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A generalization of the Lipkin model as a testing ground for many-body theories

Tesi Magistrale di
Riccardo Romano
Matricola 898601

Relatore:
Prof. Gianluca Colò

Correlatore:
Dott. Xavier Roca-Maza

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Alla mia famiglia

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Introduction

The nuclear many-body problem can be approached using many different techniques. All the methods which have been developed in nuclear physics rely on specific approximations which allow to simplify the problem. Although different in formalism, some of these methods seems to be related in spirit, if not completely equivalent. It is hard to understand these similarities in physical system which are usually characterized by many degrees of freedom.

A way to check the validity of the approximation methods is to use a solvable model as a testing ground [2, 3]. Such models should be simple enough to be solved exactly, yet not too trivial, since their aim is to mimic real systems. By comparing the results of the approximated techniques with the exact values, an estimate of the quality of the approximations can be made. Also, this procedure can suggest the situation in which each approximation method works best.

In this thesis, we will focus on one of these simple solvable models, which has been introduced by Lipkin, Meshkov and Glick in 1965 [4]. The model can be solved exactly using the angular-momentum representation, and it offers non-trivial features. In his original formulation, it is a two-level model with nucleons of one type which interact through constant potentials. The model assumes two kinds of potentials: a particle-particle (pairing) force and a particle-hole force. Despite this first formulation, since the Hamiltonian of this system is diagonal in the angular-momentum basis, the model is also suitable to describe a set of interacting spins. Indeed, due to its variety of configurations, the Lipkin model have been extensively applied in many areas of physics. Its applications include the study of quantum phase transitions [5], quantum metrology [6], the non equilibrium dynamic of the Ising model [7], etc. In nuclear physics, the Lipkin model have been intensively used to test many-body approximations. The literature on the subject is extensive, and we will cite a few here to illustrate: the Operator Boson Expansion (OBE) [8], Extended Coupled Cluster techniques (ECC) [9], the Density Functional Theory (DFT) [10], etc.

Mean-field theories, in particular, represent one of the most successful theoretical approaches to the study of nuclear structure [11]. Indeed, they are the only techniques which are able to explore all nuclei (except the lightest ones). Within this picture, the Hartree-Fock (HF) and the Random Phase Approximation (RPA) have been largely applied to the Lipkin model [1, 12, 13]. The tests show the overall good behavior of the mean-field in reproducing the energy levels of the system as the number of particle

increases. Furthermore, they prove the effectiveness of the RPA over the simplest shell model methods. Nevertheless, for some values of the parameters of the model, the Hartree-Fock ground state fails in reproducing the energy of the system. The correct result can be retrieved if a different Hartree-Fock state is assumed for these specific configurations. This feature of the Lipkin model has already been noted in the original paper [4], in which the phenomenon is described as the “insability of the Hartree-Fock state against collective excitations”. Same problems affects the RPA, due to the fact that it is still based on the Hartree-Fock ground state.

The RPA has been successful in the calculation of nuclear excitations, particularly for the collective vibrational excitations [14]. Still, the study of the spreading width of giant resonances asks for theories which include more correlations.

The aim of this work is to use the Lipkin model as a testing ground for the theories which go beyond the level of approximation of RPA. The Second Random Phase Approximation (SRPA), for example, represents a generalization of the RPA which has been very well documented [15, 16], and has been used since decades [17, 18]. Unfortunately, calculations with the SRPA are often computationally challenging, since the dimension of the RPA matrix here is raised by one order of magnitude. An alternative way to go beyond RPA is given by the Particle-Vibration Coupling (PVC) theory [19], in which the vibration is a separated degree of freedom that couples with single-particle excitations. Although extensively used [20, 21], no attempts have been made to test this technique and the SRPA on a simple system like the Lipkin model yet. To this aim, an extension of the Lipkin model will be presented in the following.

In chapter one of this thesis we review three many-body techniques which will be applied on the Lipkin model: the HF theory, the RPA and the SRPA. The results of these methods on the model are discussed in chapter two. Here, critical issues concerning the application of the techniques on the model will be highlighted. In chapter three a generalization of the Lipkin model will be presented and analyzed with the approximation methods of the previous chapters. In chapter four we show the results of the PVC method on the generalization of the Lipkin model. Chapter five reports some of the interesting features of the new model, which we believe deserve further studies. Finally, our conclusion will be drawn.

Chapter 1

The mean field approach

1.1 The static mean field

The Hamiltonian for a system of N non-relativistic particles interacting through two-body forces is

$$H = T + V = \sum_{i=1}^N t(i) + \frac{1}{2} \sum_{i \neq j}^N v(i, j), \quad (1.1)$$

where i represents the set of space, spin and isospin coordinates of the i -th nucleon. $t(i)$ is the kinetic term, while $v(i, j)$ is the two body potential. Differently from the electronic many body problem, where an external field exists due to the Coulomb potential of the nucleus, in the nuclear case the potential term is only due to the interactions among nucleons.

A full microscopic theory of the nucleus is given by the solution of the many body Schrödinger equation

$$H\Psi(1, \dots, N) = E\Psi(1 \dots N). \quad (1.2)$$

The simplest way which can be used to deal with such a problem is to describe the dynamic of the nucleons with an average potential. This approximation means that we can get rid of the two-body term, and write the Hamiltonian only with the kinetic operator and a one-body potential $U(i)$, the so called “mean field”:

$$\sum_{i=1}^N (t(i) + U(i)) \Psi(1, \dots, N) = E\Psi(1 \dots N). \quad (1.3)$$

It follows that nucleons are independent from one another. This allows to write the total wavefunction of the system as the anti-symmetrized product of single particle wavefunctions, so that the problem is completely factorized as

$$(t(i) + U(i)) \psi_i = \epsilon_i \psi_i, \quad (1.4)$$

where $E = \epsilon_1 + \dots \epsilon_A$. This procedure has originally been called “shell model”, and despite its simplicity has been widely used to obtain energy levels for closed shell nuclei. The

mean field must be built up by the action of all the nucleons interacting with each other. An analytic ansatz which yields reasonable density distributions and energy levels is the Woods-Saxon potential:

$$U_{WS}(r) = -\frac{U_0}{1 + e^{\frac{r-R}{a}}}, \quad (1.5)$$

where $R = r_0 N^{1/3}$, with $r_0 \approx 1.2$ fm. Commonly $U_0 = -50$ MeV and $a = 0.5$ MeV. Experimental findings shows that to obtain level ordering, one should correct the average field with the contribution of a two body interaction called "spin-orbit", which couples the spin angular momentum with the angular momentum of the nucleon itself.

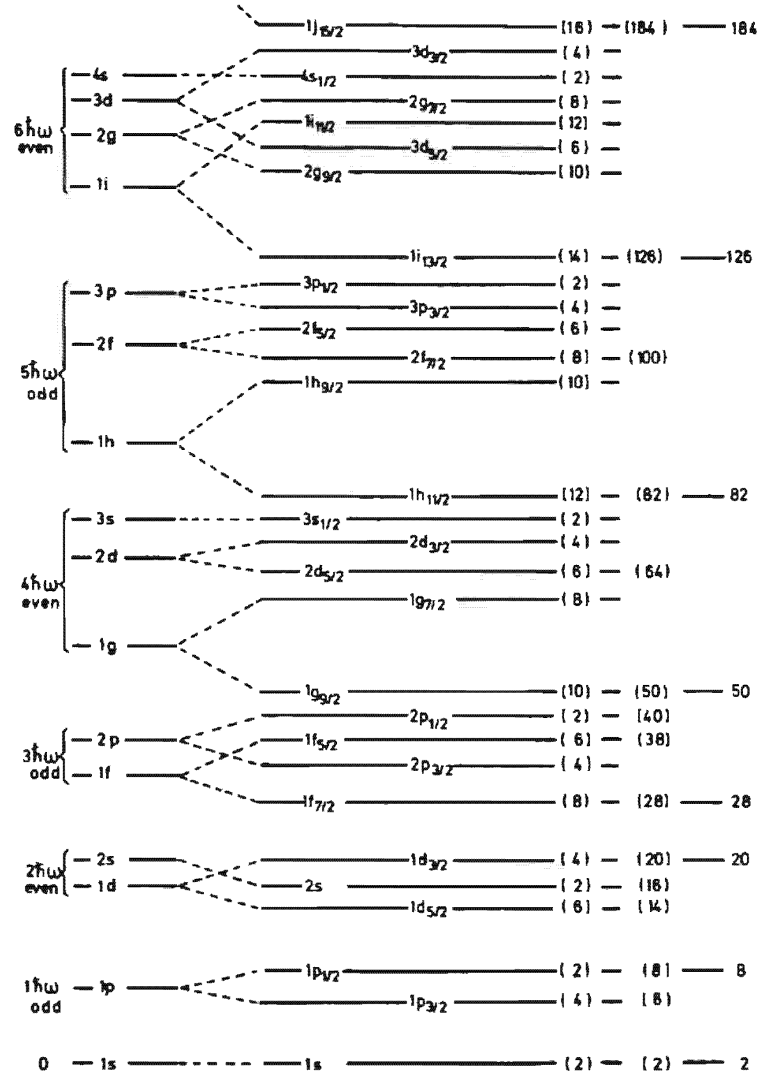


Figure 1.1: Schematic nuclear levels of the shell model with spin-orbit term. Source: [1]

1.2 The Hartree-Fock theory

Ideally, the mean field should be obtained from the two body interaction among nucleons. A way to do that is within the independent particle approximation thanks to the Hartree-Fock (HF) method.

There are many ways to obtain the Hartree-Fock equations, each of them giving a different point of view of the theory. We will discuss one of the most used derivation, which is based on the variational principle. The fundamental assumption of the Hartree-Fock theory is to take the ground state of the system as the anti-symmetric product of unknown single particle wave functions. The idea of the variational approach is to find the single particle wavefunctions as the ones which minimize the total energy of the system in this state. The derivation of the Hartree-Fock equation can also be developed in Fock space, with the aid of the Wick theorem, and it will be discussed later. Another different but highly instructive derivation of the HF equations which involves the Green's function formalism can be found in [22].

1.2.1 Variational method in configuration space

In order to provide a general picture of how Hartree-Fock methods works, we present an intuitive derivation in configuration space. The starting point is a set of N orthonormal trial single-particle states $|u_i\rangle$. The Hartree-Fock state is defined as their antisymmetric product:

$$|HF\rangle = \sqrt{N!} A(N) |u_1 \dots u_N\rangle. \quad (1.6)$$

$A(N)$ is the antisymmetrizer operator, which is defined as

$$A(N) = \frac{1}{N!} \sum_{\sigma} (-1)^{\sigma} P_{\sigma}, \quad (1.7)$$

where σ specify the permutation and P_{σ} is the coordinates permutation operator. The simplest possible permutation is the exchange of two particles, which is realized by the exchange operator P_{ij} . It's easy to see that $P_{ij}^2 = 1$ so that it is idempotent and hermitian. Since every permutation can be written as product of exchange of particles, also P_{σ} is Hermitian and idempotent and so it is $A(N)$. Note that a transformation of the single particle states by means of a unitary matrix preserves the orthogonality, and the Slater state build with the new states is equivalent to the old one.

Consider (1.1) as the Hamiltonian for the system. It can be shown that the antisymmetrizer operator commutes with it. The expectation value of Hamiltonian in this state

can be obtained with the following steps:

$$\begin{aligned}
\langle \text{HF} | T | \text{HF} \rangle &= N! \langle u_1 \dots u_N | A(N) T A(N) | u_1 \dots u_N \rangle \\
&= \sum_{\sigma} \sum_i^A \langle u_{\sigma_1} \dots u_{\sigma_N} | u_1 \dots t u_i \dots u_N \rangle \\
&= \sum_i^N \sum_{\sigma} \delta_{\sigma_1, 1} \dots \langle u_{\sigma_j} | t u_i \rangle \dots \delta_{\sigma_N, N} \\
&= \sum_i^N \langle u_i | t | u_i \rangle,
\end{aligned} \tag{1.8}$$

and

$$\begin{aligned}
\langle \text{HF} | V | \text{HF} \rangle &= N! \langle u_1 \dots u_N | A(N) V A(N) | u_1 \dots u_N \rangle \\
&= \frac{1}{2} \sum_{\sigma} \sum_{i \neq j}^N \langle u_{\sigma_1} \dots u_{\sigma_N} | v(i, j) | u_1 \dots u_i \dots u_j \dots u_N \rangle \\
&= \frac{1}{2} \sum_{\sigma} \sum_{i \neq j}^N \delta_{\sigma_1, 1} \dots \langle u_{\sigma_i} u_{\sigma_j} | v | u_i u_j \rangle \dots \delta_{\sigma_N, N} \\
&= \frac{1}{2} \sum_{i \neq j}^N (\langle u_i u_j | v | u_i u_j \rangle - \langle u_j u_i | v | u_i u_j \rangle) \\
&= \frac{1}{2} \sum_{i \neq j}^N \langle u_i u_j | v | u_i u_j - u_j u_i \rangle,
\end{aligned} \tag{1.9}$$

giving

$$\langle \text{HF} | H | \text{HF} \rangle = \sum_i^N \langle u_i | t | u_i \rangle + \frac{1}{2} \sum_{i \neq j}^N \langle u_i u_j | \bar{v} | u_i u_j \rangle. \tag{1.10}$$

Here, the potential is antisymmetrized, namely

$$\bar{v} = v(1 - P_{1,2}), \tag{1.11}$$

where $P_{1,2}$ is the exchange operator. Note that the expression involves one or two particles at a time, the other being spectators. The interaction term contains both a direct term and an exchange one. The single particle states are defined by minimizing the total energy (1.10). The procedure must be carried out enforcing orthogonality and normalization, so that the quantity to be minimized is the functional:

$$E_{\text{HF}}[u_1 \dots u_N] = \langle \text{HF} | H | \text{HF} \rangle - \sum_{ij} \epsilon_{ij} (\langle u_i | u_j \rangle - \delta_{ij}), \tag{1.12}$$

where ϵ_{ij} are the Lagrange multipliers.

$$\begin{aligned}\delta E_{\text{HF}} &= E_{\text{HF}}[u_1 \dots u_k + \eta_k \dots u_N] - E_{\text{HF}}[u_1 \dots u_N] \\ &= \langle \eta_k | t | u_k \rangle + \sum_j \langle \eta_k u_j | \bar{v} | u_k u_j \rangle - \sum_j \epsilon_{kj} \langle \eta_k | u_j \rangle + \\ &\quad \langle u_k | t | \eta_k \rangle + \sum_j \langle u_k u_j | \bar{v} | \eta_k u_j \rangle - \sum_j \epsilon_{kj} \langle u_j | \eta_k \rangle.\end{aligned}\tag{1.13}$$

The minimization condition is $\delta E_{\text{HF}} = 0$. It can be shown that if $\langle \eta | u \rangle + \langle \eta | u \rangle^* = 0$ for all η , then $|u\rangle = 0$. Furthermore, as we already noted, since the Slater determinant is left unchanged by a unitary transformation, there is a degeneracy in the solution. We may pick that one for which ϵ_{ij} : $\sum_j \epsilon_{ij} |u_j\rangle = \epsilon_i |u_i\rangle$. Then we obtain the set of N Hartree-Fock equations:

$$t |u_i\rangle + \sum_j \langle \cdot | u_j | \bar{v} | u_i u_j \rangle = \epsilon_i |u_i\rangle.\tag{1.14}$$

The presence of the exchange term replaces the N single Hartree equations (1.4) with a system of N coupled equations, which is computationally much more difficult. This is more clear when (1.14) is written in position representation:

$$\begin{aligned}-\frac{\hbar^2 \nabla^2}{2m} u_i(r) + \sum_j \int d^3 r' |n(r')|^2 \bar{v}(r, r') u_i(r) + \\ \sum_j \int d^3 r' u_j^*(r') \bar{v}(r, r') u_j(r) u_i(r') = \epsilon_i u_i(r).\end{aligned}\tag{1.15}$$

One can see that the potential term depends itself by the single-particle wavefunction. As a consequence, to solve these equation one needs to start with an ansatz for the single-particle density. The solution of the equations is a new density which can be inserted again in the Hartree-Fock equations. The cycle stops when convergence is obtained, namely when the resulting density does not change appreciably when repeating the procedure.

