(S_+)_{41}$ | $(S_+)_{34}$ | $(S_+)_{43}$ |
|---|---|---|---|---|---|---|---|---|
| $p = 6$ | −11.412 36 | 20.695 98 | −15.424 98 | 28.816 47 | −0.019 3243 | −0.202 6039 | −18.140 06 | 34.819 12 |
| $p = 8$ | −11.412 36 | 20.695 98 | −15.424 99 | 28.816 47 | −0.019 3270 | −0.202 6011 | −18.139 37 | 34.819 04 |
| $p = 10$ | −11.412 36 | 20.695 98 | −15.424 99 | 28.816 47 | −0.019 3270 | −0.202 6011 | −18.139 37 | 34.819 04 |
| Diag. | −11.412 37 | 20.695 98 | −15.425 00 | 28.816 47 | −0.019 3270 | −0.202 6013 | −18.139 37 | 34.819 05 |

The first six energy eigenvalues are as follows: 0, 0, 1.925 2507, 1.925 2507, 3.834 9946, 3.834 9946. Within the $p = 6$ subspace, the matrix elements of the $\mathfrak{su}(2)$ generators for $\alpha = 0.7$ are

$$S_0 = \begin{pmatrix} -32.192 & 0 & 10.163 & 0 & 0.224 & 0 \\ 0 & -32.192 & 0 & 10.163 & 0 & 0.224 \\ 10.163 & 0 & -32.511 & 0 & 14.351 & 0 \\ 0 & 10.163 & 0 & -32.511 & 0 & 14.351 \\ 0.224 & 0 & 14.351 & 0 & -32.840 & 0 \\ 0 & 0.224 & 0 & 14.351 & 0 & -32.840 \end{pmatrix},$$

$$S_+ = \begin{pmatrix} 0 & -145.957 & 0 & 4.929 & 0 & 0.385 \\ 145.957 & 0 & -4.929 & 0 & -0.385 & 0 \\ 0 & -9.425 & 0 & -144.789 & 0 & 6.909 \\ 9.425 & 0 & 144.789 & 0 & -6.909 & 0 \\ 0 & 0.068 & 0 & -13.331 & 0 & -143.615 \\ -0.068 & 0 & 13.331 & 0 & 143.615 & 0 \end{pmatrix}.$$

These matrix elements are quite different from the $\alpha = 0.3$ values listed in tables 3 and 4. When the equations-of-motion procedure increments $\alpha$ in small steps from 0.3 to 0.7, the matrix elements evolve slowly from their values listed in tables 3 and 4 to the above matrices. For any finite value of $N$ the matrix elements all evolve continuously, even if rapidly in the transition region, as functions of $\alpha$.

For $\alpha = 0.3$, $S_0$'s diagonal elements dominate with a value close to $-j = -N/2$; for $\alpha = 0.7$, the magnitude of the diagonal elements is reduced to about $-j/10$ and the matrix elements on the second diagonal are about one-third of the diagonal values. Yet $S_0$ at $\alpha = 0.7$ remains approximately a sparse band matrix. The $S_+$ matrix for both $\alpha = 0.3$ and 0.7 is tridiagonal, but the magnitudes of the entries are qualitatively different. The magnitudes of the off-diagonal entries of $S_+$ at $\alpha = 0.7$ are as large as the diagonal entries of $S_0$ at $\alpha = 0.3$. The matrix elements of $S_0$ and $S_+$ at $\alpha = 0.7$ show an interesting doubling that is associated with the twofold degeneracy of the energy spectrum.

The twofold degeneracy of the low-energy spectrum at $\alpha = 0.7$ and $N = 299$ is an interesting phenomenon which depends on the large particle number $N$. Figure 1 shows the