The obtained single particle states allows the total Hartree-Fock energy (1.10) to be computed. Projecting (1.14) on the solution $|u_i\rangle$ gives ϵ_i , which have the significance of the single particle HF energy

$$\epsilon_i = t_{ii} + \sum_j \bar{v}_{ijij},\tag{1.16}$$

which allows to write the total HF energy of the system as

$$\begin{aligned}E_{\text{HF}} &= \sum_i \epsilon_i - \frac{1}{2} \sum_{i \neq j}^N \bar{v}_{ijij}. \\ &= \frac{1}{2} \sum_i (t_{ii} + \epsilon_i).\end{aligned}\tag{1.17}$$

The HF determinant is constructed selecting the lowest single-particle states obtained by the minimization procedure. The occupied levels form the “Fermi sea”, which shows

a sharp “Fermi surface”. The variational derivation in configuration space do not make clear how the approximation is good, and cannot describe the existence of excited states. In the following section a different derivation is presented.

1.2.2 Wick theorem method in Fock space

The advantage of using second quantization is to incorporate the anti-symmetric nature of fermions and Pauli principle directly in the definition of creation and annihilation operators. Fermion operators must obey the following commutation relations

$$\begin{aligned}\{a_\mu, a_{\mu'}^\dagger\} &= \delta_{\mu\mu'} \\ \{a_\mu, a_{\mu'}\} &= \{a_\mu^\dagger, a_{\mu'}^\dagger\} = 0.\end{aligned}\tag{1.18}$$

In second quantization, the Hamiltonian (1.1) takes the form:

$$H = \sum_{\nu\nu'}^N t_{\nu\nu'} a_\nu^\dagger a_{\nu'} + \frac{1}{4} \sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} a_\mu^\dagger a_\nu^\dagger a_{\nu'} a_{\mu'},\tag{1.19}$$

whereas the analog of the Slater determinants is

$$|\text{HF}\rangle = \prod_i a_i^\dagger |0\rangle,\tag{1.20}$$

where i denotes the states inside the Fermi surface and $|0\rangle$ is the particle vacuum state. The single-fermion basis for which $|\text{HF}\rangle$ is a good approximation of the ground state is still to be chosen. To this aim, we can use the Wick theorem (see [22]) in order to write the two-body interaction in normal order with respect to the $|\text{HF}\rangle$ state ¹:

$$\begin{aligned}H &= \sum_{\nu\nu'}^N \left(t_{\nu\nu'} + \frac{1}{4} \sum_\mu \bar{v}_{\mu\nu\mu\nu} \right) a_\nu^\dagger a_{\nu'} \\ &\quad - \frac{1}{2} \sum_{\mu\nu} \bar{v}_{\mu\nu\mu\nu} + \frac{1}{4} \sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} : a_\mu^\dagger a_\nu^\dagger a_{\nu'} a_{\mu'} : \end{aligned}\tag{1.21}$$

The Hartree-Fock approximation consists in choosing a single particle basis which diagonalize the one-body term:

$$t_{\nu\nu'} + \frac{1}{4} \sum_\mu \bar{v}_{\mu\nu\mu\nu} = \delta_{\nu\nu'} \epsilon_\nu.\tag{1.22}$$

This is the Hartree-Fock equation in the Fock space and corresponds to (1.14) in matrix form. The self-consistent nature lies in the fact that the HF states depends itself on the

¹The HF state is here regarded as a particle-hole vacuum, see Appendix A

single particle states. Substituting this in the many-body Hamiltonian (1.19) gives

$$\begin{aligned} H &= \sum_{\nu}^N \epsilon_{\nu} a_{\nu}^{\dagger} a_{\nu} - \frac{1}{2} \sum_{ij} \bar{v}_{ijij} + \frac{1}{4} \sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} : a_{\mu}^{\dagger} a_{\nu}^{\dagger} a_{\nu'} a_{\mu'} : \\ &= H_0 + \frac{1}{4} \sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} : a_{\mu}^{\dagger} a_{\nu}^{\dagger} a_{\nu'} a_{\mu'} : \end{aligned} \quad (1.23)$$

where i and j refer to states below Fermi and where H_0 is the one-body Hamiltonian which is usually written in terms of the single-particle Hamiltonian h :

$$\begin{aligned} H_0 &= \sum_{\nu}^N \epsilon_{\nu} a_{\nu}^{\dagger} a_{\nu} - \frac{1}{2} \sum_{ij} \bar{v}_{ijij} \\ &= \sum_{\nu} h_{\nu\nu}. \end{aligned} \quad (1.24)$$

This reveals the nature of the HF determinant as the ground state for the one-body Hamiltonian H_0 . This formulation also enlightens the form of the residual interaction, which is the term in the Hamiltonian which is not diagonalized in the HF approximation. The HF energy is thus

$$\langle \text{HF} | H_0 | \text{HF} \rangle = \sum_i^N \epsilon_i - \frac{1}{2} \sum_{ij} \bar{v}_{ijij}, \quad (1.25)$$

as in (1.10). It is instructive to consider the HF equation (1.22) when ν refers to a state above the Fermi (m) surface and ν' to a state below (i). It reads:

$$t_{mi} + \frac{1}{4} \sum_{\mu} \bar{v}_{\mu m \mu i} = 0, \quad (1.26)$$

It tells us that the one-body Hamiltonian is characterized by 0 matrix element connecting particles above and below the Fermi surface. We will see in the next sections how in the simplest theory for excited states this feature of the HF determinant forbids any correlations between the ground and the excited states.

1.3 Equation of motion method

In the following, we shall develop the equation of motion method [23] since it will be useful in order to derive the RPA and SRPA equations. We start from a set of exact eigenvalues and eigenvectors of our Hamiltonian

$$H |\nu\rangle = E_{\nu} |\nu\rangle. \quad (1.27)$$

It is possible to define construction and destruction operator such as

$$Q_{\nu}^{\dagger} |0\rangle = |\nu\rangle \quad \text{and} \quad Q_{\nu} |0\rangle = 0. \quad (1.28)$$

From this we have:

$$\begin{aligned} [H, Q_\nu^\dagger] |0\rangle &= \omega_\nu Q_\nu^\dagger |0\rangle \\ [H, Q_\nu] |0\rangle &= 0, \end{aligned} \quad (1.29)$$

where $\omega_\nu = E_\nu - E_0$ is the excitation energy. In order to find an equation which is not only operatorial, these equations must be projected on a state. This state can be written by means of a generic operator R , must can be written in terms of Q_ν in order to be left with nonzero expectation values:

$$\begin{aligned} \langle 0 | R [H, Q_\nu^\dagger] | 0 \rangle &= \omega_\nu \langle 0 | R Q_\nu^\dagger | 0 \rangle \\ \langle 0 | R^\dagger [H, Q_\nu] | 0 \rangle &= 0. \end{aligned} \quad (1.30)$$

Adding an equation to the Hermitian conjugate of the other gives

$$\begin{aligned} \langle 0 | [R, [H, Q_\nu^\dagger]] | 0 \rangle &= \omega_\nu \langle 0 | [R, Q_\nu^\dagger] | 0 \rangle \\ \langle 0 | [R^\dagger, [H, Q_\nu]] | 0 \rangle &= -\omega_\nu \langle 0 | [R^\dagger, Q_\nu] | 0 \rangle. \end{aligned} \quad (1.31)$$

Another possible choice would have been to subtract one of the (1.30) to the other, which would have given anti-commutators instead of commutators. Since one equation is the complex conjugate of the other, it is actually necessary to solve only one of the two. The equation of motion we want to solve is thus

$$\langle 0 | [R, [H, Q_\nu^\dagger]] | 0 \rangle = \omega_\nu \langle 0 | [R, Q_\nu^\dagger] | 0 \rangle. \quad (1.32)$$

In practice, one needs to use some approximations for the ground state $|0\rangle$. Unfortunately, the hermiticity of the equation is no more guaranteed, and to retain that sometimes one needs to consider an alternative form of the equation of motion [23]:

$$\langle 0 | [R, H, Q_\nu^\dagger] | 0 \rangle = \omega_\nu \langle 0 | [R, Q_\nu^\dagger] | 0 \rangle, \quad (1.33)$$

where we define

$$[R, H, Q_\nu^\dagger] = \frac{[R, [H, Q_\nu^\dagger]] + [[R, H], Q_\nu^\dagger]}{2}. \quad (1.34)$$

Equation (1.33) is completely equivalent to the previous equation of motion for the exact ground state, in fact, for a state that is stationary:

$$\begin{aligned} \langle 0 | [[R, Q_\nu^\dagger], H] | 0 \rangle &= i \frac{d}{dt} \langle 0 | [R, Q_\nu^\dagger] | 0 \rangle \\ &= 0. \end{aligned} \quad (1.35)$$

When using an approximate ground state, though, this relation may not hold exactly. This version of the equation of motion is preferable in real calculations, because it maintains exact orthogonality relations among its solution [14].

1.4 The dynamical mean-field

Using independent particle models and a suitable effective interaction the basic properties of the spectra of many nuclei can be explained. Nevertheless, there exist many excited states with features that cannot be easily reproduced within the framework of shell model excitations. For example, in ^{16}O we see around 22 MeV a 5 MeV broad resonance usually called the “giant dipole”. There are many states like that. These “Giant Resonances” lie in the energy range of $\approx 10\text{--}30$ MeV and emerge on the background of other excited states. It turns out that these excitations can only be explained if we suppose that many nucleons can behave collectively inside the nucleus, in a similar fashion as vibrations in the liquid drop model [1].

This behavior can be achieved microscopically if one consider correlations between the excited states, or “configurations”. The Tamm-Dancoff Approximation (TDA) represents the first step in this directions, and it is based on a HF basis. Ground state correlations are taken into account if a more general basis is adopted, and this is done within the Random Phase Approximation (RPA). A larger basis is taken in the Second Random Phase Approximation (SRPA).

1.4.1 The Tamm-Dancoff Approximation

We have seen that the HF state is built filling with nucleons the single particle states up to the Fermi level. Actually, the HF one-body Hamiltonian (1.24) can also be used with a basis which contains excited states. Nonetheless, this is not satisfactory since it still leaves apart the residual interaction completely. We want now to incorporate excited states inside the theory and also include correlations between them.

The first excitation is the promotion of a particle outside the Fermi level, and it’s called 1p-1h excitation. We can construct it in second quantization as

$$a_m^\dagger a_i |\text{HF}\rangle. \quad (1.36)$$

where from now on m, n, p and q refers to state above Fermi, while i, j, k and l below. Each the 1p-1h, 2p-2h, 3p-3h, $\dots$, Np-Nh excitations is a complete set which is orthogonal to the others and that can be used to expand the many-body wave functions of the ground or the excited states. We can write, thus

$$\begin{aligned} |\text{HF}\rangle &= X_0^0 |\text{HF}\rangle + \sum_{mi} X_{mi}^0 a_m^\dagger a_i |\text{HF}\rangle + \dots \\ |\nu\rangle &= X_0^\nu |\text{HF}\rangle + \sum_{mi} X_{mi}^\nu a_m^\dagger a_i |\text{HF}\rangle + \dots \end{aligned} \quad (1.37)$$

The exact diagonalization of the Hamiltonian in the whole space of Np-Nh is a formidable task which cannot be solved. To deal with this situation, the standard way is to truncate the problem to a finite space. The simplest choice is to consider only 1p-1h excitation, which are the lowest configurations in energy, and therefore most important for low-lying

states. Using this approximation (Tamm-Dancoff), the ground state remain $|\text{HF}\rangle$, while the excited state is given retaining only the second term:

$$\begin{aligned} |\text{HF}\rangle &= |\text{HF}\rangle \\ |\nu\rangle &= \sum_{mi} X_{mi}^\nu a_m^\dagger a_i |\text{HF}\rangle. \end{aligned} \quad (1.38)$$

Of course, this means that no correlations are not taken into account for the ground state. This is a consequence of the HF condition discussed previously, see (1.26). Once the basis where the Hamiltonian is diagonal is defined, we can project the Schrödinger equation on a generic state

$$\langle \text{HF} | R^\dagger H | \nu \rangle = E_\nu \langle \text{HF} | R^\dagger | \nu \rangle, \quad (1.39)$$

where R is be written in terms of (1.38), as explained before for the TDA. In this case, $R = a_m^\dagger a_i$, so that:

$$\sum_{nj} X_{nj}^\nu \langle \text{HF} | a_i^\dagger a_m H a_n^\dagger a_j | \text{HF} \rangle = \sum_{nj} X_{nj}^\nu E_\nu \langle \text{HF} | a_i^\dagger a_m a_n^\dagger a_j | \text{HF} \rangle, \quad (1.40)$$

which can be written in a more convenient form using the Wick theorem:

$$\sum_{nj} A_{minj} X_{nj}^\nu = \omega_\nu X_{mi}^\nu, \quad (1.41)$$

where

$$A_{minj} = \langle \text{HF} | a_i^\dagger a_m [H, a_n^\dagger a_j] | \text{HF} \rangle. \quad (1.42)$$

Here, $\omega_\nu = E_\nu - E_{\text{HF}}$ is the excitation energy. If we consider a general Hamiltonian composed by a kinetic term and a two-body interaction like (1.19), the commutators in A_{minj} can be calculated. Using Wick theorem, one gets:

$$A_{minj} = (\epsilon_m - \epsilon_i) \delta_{mn} \delta_{ij} + \bar{v}_{mj in}, \quad (1.43)$$

where the matrix element of the interaction comes from the diagonalization of a part of the residual interaction. For many purposes it turns useful to represent the matrix elements of the interaction graphically. In many body calculations, this is usually done in the particle-hole representation, and the procedure is described in detail in Appendix A. The graphical representation of $\bar{v}_{mj in}$ in Fig. 1.2 shows the annihilation of a particle-hole pair into another particle-hole pair. For this reason, we refer to this matrix element as $1p\text{-}1h \rightarrow 1p\text{-}1h$.

1.4.2 The Random Phase Approximation

The RPA is the simplest theory of excited states which allows to include correlations inside the ground state. This is in contrast with the TDA, whose ground state, as we have seen, has a pure independent-particle character. Both TDA and RPA equations can be derived using the equation of motion method, namely from (1.32). TDA equations

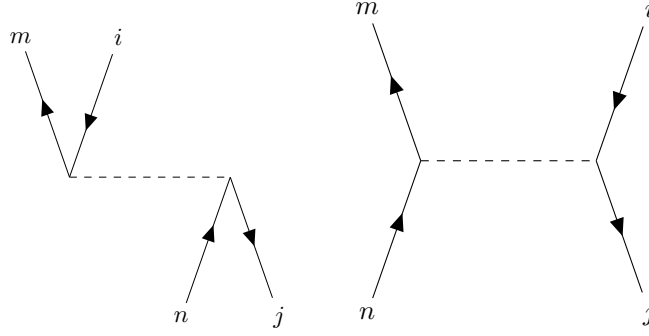


Figure 1.2: Direct and exchange part of the 1p-1h interaction matrix element of (1.43)

follows taking $|0\rangle = |\text{HF}\rangle$ and writing $Q_\nu^\dagger$ as the simplest possible excitation operator, that is the operator which creates a particle above Fermi and destroys a particle below Fermi, namely:

$$Q_\nu^\dagger = \sum_{mi} X_{mi}^\nu a_m^\dagger a_i. \quad (1.44)$$

In this theory, $R = a_m^\dagger a_i$. The RPA theory represents the most straightforward generalization to this choice. Here we take as excitation operator

$$Q_\nu^\dagger = \sum_{mi} X_{mi}^\nu a_m^\dagger a_i - \sum_{mi} Y_{mi}^\nu a_i^\dagger a_m. \quad (1.45)$$

This new operator leads a different ground state, which is defined by

$$\begin{aligned} Q_\nu |\text{RPA}\rangle &= 0. \\ Q_\nu^\dagger |\text{RPA}\rangle &= |\nu\rangle. \end{aligned} \quad (1.46)$$

This represents a more general ground state than $|\text{HF}\rangle$. Now, we have two kinds of operators R , one for each term in the definition of $Q_\nu^\dagger$. Starting from the equation of motion (1.33) we get two set of equations:

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_m, H, Q_\nu^\dagger] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [a_i^\dagger a_m, Q_\nu^\dagger] | \text{RPA} \rangle \\ \langle \text{RPA} | [a_m^\dagger a_i, H, Q_\nu^\dagger] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [a_m^\dagger a_i, Q_\nu^\dagger] | \text{RPA} \rangle. \end{aligned} \quad (1.47)$$

Next steps can be made within the “quasi-boson approximation” (QBA), which consists in taking all the expectation values on HF states. The name comes from the fact that the approximation would be an exact relation if particle-hole operators obeyed the boson commutation relation². The approximation reads:

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{RPA} \rangle &\simeq \langle \text{HF} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{HF} \rangle \\ &= \delta_{ij} \delta_{mn} \end{aligned} \quad (1.48)$$

²This also explains the choice of taking commutators instead of anti-commutators when writing the equation of motion, which allows simple evaluation of the commutators on RHS of the equations of motion [14].

Note that with this approximation for the ground state, the condition (1.35) is still satisfied, thus the simpler equation of motion (1.32) can be used for our calculations. This result is a consequence of the HF equations, which can also be expressed as $\langle \text{HF} | [a_\mu^\dagger a_\nu, H] | \text{HF} \rangle = 0$, and applies since the commutator of two one-body operator is also a one-body operator. If we use the definition of the excitation equation (1.45) in the equation of motion we end up with

$$\begin{aligned} \sum_{pk} (A_{mi,pk} X_{pk}^\nu + B_{mi,pk}^\nu Y_{pk}^\nu) &= \omega_\nu X_{mi}^\nu \\ \sum_{pk} (-B_{mi,pk}^* Y_{pk}^\nu - A_{mi,pk}^* X_{pk}^\nu) &= \omega_\nu Y_{mi}^\nu. \end{aligned} \quad (1.49)$$

Here we have exploited the anti-commutation relations at the r.h.s. and we have defined

$$\begin{aligned} A_{mi,pk} &\equiv \langle \text{HF} | [a_i^\dagger a_m, [H, a_p^\dagger a_k]] | \text{HF} \rangle \\ B_{mi,pk} &\equiv -\langle \text{HF} | [a_i^\dagger a_m, [H, a_k^\dagger a_p]] | \text{HF} \rangle, \end{aligned} \quad (1.50)$$

and

$$\begin{aligned} A_{mi,pk}^* &= \langle \text{HF} | [a_m^\dagger a_i, [H, a_k^\dagger a_p]] | \text{HF} \rangle \\ B_{mi,pk}^* &= -\langle \text{HF} | [a_m^\dagger a_i, [H, a_p^\dagger a_k]] | \text{HF} \rangle. \end{aligned} \quad (1.51)$$

We can easily see that

$$\begin{aligned} A_{mi,pk} &= A_{pk,mi}^* \quad (\text{Hermitian}) \\ B_{mi,pk} &= B_{pk,mi} \quad (\text{symmetric}). \end{aligned} \quad (1.52)$$

Eventually one can write the equations all together in matrix form:

$$\begin{pmatrix} A - \omega & B \\ B^* & A^* + \omega \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = 0, \quad (1.53)$$

This is called ‘‘RPA equation’’. We get back to the TDA approximation by putting $Y = 0$, which leaves us with $AX = \omega X$. Using a general Hamiltonian composed by a kinetic term and a two-body interaction like (1.19), the commutators in (1.50) can be computed. With the Wick theorem we obtain:

$$\begin{aligned} A_{minj} &= (\epsilon_m - \epsilon_i) \delta_{mn} \delta_{ij} + \bar{v}_{mj in} \\ B_{minj} &= \bar{v}_{mnij}, \end{aligned} \quad (1.54)$$

where ϵ are here the HF single particle energies and the matrix elements of the two body force are antisymmetrized. As expected, A is the TDA matrix. The novelty in RPA is represented by the presence of $\bar{v}_{mnij}$ matrix element, which is displayed graphically in Fig. 1.3 in particle-hole representation. Here, the interaction create two particle-hole pairs from the vacuum, and this is why sometimes the interaction is referred as virtual 2p-2h [1]. It must be emphasized, though, that the excitations space is still given by 1p-1h states.

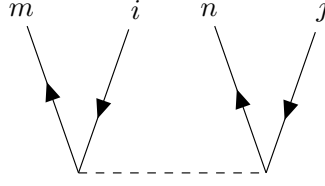


Figure 1.3: Direct part of the 1p-1h interaction matrix element of the B matrix of (1.54). The exchange part is obtained substituting j with i .

The diagonalization of the RPA matrix gives the excitation energy ω_ν and the amplitudes X_{mi}^ν and Y_{mi}^ν . It is easy to demonstrate that

$$\begin{aligned} X_{mi}^{*\nu} &= \langle \nu | a_m^\dagger a_i | 0 \rangle \\ Y_{mi}^{*\nu} &= \langle \nu | a_i^\dagger a_m | 0 \rangle, \end{aligned} \quad (1.55)$$

which means that they represent the overlap of the excited state ν , called RPA *phonon*, with a particle-hole pair acting on a ground state. They are a measure of how much the excited state is built by means of a particular particle-hole excitation. The values of X_{mi} and Y_{mi} define completely the excitation operator $Q_\nu^\dagger$ as the phonon creation operator. Consider now a general perturbing external field

$$F = \sum_{\mu\mu'} f_{\mu\mu'} a_\mu^\dagger a_\mu. \quad (1.56)$$

The transition matrix element for this operator in RPA is given by

$$\langle \nu | F | 0 \rangle = \sum_{mi} (X_{mi}^{*\nu} f_{mi}^* + Y_{mi}^{*\nu} f_{im}^*). \quad (1.57)$$

The probability for the excitation to occur at a given energy is given by the strength function. It is defined as the sum over all transition probability which contribute to a given energy excitation. It describes the response of a nucleus to the external perturbation:

$$S(\omega) = \sum_\nu |\langle \nu | F | 0 \rangle|^2 \delta(\omega - \omega_\nu), \quad (1.58)$$

It is easy to see that for a given energy the strength function is maximum when there are many amplitudes of roughly equal value. They add constructively, since the magnitude of the transition probability increases with the number of particle-hole excitation. This situation can be understood in terms of many particles which contribute in a cooperative fashion to produce a collective behavior of the nucleus. This particular excited state is called Giant Resonance (GR).

Higher configuration, like 2p-2h excitation, do not have a dominant part of the wavefunction in a Giant Resonance state. They would give rise, however, to a spreading of the transition strength of the GR, whereas in the standard RPA theory it is a discrete state.

Formal proprieties of RPA

The formal properties of the RPA equations have been investigated by Thouless [24]. These properties are more general, since they can be obtained from the equation of motion (1.32) [23]. We simply list them for the case of RPA:

- The solutions appear in pairs having symmetric positive and negative eigenvalues.
- When the Thouless stability condition is satisfied, the RPA solutions have real energies.
- Center-of-mass motion or rotations of a deformed nucleus are examples of “spurious” configurations because they do not correspond to real excitation of the nucleus, since can be removed with a suitable choice of reference system. In RPA, anyway, center-of-mass momentum or angular momentum commute with the Hamiltonian and therefore produce a zero-energy solution.
- The RPA solutions are orthonormal.
- The non-spurious solutions form a complete set.
- The matrix element of any operator calculated in RPA preserves the energy-weighted sum rule.

1.4.3 The Second Random Phase Approximation

As already noted, the standard RPA technique is able to describe the centroid of giant resonance, but it fails to account for the observed decay width of heavy nuclei [25]. This is due to the lack of mixing with more complicated nuclear configurations, like 2p-2h, 3p-3h, etc. Since we assume that the nuclear Hamiltonian only contains one- and two-body parts, an initially excited 1p-1h state can mix directly only with 2p-2h configuration. The second random phase approximation (SRPA) represents an extension of the original theory along this line, which accounts for residual coupling to the 2p-2h subspace.

As in the RPA, the SRPA equations can be derived from the equations of motion, namely from (1.33). In this case, the excitation operator comprises 2p-2h components in addition to the familiar 1p-1h components:

$$\begin{aligned}
 Q_\nu^\dagger = & \sum_{mi} X_{mi}^\nu a_m^\dagger a_i - \sum_{mi} Y_{mi}^\nu a_i^\dagger a_m \\
 & + \sum_{m < n, i < j} Z_{mnij}^\nu a_m^\dagger a_n^\dagger a_j a_i - \sum_{m < n, i < j} W_{mnij}^\nu a_i^\dagger a_j^\dagger a_n a_m.
 \end{aligned} \tag{1.59}$$

We now assume the HF approximation when evaluating the ground state expectation

values:

$$\begin{aligned}
\langle \text{SRPA} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{SRPA} \rangle &\approx \langle \text{HF} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{HF} \rangle \\
&= \delta_{ij} \delta_{nm} \\
\langle \text{SRPA} | [a_i^\dagger a_j^\dagger a_m a_n, a_p^\dagger a_q^\dagger a_k a_l] | \text{SRPA} \rangle &\approx \langle \text{HF} | [a_i^\dagger a_j^\dagger a_m a_n, a_p^\dagger a_q^\dagger a_k a_l] | \text{HF} \rangle \\
&= \delta_{il} \delta_{jk} \delta_{mq} \delta_{np} - \delta_{il} \delta_{jk} \delta_{mp} \delta_{nq} \\
&\quad + \delta_{ik} \delta_{jl} \delta_{mp} \delta_{nq} - \delta_{ik} \delta_{jl} \delta_{mq} \delta_{np}.
\end{aligned} \tag{1.60}$$

While the first equation represents the same approximation made in RPA (1.48), the second one is not exactly the QBA (see Appendix B). One can repeat the same steps as in the RPA case with the new excitation operator to get the SRPA equations

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix}, \tag{1.61}$$

where

$$\begin{aligned}
\mathcal{A} &= \begin{pmatrix} A_{mi,nj} & A_{mi,pqkl} \\ A_{mni,j,pk} & A_{mni,j,pqkl} \end{pmatrix} \\
\mathcal{B} &= \begin{pmatrix} B_{mi,nj} & B_{mi,pqkl} \\ B_{mni,j,pk} & B_{mni,j,pqkl} \end{pmatrix},
\end{aligned} \tag{1.62}$$

and

$$\begin{aligned}
\mathcal{X}_\nu &= \begin{pmatrix} X^\nu \\ Z^\nu \end{pmatrix} \\
\mathcal{Y}_\nu &= \begin{pmatrix} Y^\nu \\ W^\nu \end{pmatrix}.
\end{aligned} \tag{1.63}$$

$A_{mi,nj}$ and $B_{mi,nj}$ are the usual RPA matrices (1.50), while the others reads:

$$\begin{aligned}
A_{mi,pqkl} &= \langle \text{HF} | [a_i^\dagger a_m, H, a_p^\dagger a_q^\dagger a_l a_k] | \text{HF} \rangle \\
A_{mni,j,pqkl} &= \langle \text{HF} | [a_i^\dagger a_j^\dagger a_n a_m, H, a_p^\dagger a_k] | \text{HF} \rangle \\
A_{mni,j,pqkl} &= \langle \text{HF} | [a_i^\dagger a_j^\dagger a_n a_m, H, a_p^\dagger a_q^\dagger a_l a_k] | \text{HF} \rangle,
\end{aligned} \tag{1.64}$$

and

$$\begin{aligned}
B_{mi,pqkl} &= \langle \text{HF} | [a_i^\dagger a_m, H, a_k^\dagger a_l^\dagger a_q a_p] | \text{HF} \rangle \\
B_{mni,j,pk} &= \langle \text{HF} | [a_i^\dagger a_j^\dagger a_n a_m, H, a_k^\dagger a_q] | \text{HF} \rangle \\
B_{mni,j,pqkl} &= \langle \text{HF} | [a_i^\dagger a_j^\dagger a_n a_m, H, a_k^\dagger a_l^\dagger a_q a_p] | \text{HF} \rangle,
\end{aligned} \tag{1.65}$$

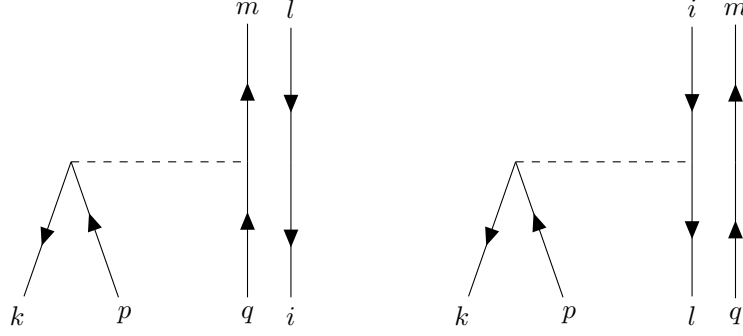


Figure 1.4: Direct part of the first (left) and second (right) interaction terms in $A_{mi,pqkl}$ of (1.68).

where, this time, the general equation of motion (1.33) must be used in order to preserve hermiticity. It can be shown that the SRPA exhibits formal properties in analogy with that listed above for the simple RPA [16], namely

$$\begin{aligned}\mathcal{A} &= \mathcal{A}^\dagger \quad (\text{Hermitian}) \\ \mathcal{B} &= \mathcal{B}^T \quad (\text{symmetric}).\end{aligned}\tag{1.66}$$

As a consequence of the use of $|\text{HF}\rangle$ as the ground state, for the B matrix we get:

$$B_{mi,pqkl} = B_{mni,j,pk} = B_{mni,j,pqkl} = 0.\tag{1.67}$$

The matrix elements can be calculated explicitly with the general Hamiltonian (1.19). In addition to the term included in the RPA, we have:

$$\begin{aligned}A_{mi,pqkl} &= a(kl)\bar{v}_{kmpq}\delta_{il} - a(pq)\bar{v}_{klpi}\delta_{mq} \\ A_{mni,j,pqkl} &= (\epsilon_m + \epsilon_n - \epsilon_i - \epsilon_j)a(pq)a(kl)\delta_{mp}\delta_{ik}\delta_{nq}\delta_{jl} + a(kl)\bar{v}_{mnpq}\delta_{ik}\delta_{jl} \\ &\quad + a(pq)\bar{v}_{ijkl}\delta_{mp}\delta_{nq} + a(mn)a(pq)a(kl)\bar{v}_{mkip}\delta_{jl}\delta_{nq},\end{aligned}\tag{1.68}$$

where $a(kl)$ is the antisymmetrizer for the indices k and l . The non-diagonal terms of the SRPA matrix $A_{mi,pqkl}$ are shown in Fig. 1.4: they are responsible of destroying two particle-hole pairs and creating one particle-hole pair. Consequently, they are referred as $2p\text{-}2h \rightarrow 1p\text{-}1h$ terms. They include correlations between the well-known $1p\text{-}1h$ subspace of RPA to the newly introduced $2p\text{-}2h$ subspace. The $A_{mni,j,pqkl}$ interaction terms are drawn in Fig. 1.5: they are the mixing terms in the $2p\text{-}2h$ subspace, namely represents $2p\text{-}2h \rightarrow 2p\text{-}2h$ processes.