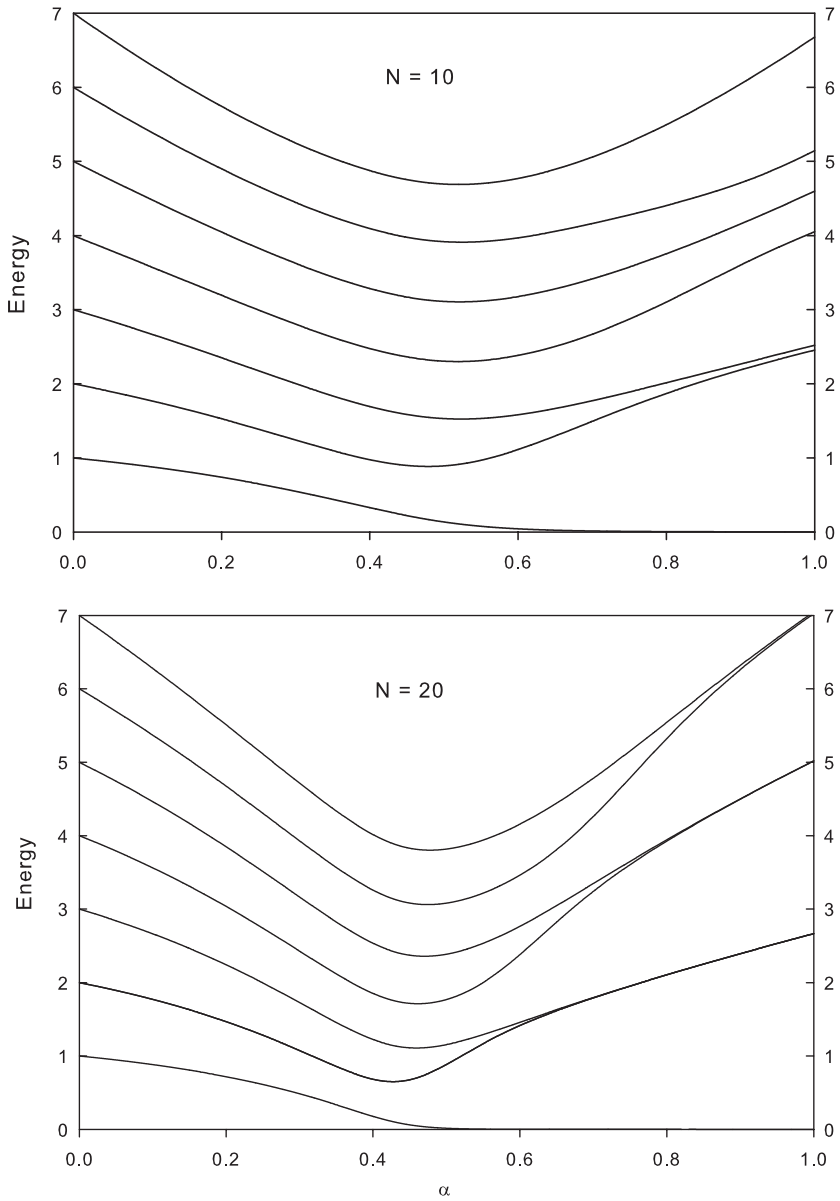


**Figure 1.** low-energy LMG spectra for $N = 10, 20$.

low-energy spectra when the particle number $N$ has the small values 10 and 20. When $N = 10$ the ground state is twofold degenerate for $\alpha > 0.6$ and the first excited state becomes nearly degenerate as $\alpha$ approaches 1. When $N = 20$, the twofold degeneracy is evident for sufficiently large $\alpha$. Although not apparent from the figures, the LMG spectra are never exactly twofold degenerate for $\alpha < 1$, but can be approximately so to high precision.

For $N = 299$ particles, figure 2 shows a transition over the interval from $\alpha \approx 0.3$ to $\alpha \approx 0.4$ in which the nondegenerate spectra change quickly to a twofold degenerate spectrum. A plot of energy differences $(\epsilon_{i+1} - \epsilon_i)$ versus $\alpha$ demonstrates that, excluding a small interval

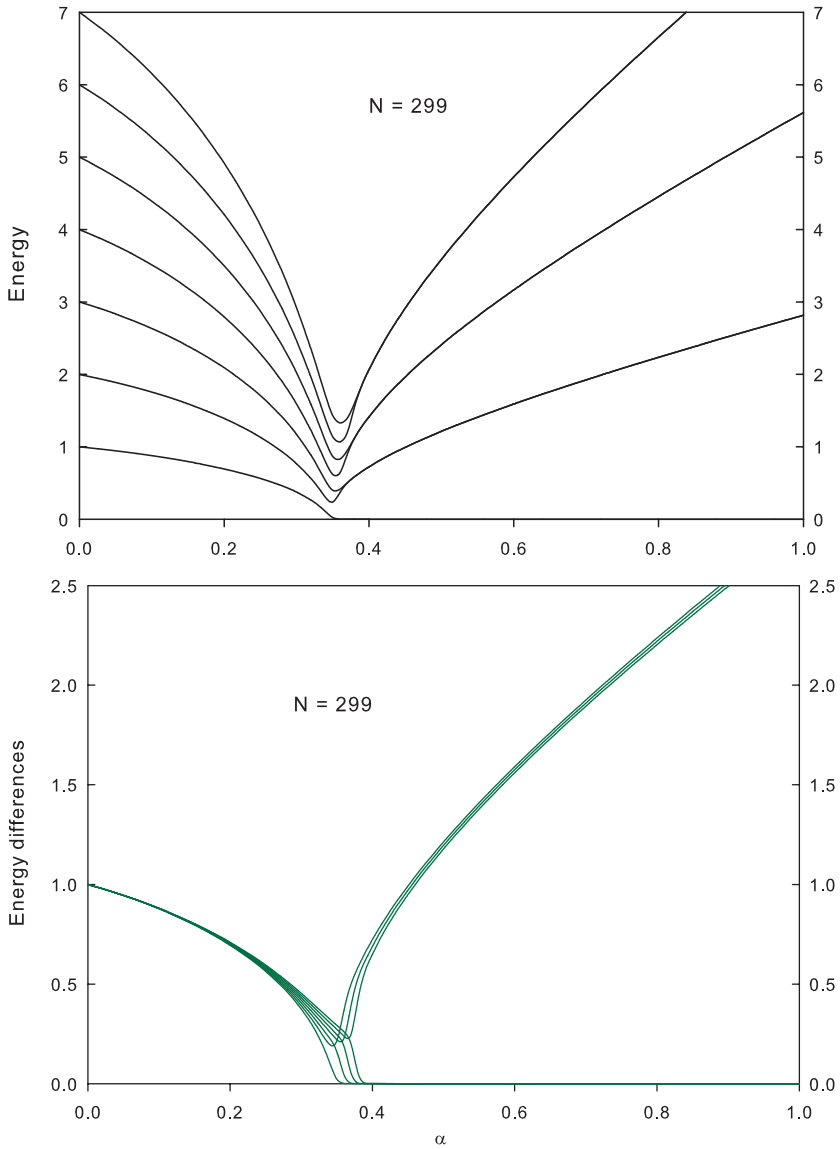


**Figure 2.** LMG low-energy spectra and energy differences for $N = 299$.

near $\alpha = 0.4$, the spectrum is that of a near perfect harmonic vibrator. The frequency of the nondegenerate spectrum decreases as $\alpha$ changes from 0 to about 0.3; the frequency of the twofold spectrum increases as $\alpha$ changes from about 0.4 to 1.

Figure 3 shows excitation energy levels and energy differences calculated with RRKK equations of motion for $N = 1000\,000$ particles. An unambiguous quantum phase transition occurs at $\alpha = 1/3$ in which the system changes from one phase, a nondegenerate harmonic vibrator, to a second phase, a twofold degenerate harmonic vibrator. A major advantage to equations of motion is that computation time, except in a small neighborhood of a critical point, does not depend on the dimension of the irreducible representation space.

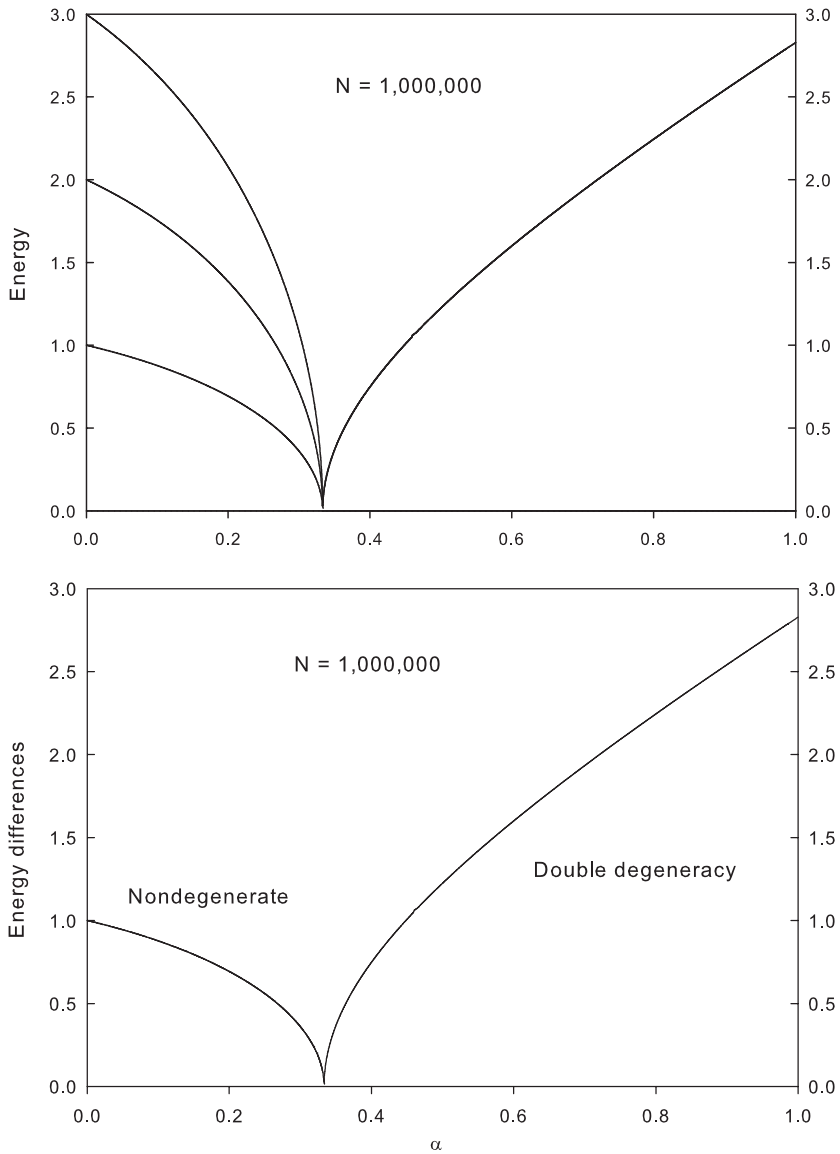


**Figure 3.** LMG low-energy spectra and energy differences for $N = 1\,000\,000$.

Computation time can increase dramatically near a phase transition point because many tiny step sizes are required to pass continuously from one phase to another. To regain computational speed, a phase transition calculation can be done in two separate fast applications, one starting to the left of the transition and ending at the critical transition point and another starting to the right of the transition and also ending at the critical point. The two separate calculations join at the transition point. This two part calculation was done for $N = 1\,000\,000$ and total computation time was about a minute on a notebook computer. In section 4.2 we report in the large $N$ limit an estimate for the starting point data at $\alpha = 1$ which was used in the two part computation. In fact, the asymptotic approximations given for large $N$

in sections 4.1 and 4.2 provide a reasonable startup for any $\alpha$, excluding a small neighborhood of the critical point $\alpha = 1/3$.

### *4.1. Analytic approximation for large particle number N and small α*

When the number of particles is large, the random phase approximation achieves an accurate formula for low-energy states. For the LMG model, this approximation is conveniently expressed in terms of a Heisenberg–Weyl boson algebra $\mathfrak{hw}(1)$, spanned by the identity $I$ and the bosons $a, a^\dagger$ for which $[a, a^\dagger] = I$. The boson mapping, $\hat{S}_+ \to \sqrt{N}a^\dagger$, $\hat{S}_- \to \sqrt{N}a$ and $\hat{S}_0 \to a^\dagger a - (N/2)I$, is then obtained from the well-known Dyson representation [56] of $\mathfrak{su}(2)$ and is valid for large $N$ and on a subspace spanned by states with $M$ values close to $-N/2$. When $\alpha = 0$, the Hamiltonian is $\hat{S}_0$ and the low-energy spectrum equals the spectrum of the boson number operator $a^\dagger a$, namely, the integers. The Heisenberg-Weyl $\mathfrak{hw}(1)$ approximation to the $\mathfrak{su}(2)$ algebra is valid on the proper subspace spanned by eigenstates of $\hat{S}_0$ with eigenvalues close to $-j = -N/2$ when $N$ is large.