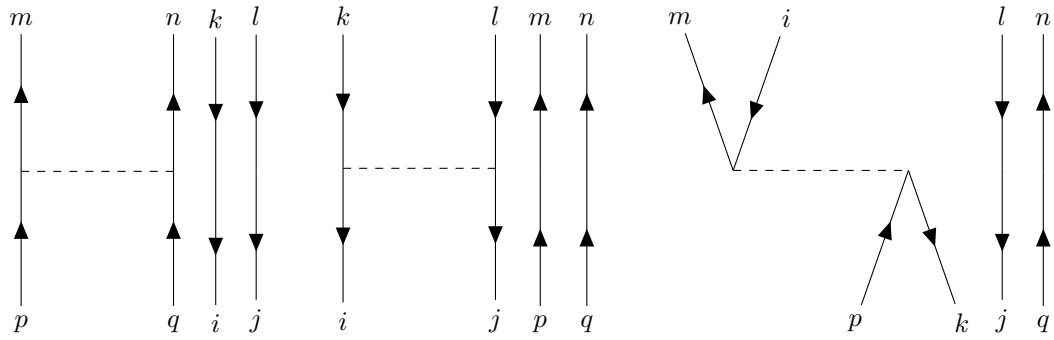


Figure 1.5: Direct part of the three interaction terms (from left to right) in $A_{mni,j,pqkl}$ of (1.68).

Chapter 2

The Lipkin model

The Lipkin-Meshkov-Glick (LMG) model [4] is an algebraic model introduced in 1965 which played an important role in nuclear theory. Because of its simplicity, it has been widely used as a testing ground for many-body approximations, with the aim of characterizing theories which go beyond the original shell model calculations [1]. Due to its $SU(2)$ structure, the LMG model can also be used to represent a set of spins, and therefore has also been used in the physics of matter and statistical physics [7].

2.1 The model

The LMG model describes a two level system where one level is situated just below the Fermi level, the other just above, separated by an energy difference of ϵ . The levels are N -fold degenerate, and the system is filled with N fermions. Each state is characterized by a quantum number σ that assumes the value $+1$ in the upper level and -1 in the lower one, and a quantum number p specifying the particular degenerate state within the shell. A two body interaction which does not change the value of p is considered.

The author proposed the following model Hamiltonian:

$$H = \sum_{p\sigma} \left(\frac{1}{2} \sigma \epsilon \right) a_{p\sigma}^\dagger a_{p\sigma} - \frac{V}{2} \sum_{pp'\sigma} a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p'-\sigma} a_{p-\sigma} - \frac{W}{2} \sum_{pp'\sigma} a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p'\sigma} a_{p-\sigma}, \quad (2.1)$$

where $a_{p\sigma}^\dagger$ and $a_{p\sigma}$ are the creation and destruction operators for a fermion in the state p, σ which satisfies the usual fermion anti-commutation relations. The first term of the Hamiltonian represents the sum of the energy the single particles have due to the external potential. The term proportional to V scatters a pair of particles from one state to another, while the term proportional to W scatters one particle up while another is scattered down.

The fact that each particle can stay in only two possible states suggested the author the use of a “quasi-spin” formulation, in which the spin-up and spin-down configurations are analogous to the upper and lower level state. In second quantization, the spin operator

in Pauli representation is

$$S^i = \sum_{p,\alpha,\alpha'} a_{p,\alpha}^\dagger S_{\alpha\alpha'}^i a_{p,\alpha'} \quad S_{\alpha\alpha'}^i = \frac{1}{2} \sigma_{\alpha\alpha'}^i, \quad (2.2)$$

where $\alpha = \uparrow, \downarrow$ is the spin quantum number and σ is the i -Pauli spin matrix:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.3)$$

In this representation, the components of the spin operator are

$$\begin{aligned} S^x &= \frac{1}{2} \sum_p \left(a_{p\uparrow}^\dagger a_{p\downarrow} + a_{p\downarrow}^\dagger a_{p\uparrow} \right) \\ S^y &= \frac{1}{2i} \sum_p \left(a_{p\uparrow}^\dagger a_{p\downarrow} - a_{p\downarrow}^\dagger a_{p\uparrow} \right) \\ S^z &= \frac{1}{2} \sum_p \left(a_{p\uparrow}^\dagger a_{p\uparrow} - a_{p\downarrow}^\dagger a_{p\downarrow} \right). \end{aligned} \quad (2.4)$$

With the corresponding ladder operator:

$$\begin{aligned} S_+ &= S^x + iS^y & S_- &= S^x - iS^y \\ &= \sum_p a_{p\uparrow}^\dagger a_{p\downarrow} & &= \sum_p a_{p\downarrow}^\dagger a_{p\uparrow} \end{aligned} \quad (2.5)$$

Similarly, in the LMG model one can introduce quasi-spin operator. In our case, the up and down configurations correspond to the upper and lower level and are represented by the quantum number $\sigma = +, -$. To lighten this difference, we will write our “quasi-spin” operators as K :

$$\begin{aligned} K_0 &= \frac{1}{2} \sum_p^N \left(a_{p,+}^\dagger a_{p,+} - a_{p,-}^\dagger a_{p,-} \right) \\ K_+ &= \sum_p^N a_{p,+}^\dagger a_{p,-} \\ K_- &= \sum_p^N a_{p,-}^\dagger a_{p,+}, \end{aligned} \quad (2.6)$$

which generate an $SU(2)$ algebraic structure. The operator K_+ and K_- scatter one particle from one level to the other one. It is easy to see that $K_- = (K_+)^\dagger$. With these operators, the LMG Hamiltonian takes the simple form:

$$\boxed{H = \epsilon K_0 - \frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (K_+ K_- + K_- K_+).} \quad (2.7)$$

Consider the following particular cases:

- In the absence of interactions ($V = 0$ and $W = 0$), the ground state is the state where all the particles lie in the lower level. The total energy is thus given by counting the number of particles in the lower state:

$$E = -\epsilon N/2. \quad (2.8)$$

- $W = 0$ and $V \neq 0$. The interaction term proportional to W does not mix configurations, because its expectation value is non-zero only when final and initial states are the same, while the term proportional to V does. Since we are interested to test many body approaches which take care of ground state correlations, this is a useful simplification. Using the definition of the ladder operator, the Hamiltonian can be rewritten as

$$H = \epsilon K_0 - V(K_x^2 - K_y^2), \quad (2.9)$$

which shows that a 180 rotation in quasi-spin space about an axis in the xy plane at an angle of 45 to the x and y axes change H into $-H$.

- Taking $W = V$ we lose the rotational symmetry and end up with a compact formulation of the LMG Hamiltonian:

$$H = \epsilon K_0 - 2V K_x^2. \quad (2.10)$$

We are going to develop the LMG model in his full formulation, but initially we will focus mostly with the behavior of V , which is responsible for mixing the ground state with the excited states, and which is also interesting due to his “pairing” nature. Nevertheless, we will consider potential W in the two different configurations listed above, following the Lipkin procedure. In the following chapters we will adopt a much broader view of the system, trying to explore other regions of the potentials.

2.2 Solution of the model

Our aim is to find a basis for the LMG Hamiltonian. First, we notice that the quasi-spin operators satisfies by construction the angular momentum commutation relations. This can be easily checked using fermion anti-commutation relations:

$$\begin{aligned} [K_+, K_-] &= 2K_0 \\ [K_0, K_{\pm}] &= \pm K_{\pm}. \end{aligned} \quad (2.11)$$

The Hamiltonian depends on operators $K_{\pm}$ and K_0 . If we define

$$K^2 \equiv \frac{1}{2}\{K_+, K_-\} + K_0^2, \quad (2.12)$$

it's easy to check it commutes with K_0 . This suggests to take a basis where both K_0 and K^2 are diagonalized; as in the standard procedure [26], we choose $|k, m\rangle$ as an orthogonal basis for the system and write

$$\begin{aligned} K^2 |k, m\rangle &= k(k+1) |k, m\rangle \\ K_0 |k, m\rangle &= m |k, m\rangle. \end{aligned} \quad (2.13)$$

Here, m correspond to the eigenvalue of the projection of the quasi-spin K_0 , while $k(k+1)$ is the total quasi-spin eigenvalue. This leads to the well known eigenvalues for the ladder operator:

$$K_{\pm} |k, m\rangle = \sqrt{k(k+1) - m(m \pm 1)} |k, m \pm 1\rangle. \quad (2.14)$$

The dimension of this basis can be deduced by the second of (2.13). The maximum eigenvalue of K_0 comes from its definition in (2.6), and corresponds to the situation where all the particles stay in the upper level, namely it is $N/2$. The minimum, instead, is given by the opposite situation and it is $-N/2$. Since every eigenvalues differ by ϵ , the number of state must be $N+1$. Hence, m corresponds to the different energy configurations the system can have, while k describe the system as a whole. Since k is equal to the maximum value of m , we must take $k = N/2$.

We can evaluate the Hamiltonian in this basis. For the diagonal elements, we get

$$\begin{aligned} \langle k, m | H | k, m \rangle &= \epsilon m - \frac{W}{2} \left(\langle k, m | K_+ \sqrt{k(k+1) - m(m-1)} | k, m-1 \rangle + \right. \\ &\quad \left. + \langle k, m | K_+ \sqrt{k(k+1) - m(m+1)} | k, m+1 \rangle \right) \\ &= \epsilon m - \frac{W}{2} \left(\sqrt{k(k+1) - m(m-1)} \sqrt{k(k+1) - (m-1)m} + \right. \\ &\quad \left. + \sqrt{k(k+1) - m(m+1)} \sqrt{k(k+1) - (m+1)m} \right) \\ &= \epsilon m - W (k(k+1) - m^2), \end{aligned} \quad (2.15)$$

while, with similar calculations:

$$\begin{aligned} \langle k, m | H | k, m+1 \rangle &= 0 \\ \langle k, m | H | k, m+2 \rangle &= -\frac{V}{2} \sqrt{k(k+1) - (m+2)(m+1)} \sqrt{k(k+1) - (m+1)m}. \end{aligned} \quad (2.16)$$

For what follows, it is convenient scale the potential V and W as

$$\begin{aligned} v &= \frac{V}{\epsilon} (N-1) \\ w &= \frac{W}{\epsilon} (N-1). \end{aligned} \quad (2.17)$$

Since the Hamiltonian is manifestly invariant for $K_{\pm} \rightarrow K_{\mp}$ transformation, it satisfy the Hermiticity property. As an example, we write down the explicit Hamiltonian for a system composed of 3 particles. Here, $k = 3/2$ and m can assume 4 values. The resulting Hamiltonian reads:

$$\frac{H_3}{\epsilon} = \begin{pmatrix} -\frac{3}{2} - \frac{3}{2} \frac{w}{N-1} & 0 & -\sqrt{3} \frac{v}{N-1} & 0 \\ 0 & -\frac{1}{2} - \frac{7}{2} \frac{w}{N-1} & 0 & -\sqrt{3} \frac{v}{N-1} \\ -\sqrt{3} \frac{v}{N-1} & 0 & \frac{1}{2} - \frac{7}{2} \frac{w}{N-1} & 0 \\ 0 & -\sqrt{3} \frac{v}{N-1} & 0 & \frac{3}{2} - \frac{3}{2} \frac{w}{N-1} \end{pmatrix} \quad (2.18)$$

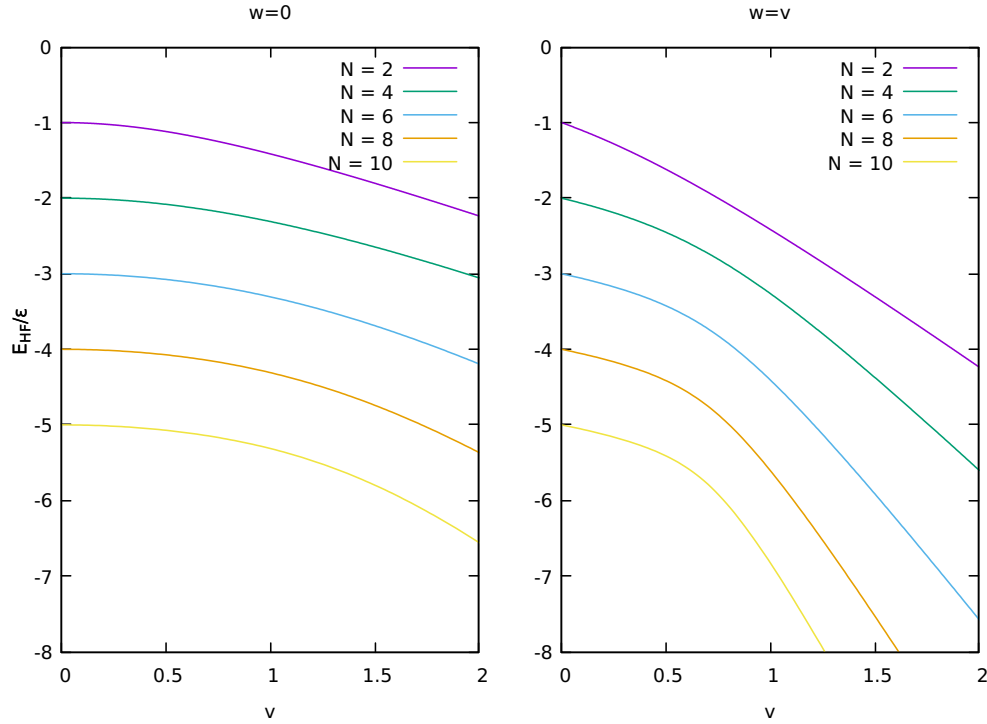


Figure 2.1: Ground state energy as a function of v for different number of particles.

As can be seen, the Hamiltonian is nonzero only on three diagonals separated by a set of zeros. This form is maintained for any N -particles LMG systems. This Hamiltonian can be diagonalized both analytically and numerically. Since the matrix is of order $N+1$, the analytical procedure only works for a small number of particle. Here, a numerical calculation has always been preferred ¹.

In fig. 2.1 the ground state energy for a system composed of different number of particles is shown. The energy of the system is decreasing due to the choice of attractive potentials.

We will focus also to the excitation energies of the system. They can be obtained simply subtracting the ground state to the eigenvalue corresponding the excitation energy we need. In 2.2 we show the first two excitation energies of a 20-particle LMG. As can be seen, the first excited state tend to the energy of the ground state, while the first on is increasing.

¹This involves the use of the Eigen C++ library. More information in http://eigen.tuxfamily.org/index.php?title=Main_Page

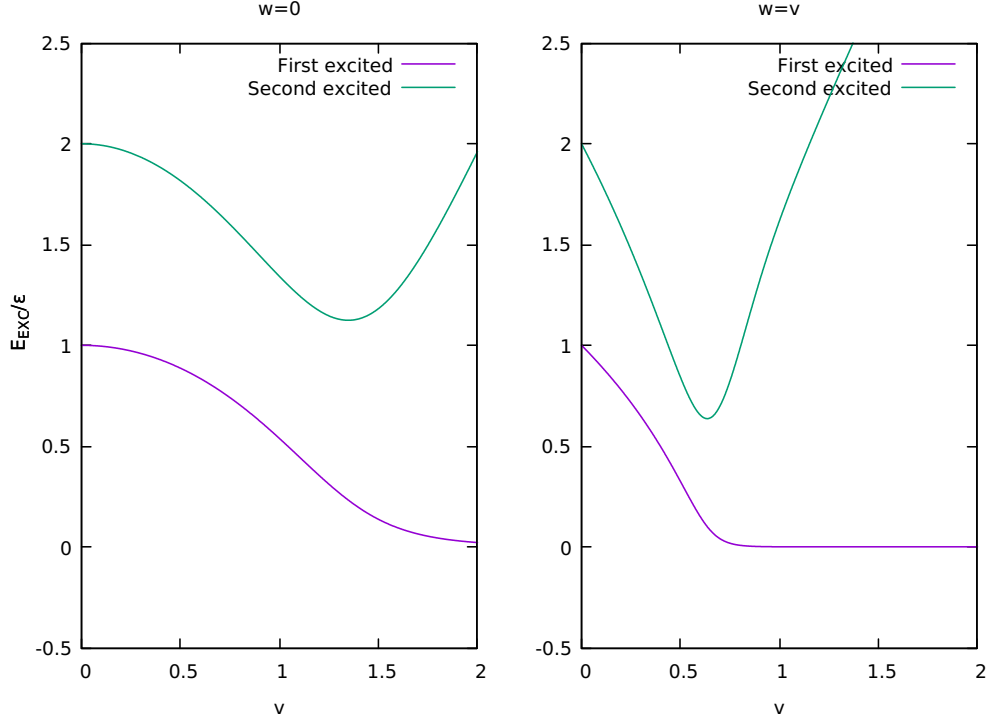


Figure 2.2: First two excitation energies for the 20-particle LMG model.

2.3 Hartree-Fock approximation

A basis where the LMG Hamiltonian is diagonalizable is already known from (2.13): each system configuration is represented by a different projection of the total quasi-spin operator. In this picture the ground state is the state where the projection on the quasi spin is minimum, and it corresponds to the case where all the particle stay on the lower energy level.

In order to develop the Hartree-Fock theory, though, we have to construct the Slater determinant. The obvious choice to this aim is to consider the state given by the product of all the particles in the lower level:

$$|\Phi_0\rangle = \prod_p a_{p,-}^\dagger |0\rangle, \quad (2.19)$$

where $|0\rangle$ is the vacuum for the particles. Nevertheless, it might be useful to consider a generalization of this state. From the theorem of Thouless [27], we know that any Slater determinant which is not orthogonal to $|\Phi_0\rangle$ can be written in the form

$$|\Phi\rangle = \prod_p \tilde{a}_{p,-}^\dagger |0\rangle, \quad (2.20)$$

where $\tilde{a}_{p,-}^\dagger$ is a linear superposition of single-particle operators. The transformation which connects them to the original single-particle operator is unitary, and can be expressed as:

$$\begin{pmatrix} \tilde{a}_{p,+} \\ \tilde{a}_{p,-} \end{pmatrix} = \begin{pmatrix} \cos \frac{\alpha}{2} & -\sin \frac{\alpha}{2} \\ \sin \frac{\alpha}{2} & \cos \frac{\alpha}{2} \end{pmatrix} \begin{pmatrix} a_{p,+} \\ a_{p,-} \end{pmatrix} \quad (2.21)$$

The case $\alpha = 0$ represents the identity transformation, and the Slater determinant is here naturally built adding all the particles on the lower state. When $\alpha \neq 0$, instead, each particle is represented as a superposition of the bare particles in the upper and lower level. This kind of transformation is widely used in many body theory when defining “quasi-particles”, as in BCS or Bogoliubov theory [22].

In order to apply the Hartree-Fock method, we need now to evaluate the Hamiltonian in this state and minimize it using α as the variational parameter. The simplest way to do that is to express the Hamiltonian in terms of the new operators, and then evaluating it on the exact ground state of the theory. We can define $\tilde{K}_+$, $\tilde{K}_0$ and $\tilde{K}_-$ using the $\tilde{a}_{p,+}$ and $\tilde{a}_{p,-}$ written above. They satisfy the angular momentum commutation relations in analogy with $K_{0,\pm}$. One can show they are connected to the old ones by the following relation:

$$\begin{pmatrix} \tilde{K}_+ \\ \tilde{K}_0 \\ \tilde{K}_- \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \cos \alpha + 1 & 2 \sin \alpha & \cos \alpha - 1 \\ -\sin \alpha & 2 \cos \alpha & -\sin \alpha \\ \cos \alpha - 1 & 2 \sin \alpha & \cos \alpha + 1 \end{pmatrix} \begin{pmatrix} K_+ \\ K_0 \\ K_- \end{pmatrix} \quad (2.22)$$

We can then rewrite the Hamiltonian in the new basis:

$$\begin{aligned} \tilde{H} = & \frac{\epsilon}{2} \left[2 \cos \alpha \tilde{K}_0 + \sin \alpha (\tilde{K}_+ + \tilde{K}_-) \right] + \frac{W}{2} \left[\tilde{K}_+^2 + \tilde{K}_-^2 - \{\tilde{K}_+, \tilde{K}_-\} \right] \\ & - \frac{V+W}{4} \left[\sin^2 \alpha \left(4\tilde{K}_0^2 - \{\tilde{K}_+, \tilde{K}_-\} \right) - \sin 2\alpha \left(\{\tilde{K}_0, \tilde{K}_+\} + \{\tilde{K}_0, \tilde{K}_-\} \right) \right. \\ & \left. + (1 + \cos^2 \alpha)(\tilde{K}_+^2 + \tilde{K}_-^2) \right]. \end{aligned} \quad (2.23)$$

Varying $\langle \Phi | \tilde{H} | \Phi \rangle$ with respect to α gives the HF equation for the LMG model. The ground state for the new Hamiltonian is build as the state where all the quasi-particles stays in the lower level, which, using the angular momentum basis, is:

$$|\text{HF}\rangle = |N/2, -N/2\rangle, \quad (2.24)$$

where we already call it $|\text{HF}\rangle$, despite it is actually the HF state only when the value of variational parameter is determined. Using (2.13) and (2.14), the spectra of the operators involved in the Hamiltonian can be found:

$$\begin{aligned} \tilde{K}_0 |N/2, -N/2\rangle &= -\frac{N}{2} |N/2, -N/2\rangle \\ \tilde{K}_+ |N/2, -N/2\rangle &= \sqrt{N} |N/2, -N/2 + 1\rangle \\ \tilde{K}_- |N/2, -N/2 + 1\rangle &= \sqrt{N} |N/2, -N/2\rangle \\ \tilde{K}_- |N/2, -N/2\rangle &= 0. \end{aligned} \quad (2.25)$$

Using v and w as in (2.17), the ground state energy and the variational condition can be computed:

$$\langle \text{HF} | \tilde{H} | \text{HF} \rangle = -N \frac{\epsilon}{2} \left(\cos \alpha + \frac{w}{N-1} + \frac{v+w}{2} \sin^2 \alpha \right) \quad (2.26)$$

$$\frac{\partial \tilde{E}_{\text{HF}}}{\partial \alpha} = N \frac{\epsilon}{2} \sin \alpha (1 - (v+w) \cos \alpha) = 0. \quad (2.27)$$

The solution of the minimization condition can be achieved analitically, and it is defined differently depending on whether the term $v+w$ is greater or smaller than one:

$$\cos \alpha_{\text{HF}} = \begin{cases} 1 & \text{for } v+w < 1 \\ \frac{1}{v+w} & \text{for } v+w > 1 \end{cases} \quad (2.28)$$

In fig 2.3 we show the dependence of the ground state energy with α for different values of the potentials $v+w$. As it can be seen on the left-hand graph, at the critical point $v=1$ the value of α in the first region where the energy is minimum become unstable. For v greater than 1, a new single particle basis must be used. This basis is now composed of quasi-particles which are superposition of particles on the upper and lower level whose relative amplitudes are weighted by α . When the potential w is turned on (see the right-hand graph), a similar behavior is found, but the value of the critical point now depends also on w . In general, we can say that $v+w$ defines a phase transition between the two energy solutions, or, in other terms, a the deformation of the system in the quasi-spin space.

The ground state energy, expressed in units of ϵ , is:

$$\frac{E_{\text{HF}}}{\epsilon} = -\frac{N}{2} \begin{cases} 1 + \frac{w}{N-1}, & \text{for } v+w < 1 \\ \frac{1+(v+w)^2}{2(v+w)} + \frac{w}{N-1}, & \text{for } v+w > 1 \end{cases} \quad (2.29)$$

The result is shown in fig. 2.4 for different numbers of particles. As it can be seen, in the first region of the potentials for $w=0$ the energy is flat. When $w=v$, instead, it assumes a linear dependence.

2.4 Random Phase Approximation

In order to develop the approximation, we need to write the RPA excitation operator for the LMG model. This problem has been already approached in [13]. The RPA operator reads

$$Q_{\nu}^{\dagger} = \sum_{mi} X_{mi}^{\nu} a_m^{\dagger} a_i - \sum_{mi} Y_{mi}^{\nu} a_i^{\dagger} a_m. \quad (2.30)$$

To this aim, two preliminary comments must be made:

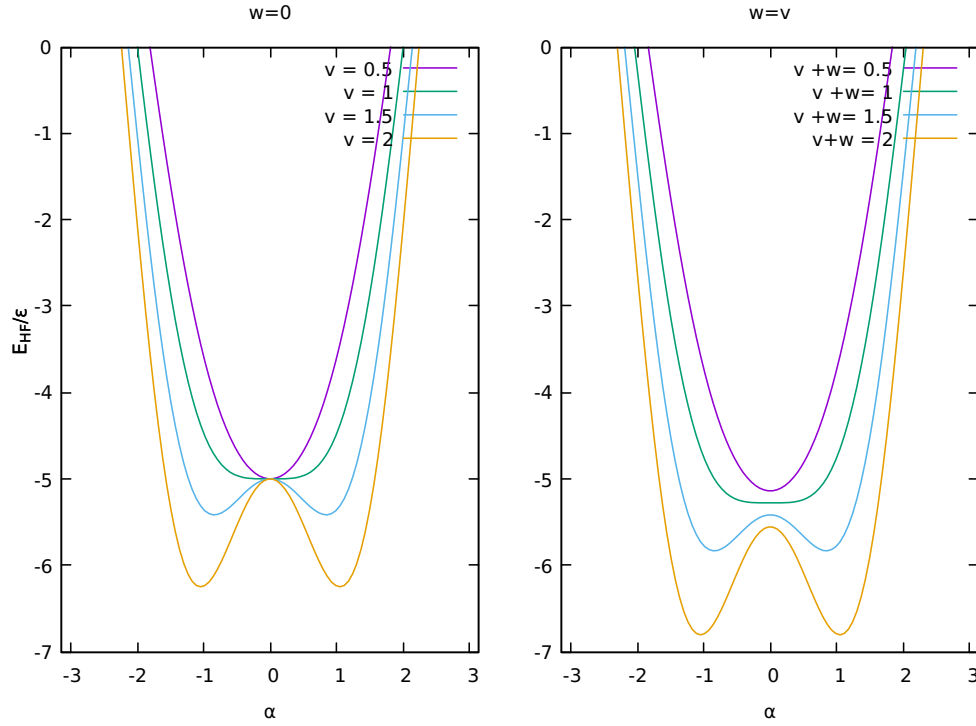


Figure 2.3: HF ground state energy as a function of α for different value of v and $v + w$ for a 10-particle LMG model.

- Since the quantum number p is left unchanged by the interaction, and the system is degenerate in p , the excitations have all the same energy and the subscript ν can be removed from the excitation operator.
- The amplitudes associated with the 1p-1h transition are all the same, so they can be pulled out from the sum.