For small positive $\alpha$ and large $N$, the excitation spectrum of the Hamiltonian $\hat{H}(\alpha)$ is approximately the same as that of the operator

$$\hat{h}_1(\alpha) = (1-\alpha)a^\dagger a + \alpha(a^\dagger a^\dagger + aa) \tag{24}$$

in the $\mathfrak{hw}(1)$ enveloping algebra. By making a canonical transformation to new bosons,

$$b^\dagger = \cosh\eta a^\dagger + \sinh\eta a \qquad b = \cosh\eta a + \sinh\eta a^\dagger, \tag{25}$$

the boson Hamiltonian is expressed as a boson number operator plus a constant,

$$\hat{h}_1(\alpha) = \omega_1 b^\dagger b + \text{ const.}, \tag{26}$$

when the parameter $\eta$ satisfies

$$\omega_1 \cosh 2\eta = 1 - \alpha \qquad \omega_1 \sinh 2\eta = 2\alpha. \tag{27}$$

The solution for the vibrational frequency is

$$\omega_1 = \sqrt{(1+\alpha)(1-3\alpha)}. \tag{28}$$

Therefore the harmonic spectrum of the boson approximation to $\hat{H}(\alpha)$ is

$$\epsilon_{i+1} = \omega_1 i, \qquad \text{for} \quad i = 1, 2, 3, \ldots. \tag{29}$$

For $N = 10^6$ the difference between the boson approximation to the energy and the RRKK calculation shown in figure 3 is less than one part in a million for the interval $0 \leqslant \alpha < 1/3 - 10^{-5}$. Note that the analytic approximation gives the correct location of the phase transition at $\alpha = 1/3$. For fewer particles and smaller dimensional representation spaces, the analytic approximation is useful for smaller $\alpha$.

### *4.2. Analytic approximation for large particle number N and α ≈ 1*

To approach the phase transition from the right side, the minimization algorithm that finds RRKK solutions requires a starting estimate, say at $\alpha = 1$. For $\alpha \approx 1$, the LMG Hamiltonian, $\hat{H}(\alpha)$, can be solved in the asymptotic limit of large $N$ using the shifted harmonic oscillator approximation [57]. To motivate and guide this approximation, figure 4 shows the ground state amplitudes of $\hat{H}(\alpha)$ with respect to the standard $\mathfrak{su}(2)M$ basis in the subspace $V_o$ when $N = 2J = 600$ and $\alpha = 1.0, 0.6$. The amplitudes of $M$ and its neighbors $M \pm 2$ differ in sign. The envelopes of the absolute values of the amplitudes appear to be Gaussian. The $\alpha = 1$

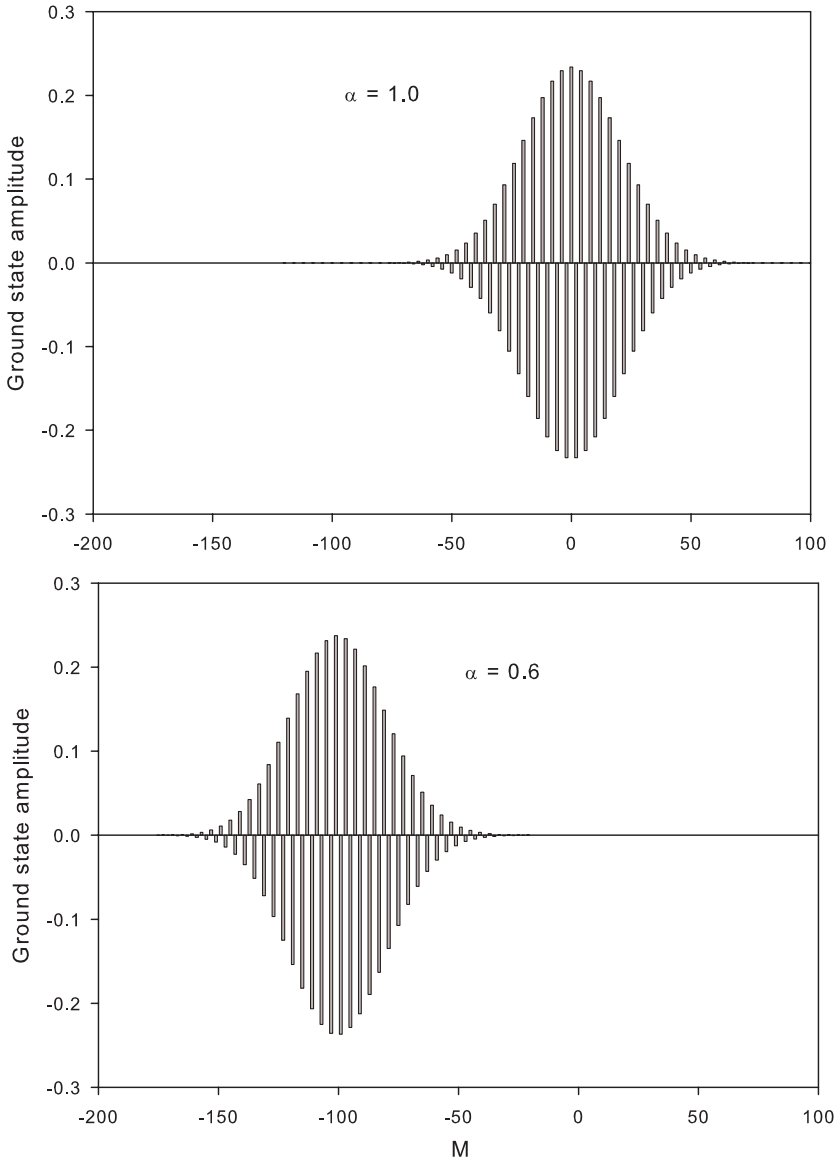


**Figure 4.** Histograms showing ground state amplitudes in the standard $M$ basis for $N = 600$ and $\alpha = 1.0, 0.6$.

distribution is centered at $M = 0$, while that of the $\alpha = 0.6$ amplitudes is shifted to the left around $M \approx -100$. The distributions are seen to be relatively narrow. For larger values of $N$ (not shown) they are even narrower.