Using the definitions of $K_{\pm}$, $Q^{\dagger}$ reduces to

$$Q^{\dagger} = \frac{1}{\sqrt{N}} (XK_{+} - YK_{-}). \quad (2.31)$$

The term $1/\sqrt{N}$ is a normalization constant and is added for later convenience. Next steps can be made following what has been done in the general case. From (1.32), the equations of motion are

$$\begin{aligned} \langle \text{RPA} | [K_{-}, [H, Q_{\nu}^{\dagger}]] | \text{RPA} \rangle &= \omega \langle \text{RPA} | [K_{-}, Q_{\nu}^{\dagger}] | \text{RPA} \rangle \\ \langle \text{RPA} | [K_{+}, [H, Q_{\nu}^{\dagger}]] | \text{RPA} \rangle &= \omega \langle \text{RPA} | [K_{+}, Q_{\nu}^{\dagger}] | \text{RPA} \rangle. \end{aligned} \quad (2.32)$$

To evaluate these expression we can make use of the QBA. Of course, this means we need to consider the Hamiltonian (2.23) and the ground state (2.24). Furthermore, $Q^{\dagger}$ must

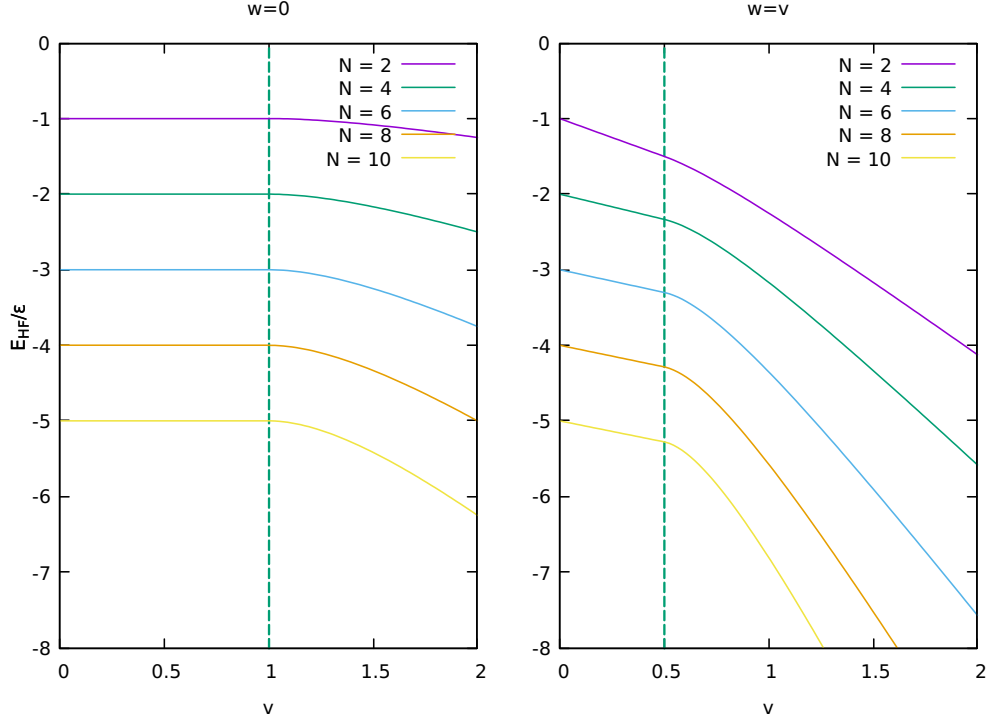


Figure 2.4: HF ground state energy as a function of v for different number of particles and w potential

be defined in term of the transformed operator. Using the action of operators $K_{\pm}$ on HF state as in (2.25), the commutators on RHS can be evaluated and we get:

$$\begin{aligned} \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N} X - \frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N} Y &= \omega X \\ \frac{\langle \text{HF} | [K_+, [H, K_+]] | \text{HF} \rangle}{N} X - \frac{\langle \text{HF} | [K_+, [H, K_-]] | \text{HF} \rangle}{N} Y &= \omega Y, \end{aligned} \quad (2.33)$$

where we have dropped all the tilde for simplicity. In order to write the equations in matrix form we can define

$$\begin{aligned} A &= \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N} \\ B &= -\frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N}. \end{aligned} \quad (2.34)$$

Since the matrix element on the second row of (2.33) are the complex conjugate of the terms on the first row, we get the RPA equation in matrix form (1.54) as in the general formulation:

$$\begin{pmatrix} A - \omega & B \\ B^* & A^* + \omega \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = 0. \quad (2.35)$$

The commutators in A and B can be computed, and the full calculation is reported in Appendix C.1. Evaluating the expressions with $\alpha = \alpha_{HF}$ as in (2.28) to fulfill the HF condition we find

$$A = \epsilon \begin{cases} 1 - w, & \text{for } v < 1 - w \\ \frac{3(v+w)^2 - 1}{2(v+w)} - w, & \text{for } v > 1 - w \end{cases} \quad (2.36)$$

$$B = \epsilon \begin{cases} -v, & \text{for } v < 1 - w \\ -\frac{1 + (v+w)^2}{2(v+w)} + w, & \text{for } v > 1 - w \end{cases} \quad (2.37)$$

We notice that the first region solution reflects for both A and B what we already found for a general Hamiltonian in (1.54). This is because with this choice of α , the unitary transformation in (2.21) reduces to the identity, and the trivial HF ground state (2.19) is retrieved. We recognize w as the $\bar{v}_{mjn}$ term, while v is the $\bar{v}_{mnij}$ force. A different situation characterizes the second region, which is described by a basis which is different from the HF by a unitary transformation, and shows non-trivial solution. Since both A and B are manifestly real, the RPA equations reads:

$$\begin{pmatrix} A - \omega & B \\ B & A + \omega \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = 0. \quad (2.38)$$

The eigenvalue problem can now be solved. The diagonalization of the matrix lead to

$$\omega = \sqrt{A^2 - B^2} \quad \text{and} \quad X = \frac{B}{\omega - A} Y, \quad (2.39)$$

where we selected only the positive eigenvalue. The problem is completely defined if one looks at the condition the RPA amplitudes must satisfy for the excited states to be orthonormal

$$\begin{aligned} \langle \nu | \nu \rangle &= 1 = \langle \text{RPA} | QQ^\dagger | \text{RPA} \rangle \\ &= \langle \text{RPA} | [QQ^\dagger] | \text{RPA} \rangle \\ &\simeq \langle \text{HF} | [QQ^\dagger] | \text{HF} \rangle \\ &= (X^* X - Y Y^*), \end{aligned} \quad (2.40)$$

where in the last step we used the definition of excitation operator $Q^\dagger$ in (2.31) and relations (2.25) for the action of $K_\pm$ on the HF state. The normalization condition is thus:

$$|X|^2 - |Y|^2 = 1. \quad (2.41)$$

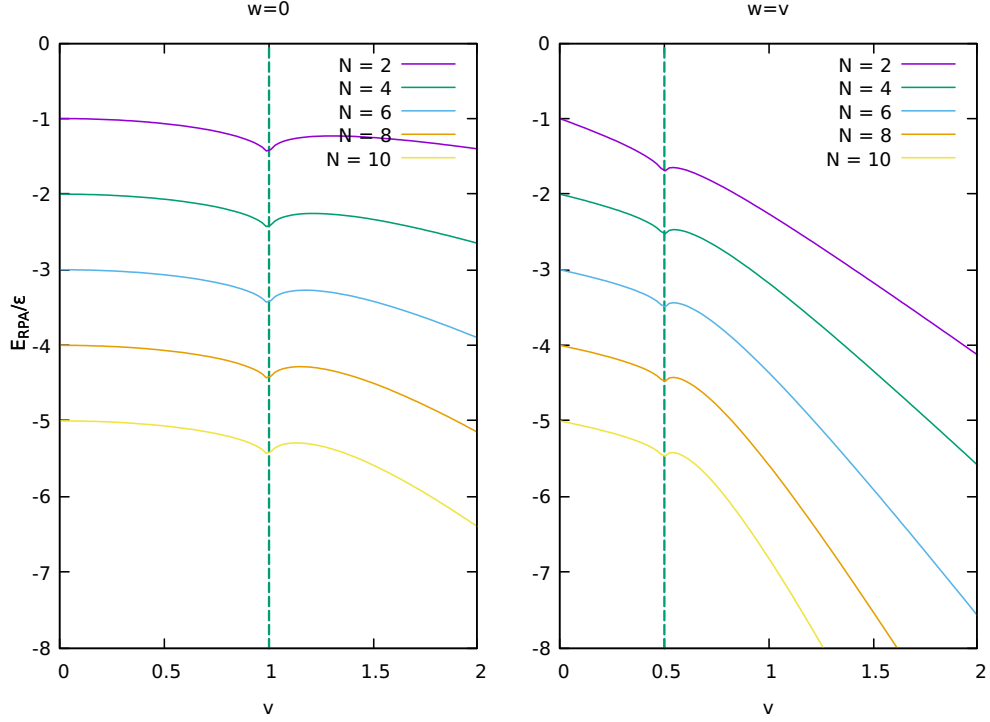


Figure 2.5: RPA ground state energy as a function of v for different number of particles and w potential

2.4.1 Ground state energy

The RPA ground state energy can be obtained with the steps described in [1]. We are not going to get through the calculation; using (2.39) and (2.41) we obtain:

$$\begin{aligned} E_{\text{RPA}} &= E_{\text{HF}} + \omega |Y|^2 \\ &= E_{\text{HF}} + \frac{\sqrt{A^2 - B^2} - A}{2}. \end{aligned} \quad (2.42)$$

The result is shown in Fig. 2.5. As can be seen, the RPA ground state energy presents a bump at the value of the potential where the domain of the solution change. It is clearly an artifact of the approximation, since the exact result does not present it. This behavior seems to be avoided using a better approximation than QBA: calculations with SCRPA show better agreements with the analytic solution [1].

We now compare the approximation methods taken into account and the exact solution. In Fig. 2.6 the the 4-particles and the 20-particles LMG model ground state energy is shown for the exact solution, the Hartree-Fock approximation and the RPA.

- For $w = 0$, the RPA solution follows quite closely the analytic one, while the HF solution is slightly higher in energy. In the second region, in particular, the agreement between RPA and the exact result is excellent.

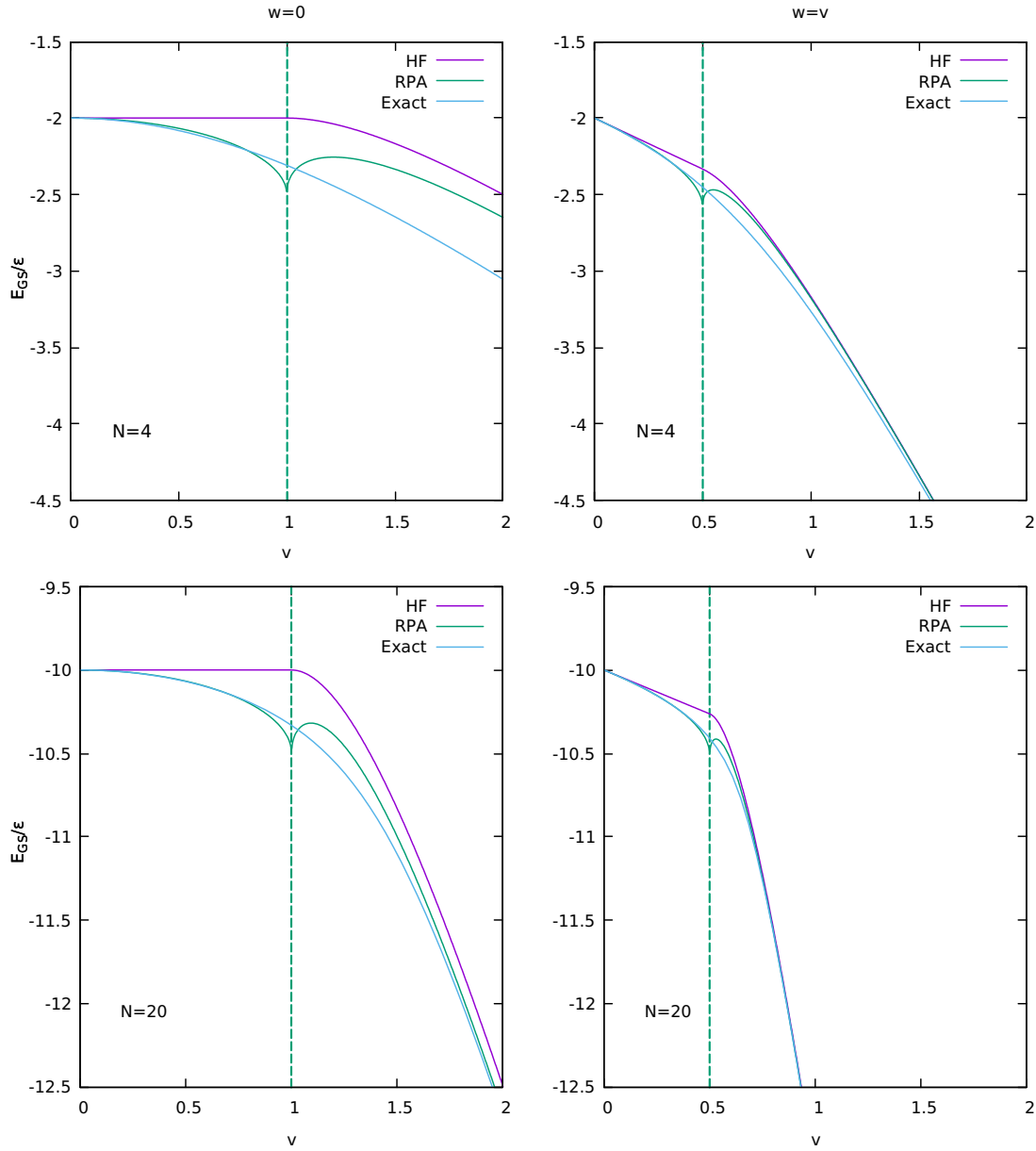


Figure 2.6: Ground state energy comparison for the system of 4 particles (above) and 20 particles (below) with HF, RPA and the exact solution.

- In the $w = v$ case, things gets even better for the RPA solution, which follows remarkably the real one, while the HF one still remain a bit departed. It must be noted that in the second region the RPA energy tend to the HF energy. This is due to the fact that here

$$B = -\frac{\epsilon}{4w}, \quad (2.43)$$

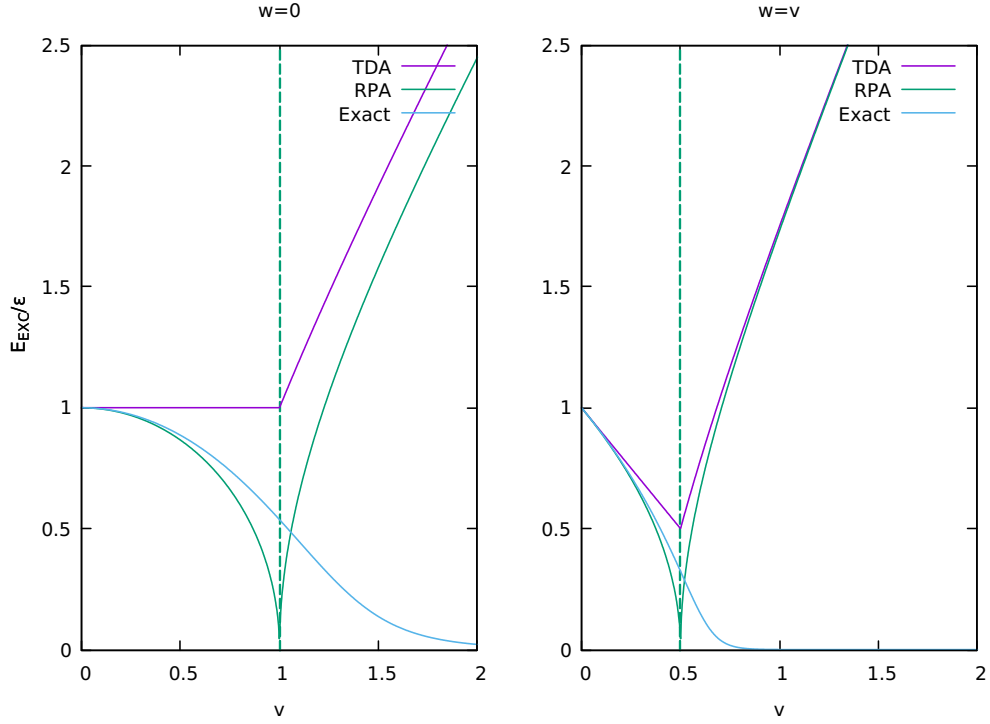


Figure 2.7: Excitation energy comparison with RPA, TDA and exact excitation energy.

so that for high value of w , $B \rightarrow 0$, and consequently the RPA matrix reaches the limiting case of TDA matrix.