The SHA shows that, in the large-$N$ asymptotic limit, the amplitudes obey a differential equation whose solution is a Gaussian function. For $\alpha \approx 1$, suppose $|\psi\rangle$ is a low-energy eigenstate of $\hat{H}(\alpha)$ belonging to the eigenvalue $E$, and let $x = M/J \ll 1$. To find the differential equation, first change the standard basis to $|x\rangle = \pm|M\rangle$ by choosing phase signs so that all the amplitudes, $\psi(x) = \langle x|\psi\rangle$, are positive. When $x \ll 1$, the matrix elements of

the $\mathfrak{su}(2)$ operators in the new basis are approximately

$$\begin{aligned}\langle x|\hat{S}_0|\psi\rangle &= \frac{N}{2}x\psi(x)\\ \langle x|\hat{S}_+^2|\psi\rangle &\approx -\frac{N^2}{4}(1-x^2)\psi\left(x-\frac{4}{N}\right)\\ \langle x|\hat{S}_-^2|\psi\rangle &\approx -\frac{N^2}{4}(1-x^2)\psi\left(x+\frac{4}{N}\right).\end{aligned} \tag{30}$$

By making Taylor series expansions for the amplitudes $\psi\left(x\pm\frac{4}{N}\right)$, the Hamiltonian eigenvalue problem is approximately equivalent to the following differential equation for the amplitudes,

$$E\psi(x) = (1-\alpha)\frac{N}{2}x\psi(x) - \frac{N\alpha}{2}(1-x^2)\left(\psi(x)+\frac{8}{N^2}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}(x)\right) \tag{31}$$

$$= -\frac{4\alpha}{N}(1-x^2)\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}(x) + \frac{N\alpha}{2}((x-\bar{x})^2-\bar{x}^2-1)\psi(x), \tag{32}$$

where

$$\bar{x} = -\frac{1-\alpha}{2\alpha}. \tag{33}$$

This Schrödinger-like equation has a harmonic oscillator potential well, which is deep and narrow for large $N$. In the asymptotic limit, the solutions $\psi(x)$ are near zero outside a narrow interval centered at $x=\bar{x}$. This concurs with the numerical calculations shown in figure 4. Only a small error will result if the $x$-dependent coefficient of the second derivative is replaced by a constant,

$$\frac{1}{2B}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}(x) + \frac{1}{2}B\omega_2^2(x-\bar{x})^2\psi(x) = \left(E+\frac{N\alpha}{2}(\bar{x}^2+1)\right)\psi(x), \tag{34}$$

where $B = 2\alpha N/((3\alpha-1)(\alpha+1))$ and

$$\omega_2 = \sqrt{2(3\alpha-1)(\alpha+1)}. \tag{35}$$

Hence, in the SHA, the excitation energies are

$$\epsilon_{i+1} = \omega_2 i \qquad \text{for} \quad i = 1, 2, \ldots. \tag{36}$$

For $N = 10^6$ the SHA and the RRKK numerical calculations of figure 3 for the low-energy excitation spectrum agree to within one part in $10^6$ over the interval $0.34 < \alpha \leqslant 1$. Note that the SHA for large particle number yields the correct location of the quantum phase transition at $\alpha = 1/3$.

The starting estimates at $\alpha = 1$ for the LMG $\mathfrak{su}(2)$ operators in a small $p$-dimensional subspace spanned by the least energy states are the following band matrices:

$$\hat{S}_0 = \begin{pmatrix} 0 & a_2 I & 0 & \cdots \\ a_2 I & 0 & a_4 I & \cdots \\ 0 & a_4 I & 0 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix}, \qquad a_i^2 = \frac{N}{2\sqrt{8}}i, \qquad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hat{S}_+ = \begin{pmatrix} b_0 J & -a_1 J & 0 & \cdots \\ a_1 J & b_1 J & -a_2 J & \cdots \\ 0 & a_2 J & b_2 J & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix}, \qquad b_i = \frac{N}{2} - i, \qquad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

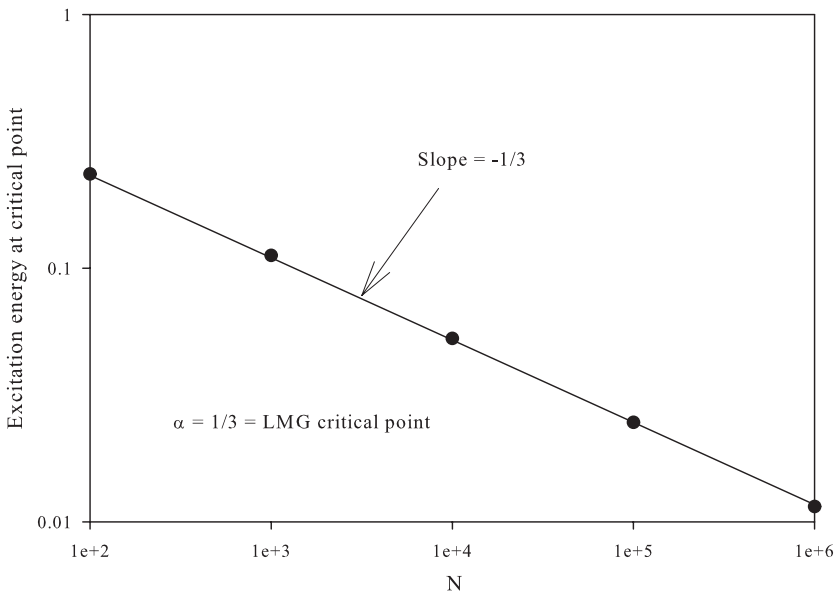


**Figure 5.** Log–Log plot of excitation energy at the critical point versus the number of fermions.

### *4.3. Critical exponents*

At the critical point $\alpha = 1/3$, asymptotic scaling properties, with respect to the number of fermions $N \to \infty$, are of considerable interest in statistical physics. Equations of motion provide an effective tool for revealing scaling dependences of excitation energies and matrix elements because the RRKK method determines solutions for large particle number.

If a positive quantity, denoted by $Q$, obeys an asymptotic power law with a critical exponent $c$,

$$Q/N^c \overset{N\to\infty}{\longrightarrow} A, \qquad A = \text{constant}, \tag{37}$$

then $\log Q$ depends linearly on $\log N$,

$$\log Q \overset{N\to\infty}{\sim} c \log N + \log A. \tag{38}$$

The asymptotic slope of a $\log Q$ versus $\log N$ plot equals the critical exponent.

Figure 5 plots the logarithm of the excitation energy $\epsilon_2 - \epsilon_1$ at $\alpha = 1/3$ versus the logarithm of $N$ for $N \leqslant 10^6$. The critical exponent is $-1/3$ as was also obtained in [40] and [17] for the quartic oscillator, and by Dusuel and Vidal [38] and Leyvraz and Heiss [39] for a number of models, including the LMG. The critical exponent, $-1/3$, for excitation energy level scaling has also been obtained for the U(5)-O(6) quantum phase transition in the interacting boson model [40, 41]. The LMG and U(5)-O(6) quantum phase transitions belong to the same universality class as the liquid–gas and ferromagnetic second-order thermodynamic phase transitions [43].

Figures 6 and 7 plot logarithms of two typical matrix elements, $-(S_+)_{12}$ and $-(S_0)_{13}$, evaluated at the critical point versus the logarithm of $N$. Again a straight line plot fits the RRKK solutions for $N \leqslant 10^6$. The critical exponent for $-(S_+)_{12}$ is $+2/3$ and that for $-(S_0)_{13}$ is $+1/3$. The critical exponents for other matrix elements may be determined similarly by numerical computation. Hellemans *et al* [42] report the deformation's critical exponent for the U(5)-O(6) quantum phase transition.