In all the cases considered, the RPA and HF solutions converge for large values of the interaction v and w . Also, it is evident that the solutions of the effective theories shows better agreement with the exact when the number of the particles composing the system increases, attesting the better reliability of the mean field in the thermodynamic limit.

2.4.2 Excited state

In Fig. 2.7 the first excitation energy of the system with respect to v for RPA, TDA and the exact solution is shown. The exact result has been obtained subtracting the ground state to the first eigenvalue, while for the RPA and TDA case the excitation energy is ω . This plot reveal the breakdown of the RPA and TDA the HF when choosing a basis which is not the original HF one. In order to study this behavior in more detail, we evaluated the RPA amplitudes. They can be obtained using the result of the diagonalization procedure

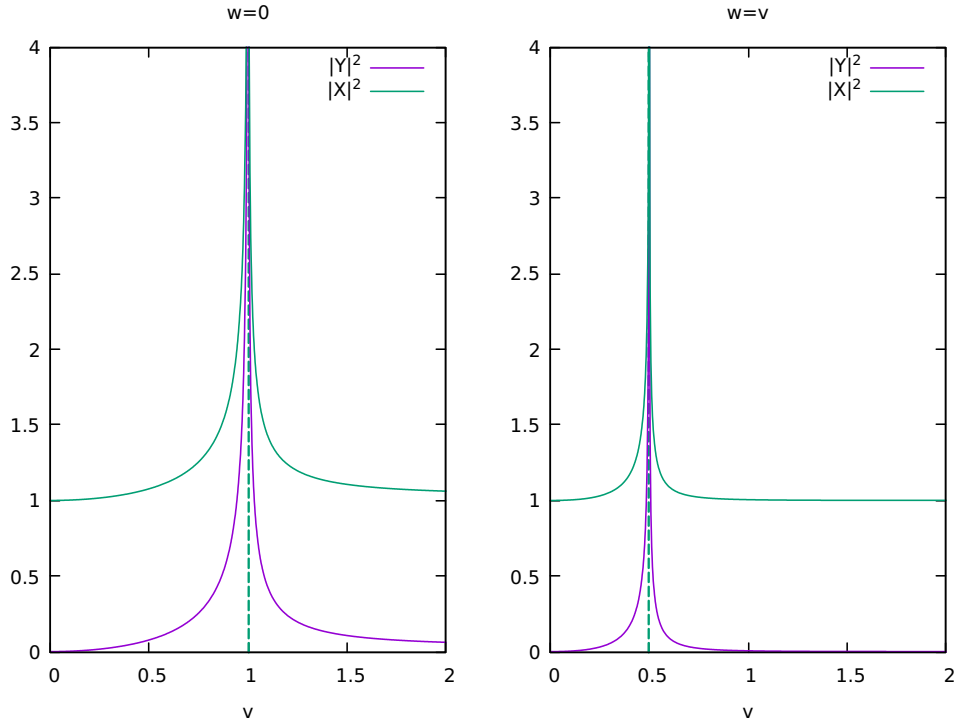


Figure 2.8: RPA excitation amplitudes

(2.39) and the normalization condition (2.41):

$$|Y|^2 = \frac{1}{\left(\frac{B}{\omega-A}\right)^2 - 1} \quad (2.44)$$

$$|X|^2 = 1 + |Y|^2.$$

In Fig. 2.8 the square modulus of $|X|$ and $|Y|$ as function of the potential v is shown. For $v = 1$ and $w = 0$ or $v = w = 0.5$ both probabilities diverge. This behavior can be understood analytically looking at the RPA matrix. Coming from the left of v potential, the RPA matrix looks

$$\text{RPA} = \begin{pmatrix} 1-w & -v \\ v & 1-w \end{pmatrix} \quad (2.45)$$

For v approaching to 1 and $w = 0$, or for both v and w approaching to 0.5, the elements on the diagonal are almost equal to the elements outside. It is easy to check that the diagonalization of such a matrix involves 0 energy eigenvalues and eigenvectors whose absolute value is infinite. Since RPA is build assuming small values of $|Y|$, this result is clearly not acceptable.

These results reveal the incapacity of the RPA to describe the excited state of the system in some regions of the potentials. This was already noted in the Lipkin's

original paper, and might represent an artifact of mean field theories with this simplified Hamiltonian [4]. In the following, we will try to answer to this fundamental question presenting the application of the SRPA with the aim of understanding its effectiveness with the LMG model.

2.5 Second Random Phase Approximation

The derivation of the SRPA equations has been widely described in [16] or [15], but no attempts have been made to develop them for the LMG model. In the SRPA framework, we have seen that $Q_\nu^\dagger$ operator contains 2p-2h terms in addition to 1p-1h terms of RPA:

$$\begin{aligned} Q_\nu^\dagger = & \sum_{mi} X_{mi}^\nu a_m^\dagger a_i - \sum_{mi} Y_{mi}^\nu a_i^\dagger a_m \\ & + \sum_{m<n, i<j} Z_{mni}^\nu a_m^\dagger a_n^\dagger a_j a_i - \sum_{m<n, i<j} W_{mni}^\nu a_i^\dagger a_j^\dagger a_n a_m. \end{aligned} \quad (2.46)$$

The fermion anti-commutation relations allow us to write the product of four creation and annihilation operators as the product of two 1p-1h operators. Since the amplitudes associated with a specific state are all the same, they can be pulled out from the sum, and using the definitions of $K_\pm$, the excitation operator $Q_\nu^\dagger$ can be written as

$$Q_\nu^\dagger = \frac{1}{\sqrt{N}} (X_\nu K_+ - Y_\nu K_-) + \frac{1}{\sqrt{2N(N-1)}} (Z_\nu K_+ K_+ - W_\nu K_- K_-), \quad (2.47)$$

where the normalization factors are added for later convenience. Consider now the RPA motion equation (1.32). We will see that, in this case, hermiticity is retained, although (1.35) is not satisfied. With the definition of operator $Q_\nu^\dagger$ as in SRPA, we now have 4 different kind of operator R. This lead to a set of 4 equations:

$$\begin{aligned} \langle \text{RPA} | [K_-, [H, Q_\nu^\dagger]] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [K_-, Q_\nu^\dagger] | \text{RPA} \rangle \\ \langle \text{RPA} | [K_- K_-, [H, Q_\nu^\dagger]] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [K_- K_-, Q_\nu^\dagger] | \text{RPA} \rangle \\ \langle \text{RPA} | [K_+, [H, Q_\nu^\dagger]] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [K_+, Q_\nu^\dagger] | \text{RPA} \rangle \\ \langle \text{RPA} | [K_+ K_+, [H, Q_\nu^\dagger]] | \text{RPA} \rangle &= \omega_\nu \langle \text{RPA} | [K_+ K_+, Q_\nu^\dagger] | \text{RPA} \rangle. \end{aligned} \quad (2.48)$$

Here, the excitation energy conserves the subscript ν since we now have two way to excite the system. Again, these equation can be evaluated with the approximation as in (1.60), and that means we need to use HF Hamiltonian (2.23) and the ground state (2.24).

Putting (2.47) in the equation of motions and evaluating RHS commutators we get

$$\begin{aligned}
& \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N} X_\nu - \frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N} Y_\nu \\
& + \frac{\langle \text{HF} | [K_-, [H, K_+ K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} Z_\nu - \frac{\langle \text{HF} | [K_-, [H, K_- K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} W_\nu = \omega_\nu X_\nu \\
& \frac{\langle \text{HF} | [K_- K_-, [H, K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} X_\nu - \frac{\langle \text{HF} | [K_- K_-, [H, K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} Y_\nu \\
& + \frac{\langle \text{HF} | [K_- K_-, [H, K_+ K_+]] | \text{HF} \rangle}{2N(N-1)} Z_\nu - \frac{\langle \text{HF} | [K_- K_-, [H, K_- K_-]] | \text{HF} \rangle}{2N(N-1)} W_\nu = \omega_\nu Z_\nu \\
& \frac{\langle \text{HF} | [K_+, [H, K_+]] | \text{HF} \rangle}{N} X_\nu - \frac{\langle \text{HF} | [K_+, [H, K_-]] | \text{HF} \rangle}{N} Y_\nu \\
& + \frac{\langle \text{HF} | [K_+, [H, K_+ K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} Z_\nu - \frac{\langle \text{HF} | [K_+, [H, K_- K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} W_\nu = \omega_\nu Y_\nu \\
& \frac{\langle \text{HF} | [K_+ K_+, [H, K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} X_\nu - \frac{\langle \text{HF} | [K_+ K_+, [H, K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} Y_\nu \\
& + \frac{\langle \text{HF} | [K_+ K_+, [H, K_+ K_+]] | \text{HF} \rangle}{2N(N-1)} Z_\nu - \frac{\langle \text{HF} | [K_+ K_+, [H, K_- K_-]] | \text{HF} \rangle}{2N(N-1)} W_\nu = \omega_\nu W_\nu.
\end{aligned} \tag{2.49}$$

Again, we have dropped all the tilde for simplicity. We notice that some matrix elements have the same form but appear with all + and - inverted. One can show they represent the same quantity apart from a complex conjugation. The equations can then be written in a simpler form as:

$$\begin{aligned}
A_{1,1} X_\nu + A_{1,2} Z_\nu + B_{1,1} Y_\nu + B_{1,2} W_\nu &= \omega_\nu X_\nu \\
A_{2,1} X_\nu + A_{2,2} Z_\nu + B_{2,1} Y_\nu + B_{2,2} W_\nu &= \omega_\nu Z_\nu \\
B_{1,1}^* X_\nu + B_{1,2}^* Z_\nu + A_{1,1}^* Y_\nu + A_{1,2}^* W_\nu &= -\omega_\nu Y_\nu \\
B_{2,1}^* X_\nu + B_{2,2}^* Z_\nu + A_{2,1}^* Y_\nu + A_{2,2}^* W_\nu &= -\omega_\nu W_\nu,
\end{aligned} \tag{2.50}$$

where

$$\begin{aligned}
A_{1,1} &= \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N} \\
A_{1,2} &= \frac{\langle \text{HF} | [K_-, [H, K_+ K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} \\
A_{2,1} &= \frac{\langle \text{HF} | [K_- K_-, [H, K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} \\
A_{2,2} &= \frac{\langle \text{HF} | [K_- K_-, [H, K_+ K_+]] | \text{HF} \rangle}{2N(N-1)},
\end{aligned} \tag{2.51}$$

and

$$\begin{aligned}
B_{1,1} &= -\frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N} \\
B_{1,2} &= -\frac{\langle \text{HF} | [K_-, [H, K_- K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} \\
B_{2,1} &= -\frac{\langle \text{HF} | [K_- K_-, [H, K_-]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} \\
B_{2,2} &= -\frac{\langle \text{HF} | [K_- K_-, [H, K_- K_-]] | \text{HF} \rangle}{2N(N-1)}.
\end{aligned} \tag{2.52}$$

The matrix elements $A_{1,1}$ and $B_{1,1}$ are the usual RPA matrix elements, while $A_{1,2}$ describe the coupling of 1p-1h states to 2p-2h states and $A_{2,2}$ gives the mixing matrix elements among 2p-2h states themselves. We can then write (2.50) in matrix notation as in his general formulation (1.61):

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix}, \tag{2.53}$$

where

$$\begin{aligned}
\mathcal{A} &= \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \\
\mathcal{B} &= \begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix},
\end{aligned} \tag{2.54}$$

and

$$\begin{aligned}
\mathcal{X}_\nu &= \begin{pmatrix} X_\nu \\ Z_\nu \end{pmatrix} \\
\mathcal{Y}_\nu &= \begin{pmatrix} Y_\nu \\ W_\nu \end{pmatrix}.
\end{aligned} \tag{2.55}$$

We need now to obtain the explicit form of the elements of $\mathcal{A}$ and $\mathcal{B}$ matrices. As in RPA, this can be achieved using the HF Hamiltonian (2.23) and the ground state (2.24). All the calculation are reported in C.1. Using the correct value for the variational parameter

α for the HF approximation, we end up with:

$$A_{1,2} = \frac{\epsilon}{\sqrt{N-1}} \begin{cases} 0, & \text{for } v < 1-w \\ \frac{\sqrt{2(v+w)^2-2}}{v+w}, & \text{for } v > 1-w \end{cases}$$

$$A_{2,2} = \frac{\epsilon}{(N-1)} \begin{cases} 2(N-1) - 2w(N-2), & \text{for } v < 1-w \\ \frac{3(v+w)^2(N-2) + 4 - N}{v+w} - 2w(N-2), & \text{for } v > 1-w \end{cases} \quad (2.56)$$

$$A_{2,1} = A_{1,2}$$

$$B_{1,2} = B_{2,1} = B_{2,2} = 0.$$

Where the $A_{2,1} = A_{1,2}$ result guarantees the hermiticity of the equations and allows us to use the equation of motion (1.32) instead of (1.33). The last relation is clearly a consequence of the quasi-boson approximation.

As we have already pointed out, $\mathcal{A}$ and $\mathcal{B}$ matrices exhibit symmetries in complete analogy with the simple RPA. Furthermore, since our matrix elements are all real, the second RPA matrix can be reduced as:

$$\begin{pmatrix} A_{1,1} & A_{1,2} & B_{1,1} & 0 \\ A_{1,2} & A_{2,2} & 0 & 0 \\ -B_{1,1} & 0 & -A_{1,1} & -A_{1,2} \\ 0 & 0 & -A_{1,2} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X_\nu \\ Z_\nu \\ Y_\nu \\ W_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X_\nu \\ Z_\nu \\ Y_\nu \\ W_\nu \end{pmatrix} \quad (2.57)$$

As in RPA, the problem is completely defined once the SRPA orthonormality relation for the amplitudes is determined. It reads:

$$|X_\nu|^2 - |Y_\nu|^2 + |Z_\nu|^2 - |W_\nu|^2 = 1. \quad (2.58)$$

2.5.1 Excited states

The eigenvalue problem can be solved in order to find the excitation energies. The diagonalization of the matrix gives two results:

$$\omega_{1,2} = \sqrt{\frac{A_{1,1}^2 + 2A_{1,2}^2 + A_{2,2}^2 - B_{1,1}^2}{2}} \pm \frac{1}{2} \sqrt{\begin{aligned} & A_{1,1}^4 + A_{2,2}^4 + B_{1,1}^4 - 2B_{1,1}^2(A_{1,1}^2 + 2A_{1,2}^2 \\ & - A_{2,2}^2) + 4A_{1,1}^2A_{1,2}^2 - 2A_{1,1}^2A_{2,2}^2 \\ & + 4A_{1,2}^2A_{2,2}^2 + 8A_{1,1}A_{1,2}^2A_{2,2}, \end{aligned}} \quad (2.59)$$

As can be seen, for $A_{1,2}$ and $A_{2,2}$ equal to zero we come back to the standard RPA excitation energy.