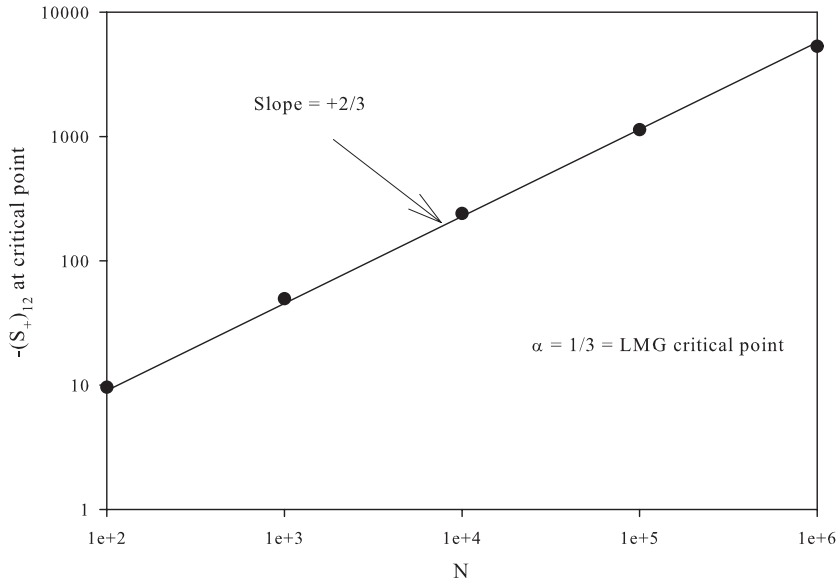


**Figure 6.** Log–Log plot of $-(S_+)_{12}$ at the critical point versus the number of fermions.

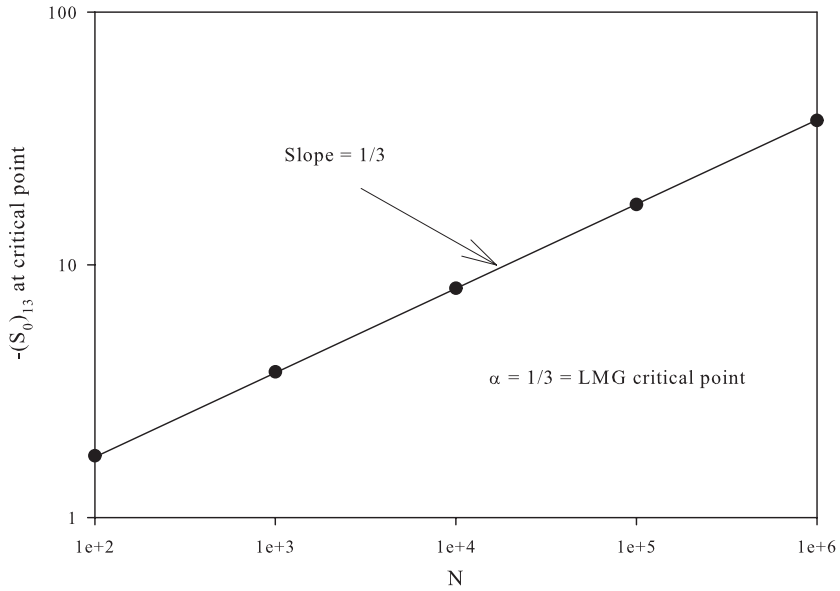


**Figure 7.** Log–Log plot of $-(S_0)_{13}$ at the critical point versus the number of fermions.

## 5. Discussion

Although matrix diagonalization is undoubtedly a powerful tool in obtaining a theoretical interpretation of the physical properties of many quantum mechanical systems, there are situations in which the equations-of-motion approach is more intellectually satisfying and more effective. First observe that a necessary condition for deriving the low-energy eigenstates of a Hamiltonian on an infinite-dimensional Hilbert space by matrix diagonalization, is that

there exists an ordered basis for the Hilbert space such that the sum of the squares of the coefficients of the expansion of the low-energy eigenstates in this basis forms a sufficiently rapidly convergent series. In practice, this usually requires that the Hamiltonian should have a suitable system of approximate symmetries to enable the construction of such a basis and enable determination of the Hamiltonian and other matrix elements in this basis. However, there are situations in which no suitable precisely-defined basis is available. As figure 4 illustrates, there are LMG Hamiltonians for which the sequence of expansion coefficients for the ground state do not begin to converge until the 300th term in the naturally-defined basis. In such a situation, the Jacobi method, for example, of finding selected eigenstates by a diagonalization algorithm, if it converged, would undoubtedly return highly excited states. In contrast, the equations-of-motion approach is not constrained by the necessity of choosing a basis.

Algebraic and other structural properties of a particular mathematical problem should be used to solve it. This guiding principle applies to both analytic and numerical solutions. Diagonalization algorithms, such as the Jacobi method, apply to any real symmetric matrix, e.g., a matrix whose entries are random numbers. For a spectrum-generating algebra, the Hamiltonian matrix is far from random and its special algebraic properties are exploited by the equations-of-motion method and reflected in its solutions.

The RRKK method also has the attractive property that it can start with simple model approximations and develop them into accurate results. For example, it can start with the results of a mean-field approximation and add the fluctuation corrections of a more precise solution.

The Lipkin–Meshkov–Glick model Hamiltonian $\hat{H}(\alpha)$, in its large particle number limit, shows a quantum or structural phase transition at $\alpha = 1/3$ in its low-energy domain. This striking phase phenomenon often occurs in the zero temperature thermodynamic limit of a system by variation of a control parameter in the Hamiltonian [44–46]. The topic has attracted the attention of many nuclear structure theorists. A historic overview of the numerous contributions to the subject in nuclear physics is given in [11]. Some recent articles given, for example, by [28, 42, 50–54]. Of particular recent interest are studies of phase transitions in excited states, cf [55] and articles referenced therein. Because the efficacy of the equations-of-motion method is not especially sensitive to the dimension of the representation space, the RRKK technique makes it possible to compute properties, including critical exponents, for systems with very large particle number, as we have demonstrated for the LMG model and, in prior work, for the quartic five-dimensional oscillator [17].

How small can the dimension $p$ of the equations-of-motion subspace be? The answer depends on the dimension $q$ of the subspace for which one wishes to obtain accurate results and the level of accuracy required. More precise results generally require a higher dimension $p$ in order to improve the accuracy of intermediate state summations. Less tightly banded and less sparse matrices, which represent Lie algebra generators in the eigenenergy basis, would make it necessary to increase $p$. When the degree of the Hamiltonian in the enveloping algebra is greater than the quadratic LMG operator of this paper, accurate intermediate state sums require a larger value for $p$. Note that $p$ must be greater than the number of low-energy states that are to be studied and large enough so that the number of independent equations is greater than the number of unknowns.

Are the Lie algebra representation matrices always band matrices? For the LMG model the answer is 'yes'. In fact, it is easily shown that the matrices are generally band diagonal whenever a mean-field approximation is valid. The general conditions for the validity of this working hypothesis of the equations-of-motion method will be explored in a following paper. Physical considerations may support the equations-of-motion hypothesis,

e.g., the representation of a Lie algebra generator may be interpreted physically as a transition operator and the transition probabilities connecting low and high energy states may be known experimentally to be small.

For large particle number $N$, a reasonable estimate of the solution may be derived for any $\alpha$ excluding a small neighborhood centered on the critical point $\alpha = 1/3$. The length $\delta$ of the difficult interval $\left(\frac{1}{3} - \frac{\delta}{2}, \frac{1}{3} + \frac{\delta}{2}\right)$ shrinks as $N$ increases. Estimates of excitation energies are given in equations (29) and (36). Matrix element estimates for any $\alpha$, excluding the critical point neighborhood, may be derived using the boson approximations of sections 4.1 and 4.2.

To investigate the small neighborhood around the critical point when $N$ is large, an equations-of-motion computation which passes continuously from $\alpha = \frac{1}{3} - \frac{\delta}{2}$ to $\alpha = \frac{1}{3} + \frac{\delta}{2}$ proceeds by making many tiny steps. The step size is of the order of $1/N$.

It is important to be aware of the conditions necessary to obtain accurate results. For example, double precision (15 significant digits) is needed for the fractional error between $S_0 S_+ - S_+ S_0$ and $S_+$ to be less than one part in $10^8$, for $\alpha$ in the neighborhood of its critical value, and the number of particles, $N$, should not exceed $10^7$. Higher machine precision is needed for larger numbers of particles. For example, an accuracy of one part in $10^8$ can be achieved on a quad precision computer (31 significant digits) for $N$ up to Avogadro's number $10^{23}$. For the LMG model the analytic asymptotic approximations of sections 4.1 and 4.2 are very accurate for such large particle number except in a tiny neighborhood of the critical point. The issue of significant digits in the LMG model becomes important when a careful study is being made of the phase transition within the tiny neighborhood of the critical point for extremely large, but finite, $N$. It should be noted, however, that the increasing fractional error with particle number can be attributed to the collapse at the critical point of the excited states to a multiply-degenerate ground state in the asymptotic $N \to \infty$ limit.

## 6. Conclusion

The equations-of-motion method is advantageous when: (1) the dimension of the quantum Hilbert space is very large and the low-energy eigenstates of interest do not have a sufficient rapidly convergent expansion in an ordered-symmetry adapted basis for matrix diagonalization methods in a truncated basis to be practicable, and (2) the desired number of low-energy eigenvalues and matrix elements (transition rates) among these states is relatively small. In addition, for a given Hamiltonian, two mathematical requirements must be verified for a successful application of the RRKK approximation method: the spectrum-generating condition and a projection property.

First a spectrum-generating algebra $\mathfrak{g}$ must be chosen for the Hamiltonian operator. For any finite-dimensional state space, a spectrum-generating algebra exists. When the Hamiltonian is an operator on an $m$-dimensional Hilbert space, the algebra $\mathfrak{u}(m)$ is spectrum generating. Suppose $H = \sum H_{ij} E_{ij}$, where $E_{ij}$ denotes the $m \times m$ matrix whose sole nonzero entry is one at the intersection of row $i$ and column $j$. The complexification of the spectrum-generating algebra $\mathfrak{u}(m)$ is the span of the set of $m^2$ matrices $\{E_{ij}, 1 \leqslant i, j \leqslant m\}$. Other choices for a spectrum-generating algebra are often possible. For example, consider the quantum state space of a system of $A$ fermions, viz., the exterior product space of $A$-copies of an $n$ dimensional single-particle space. Any Hamiltonian on this fermion state space is in the enveloping algebra of the spectrum-generating algebra $\mathfrak{u}(n)$. Although $n \ll m$, the dimension $n!/A!(n-A)!$ of the many-particle space, the dimension of the $\mathfrak{u}(n)$ algebra will, in general, be much too large for practical purposes.

Let $P$ denote the projector onto a subspace $V$ spanned by a chosen set of low-energy eigenstates of physical interest, and let $Q$ denote the projector onto a selected subspace $W$

of $V$. The second requirement is that monomial terms in the enveloping algebra satisfies a projection property relative to $P$ and $Q$. For example, the quadratic term $\hat{X}\hat{Y} \in \mathrm{U}(\mathfrak{g})$, where $\hat{X}, \hat{Y} \in \mathfrak{g}$, is approximated within the subspace $W$ by

$$Q\hat{X}\hat{Y}Q \approx Q\hat{X}P\hat{Y}Q. \tag{39}$$

The algebra commutation relations, equations (1), can be approximated, therefore, by

$$Q\hat{X}_\alpha P\hat{X}_\beta Q - Q\hat{X}_\beta P\hat{X}_\alpha Q \approx \sum_\gamma C^\gamma_{\alpha\beta} Q\hat{X}_\gamma Q. \tag{40}$$

Commutators involving the Hamiltonian, equation (2), and the Casimir polynomials must satisfy similar projection equations.

When the matrices representing the Lie algebra elements with respect to the eigenenergy basis are approximately band diagonal, the projector conditions can be satisfied. The projection requirements guarantee that intermediate state summations in the commutator and Casimir equations can be evaluated accurately by a truncated summation. In this favorable case, errors in equations of motion created by discarding terms, e.g., those of equation (19) in the LMG model, are negligibly small.

The spectrum-generating algebra $\mathfrak{u}(m)$, where $m$ is the dimension of the state space, fails the projection property requirement because this algebra is a basis for all Hermitian operators. Not all matrices $E_{ij}$, $1 \leqslant i, j \leqslant m$, can be band diagonal in the eigenenergy or any other basis. However, in practical situations to which the equations-of-motion method applies, one is interested in large $m$-dimensional representations of a spectrum-generating algebra $\mathfrak{g}$ for which $\dim \mathfrak{g} \ll m$. In the present application, for example, we have considered representations of dimension $m$, with $m \geqslant 300$, of the 3-dimensional LMG spectrum-generating algebra $\mathfrak{su}(2)$ and observe that in all cases the matrices are band diagonal to a good approximation. We shall show in a following paper that this is a general result that follows whenever a mean-field approximation provides a reasonable first approximation for the low-energy states of interest.

The precise general conditions for a spectrum-generating algebra to satisfy the projection property are not known. Roughly speaking, we can say that the dimension of the algebra $\mathfrak{g}$ should be less than the square of the dimension of the subspace $V$. Otherwise the algebra contains operators with nontrivial matrix elements connecting low and high energy states and the projection property fails. Suppose the algebra generators can be interpreted as physically measurable transition operators. If transitions are measured and found to be small connecting low-energy states in $W$ with high energy states in $V^\perp$, then experiment supports directly the projection hypothesis.

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