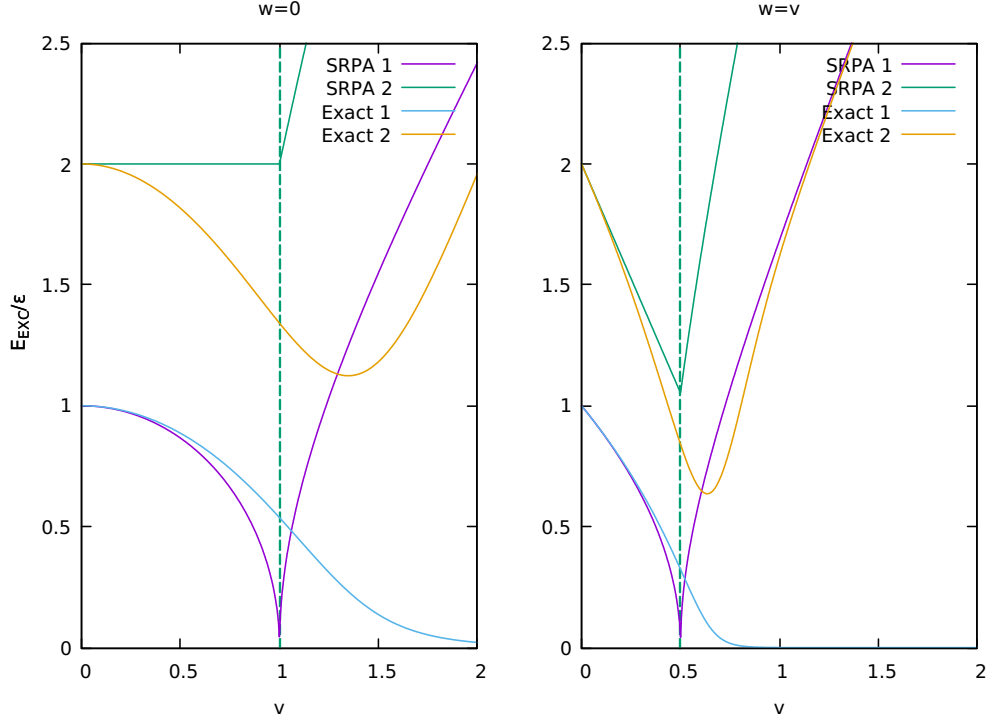


Figure 2.9: SRPA and exact excitation energy

It is worthwhile to note the excitation energies of the model in the case of small values of $v + w$, namely in the first region of definition of the solutions. Here, $A_{1,2}$ matrix is equal to 0, which means the model does not take into accounts 1p-2h and 1h-2p correlations. The excitation energies then result:

$$\begin{aligned}\omega_1 &= \omega_{RPA} \\ \omega_2 &= A_{2,2}.\end{aligned}\tag{2.60}$$

Instead, when the matrix is evaluated in the second region, namely using the a different variational parameter than the trivial solution $\alpha = 0$, 1p-2h and 1h-2p correlations are taken into account. The trivial solution for the first region is due to LMG intrinsic simplicity: the general SRPA expressions for the its matrix elements (1.68) show the dependence of $A_{1,2}$ by terms like v_{kmpq} , which are missing in the LMG model.

In Fig. 2.9 the excitation energies are shown compared to the exact solution. As in RPA, the brakedown of the theory is manifest in the second region. We conclude the impossibility for the LMG model to be described in this region by both RPA and SRPA theories.

Chapter 3

The generalized Lipkin model

The results of the previous chapter show the inadequacy of HF, RPA and SRPA to describe the LMG model for high values of the potentials. Furthermore, SRPA calculations evidences the lack of 1p-1h 2p-2h coupling, which is a consequence of the extreme simplicity of the model.

We wonder if a more complex Hamiltonian would solve the issues we encountered using the approximation methods. In this chapter we propose and analyze an extended version of the LMG model which makes use of a more general interaction. In second quantization, a general two-body force reads

$$V = \frac{1}{2} \sum_{\sigma_1, \sigma_2 \sigma_3 \sigma_4} \sum_{p, p'} \langle p\sigma_1, p'\sigma_2 | V | p\sigma_3, p'\sigma_4 \rangle a_{p, \sigma_1}^\dagger a_{p', \sigma_2}^\dagger a_{p', \sigma_4} a_{p, \sigma_3}. \quad (3.1)$$

As in LMG model, we label with p all the particular degenerate states within a given shell, and with σ the particular energy level. In this form, the interaction does not change the quantum number p . We write explicitly the various terms in σ assuming two levels:

$$\begin{aligned} V = & \frac{V_{++,--}}{2} (K_+^2 + K_-^2) + \frac{V_{+-,-+}}{2} (K_+ K_- + K_- K_+ - K_{0-} - K_{0+}) \\ & + V_{+-,+ -} K_{0+} K_{0-} \\ & + \frac{V_{--,+-}}{2} (K_- K_{0-} + K_{0-} K_+) + \frac{V_{--, -+}}{2} (K_- K_{0-} + K_{0-} K_+) \\ & + \frac{V_{++, -+}}{2} (K_+ K_{0+} + K_{0+} K_-) + \frac{V_{++, + -}}{2} (K_+ K_{0+} + K_{0+} K_-) \\ & + \frac{V_{++, ++}}{2} K_{0+}^2 + \frac{V_{--, --}}{2} K_{0-}^2, \end{aligned} \quad (3.2)$$

where we have used the quasi-spin operator defined in (2.6) and have introduced two additional operators:

$$\begin{aligned} K_{0+} &= \sum_p a_{p,+}^\dagger a_{p,+} \\ K_{0-} &= \sum_p a_{p,-}^\dagger a_{p,-}, \end{aligned} \quad (3.3)$$

which satisfy

$$\begin{aligned} [K_{0\pm}, K_+] &= \pm K_+ \\ [K_{0\pm}, K_-] &= \mp K_- \end{aligned} \quad (3.4)$$

We can write $V_{++,--}$ and $V_{+-,-+}$ as $-V$ and $-W$, following the original LMG convention. Since the interaction must be symmetric for the exchange of particles, V takes a more compact form:

$$\begin{aligned} V = & -\frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (\{K_+, K_-\} - (K_{0-} + K_{0+})) + \\ & + V_{+-,+} K_{0+} K_{0-} \\ & + V_{--,+} (K_- K_{0-} + K_{0-} K_+) \\ & + V_{++,+} (K_+ K_{0+} + K_{0+} K_-) \\ & + \frac{V_{++,++}}{2} K_{0+}^2 + \frac{V_{--,--}}{2} K_{0-}^2. \end{aligned} \quad (3.5)$$

This expression is still difficult to handle because of the presence of operators $K_{0\pm}$, which are not diagonal in angular momentum representation. Thus, we assume the following approximation:

$$\begin{aligned} V_{+-,+} = V_{++,++} = V_{--,--} &= -F \\ V_{--,+-} = V_{+-,-+} &= -G. \end{aligned} \quad (3.6)$$

This leads to

$$\begin{aligned} V = & -\frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (\{K_+, K_-\} - (K_{0-} + K_{0+})) \\ & - \frac{F}{2} (K_{0+} + K_{0-})^2 - G (K_- K_{0-} + K_{0-} K_+ + K_+ K_{0+} + K_{0+} K_-). \end{aligned} \quad (3.7)$$

The term proportional to G can be rewritten exploiting the commutation relations (3.4) to get

$$\begin{aligned} V = & -\frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (\{K_+, K_-\} - (K_{0-} + K_{0+})) \\ & - \frac{F}{2} (K_{0+} + K_{0-})^2 - G(K_+ + K_-)(K_{0+} + K_{0-} - 1). \end{aligned} \quad (3.8)$$

Since the sum of K_{0+} and K_{0-} is the total number of particles, which is a constant of the model, the total Hamiltonian can be written as:

$$\begin{aligned} H = & \epsilon K_0 - \frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (K_+ K_- + K_- K_+) \\ & - G(K_+ + K_-)(N - 1) + \frac{W}{2} N - \frac{F}{2} N^2. \end{aligned} \quad (3.9)$$

Since the number of particles is a constant of the model, we can get rid of the last two terms. The form of our generalized LMG model is thus:

$$H = \epsilon K_0 - \frac{V}{2} (K_+^2 + K_-^2) - \frac{W}{2} (K_+ K_- + K_- K_+) - G(K_+ + K_-)(N - 1).$$

(3.10)

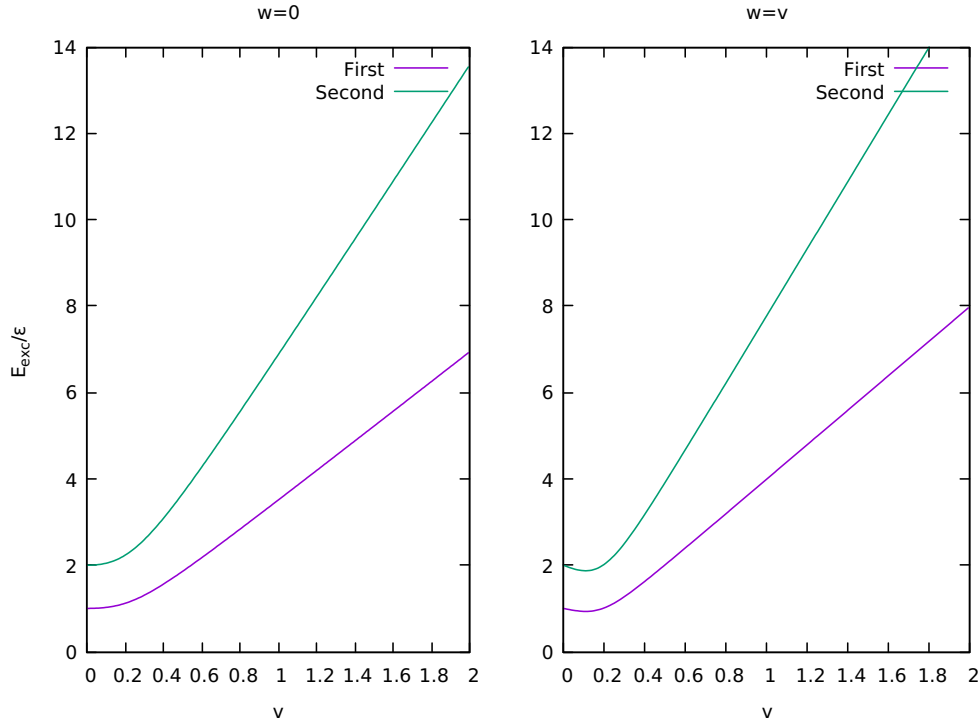


Figure 3.1: First two excitation energies for the 20-particle extended LMG

The novelty with respect of the LMG model is represented by the terms proportional to G . Despite they come from a two-body interaction, they are one-body operator: this is due by the angular commutation relation.

3.1 Solution of the model

The goal of this procedure has been to obtain a generalization of the LMG model which is still very simple to solve. Indeed, the angular momentum basis can be used as the basis for our Hamiltonian. As an example, we write down the Hamiltonian for a system composed of 3 particle, which can be compared with (2.18) :

$$\frac{H_3}{\epsilon} = \begin{pmatrix} -\frac{3}{2} - \frac{3}{4}w & -\sqrt{3}g & -\frac{\sqrt{3}}{2}v & 0 \\ -\sqrt{3}g & -\frac{1}{2} - \frac{7}{4}w & -2g & -\frac{\sqrt{3}}{2}v \\ -\frac{\sqrt{3}}{2}v & -2g & \frac{1}{2} - \frac{7}{4}w & -\sqrt{3}g \\ 0 & -\frac{\sqrt{3}}{2}v & -\sqrt{3}g & \frac{3}{2} - \frac{3}{4}w \end{pmatrix}, \quad (3.11)$$

where we have chosen

$$g = \frac{G}{\epsilon}(N-1). \quad (3.12)$$

As in the previous case, the Hamiltonian can be diagonalized both analitically and numerically. Of course, when the number of particles is too high, the analytic diagonalization is a formidable problem. Here, the numerical solution has always been preferred.

Of course, to carry on the computation we need to specify the value of g with respect of the other terms, v and w . To start, we decide to consider them as equal, and write

$$g = v, \quad (3.13)$$

but we will discuss other choices later. In Fig. 3.1 the first two excitation energies of this model are drawn with respect to v . Along the line of the LMG model, w potential has been considered in two limit cases. The right-hand graph, therefore, shows the case where all the potential are equal. As can be seen comparing with 2.2, the main difference with the standard LMG is on the first excited state, which is now an increasing function of v .

3.2 Hartree-Fock approximation

The Hartree Fock approximation can be developed along the same line of the standard LMG case. We consider again the unitary trasformation of the fermion operators as in (2.21), and the expression of the trasformed operator $\tilde{K}_\pm$ and $\tilde{K}_0$ in (2.22). Writing the model Hamiltonian (3.10) in terms of these operators we get

$$\begin{aligned} \tilde{H} = & \frac{\epsilon}{2} \left[2 \cos \alpha \tilde{K}_0 + \sin \alpha (\tilde{K}_+ + \tilde{K}_-) \right] + \frac{W}{2} \left[\tilde{K}_+^2 + \tilde{K}_-^2 - \{\tilde{K}_+, \tilde{K}_-\} \right] \\ & - \frac{V+W}{4} \left[\sin^2 \alpha \left(4\tilde{K}_0^2 - \{\tilde{K}_+, \tilde{K}_-\} \right) - \sin 2\alpha \left(\{\tilde{K}_0, \tilde{K}_+\} + \{\tilde{K}_0, \tilde{K}_-\} \right) \right. \\ & \left. + (1 + \cos^2 \alpha)(\tilde{K}_+^2 + \tilde{K}_-^2) \right] - G \left(\cos \alpha (\tilde{K}_+ + \tilde{K}_-) - 2 \sin \alpha \tilde{K}_0 \right) (N-1). \end{aligned} \quad (3.14)$$

This Hamiltonian differs from (2.23) by the terms proportional to G . Using the ground state (2.24), the ground state energy and the variational condition can be calculated:

$$\begin{aligned} \langle \text{HF} | \tilde{H} | \text{HF} \rangle &= -N \frac{\epsilon}{2} \left(\cos \alpha + \frac{w}{N-1} + \frac{v+w}{2} \sin^2 \alpha + 2g \sin \alpha \right) \\ \frac{\partial \tilde{E}_{\text{HF}}}{\partial \alpha} &= N \frac{\epsilon}{2} (\sin \alpha - (v+w) \sin \alpha \cos \alpha - 2g \cos \alpha) = 0. \end{aligned} \quad (3.15)$$

This time, the minimization condition is not trivial and must be solved numerically. In Fig. 3.2 the dependence of the HF ground state energy with the variational parameter α for different values of the potential is shown. Comparing with Fig. 2.3 we notice that within this model there is no trace of discontinuity of α . Furthermore, no zero solution of α exists: the HF basis build by bare particles is never able to describe the system and a unitary transformation is always needed.

We are not going to evaluate the energy of the ground state, as did previously, but we will focus on the excitation energies only, where the approximation methods failed in reproducing the exact LMG model results.

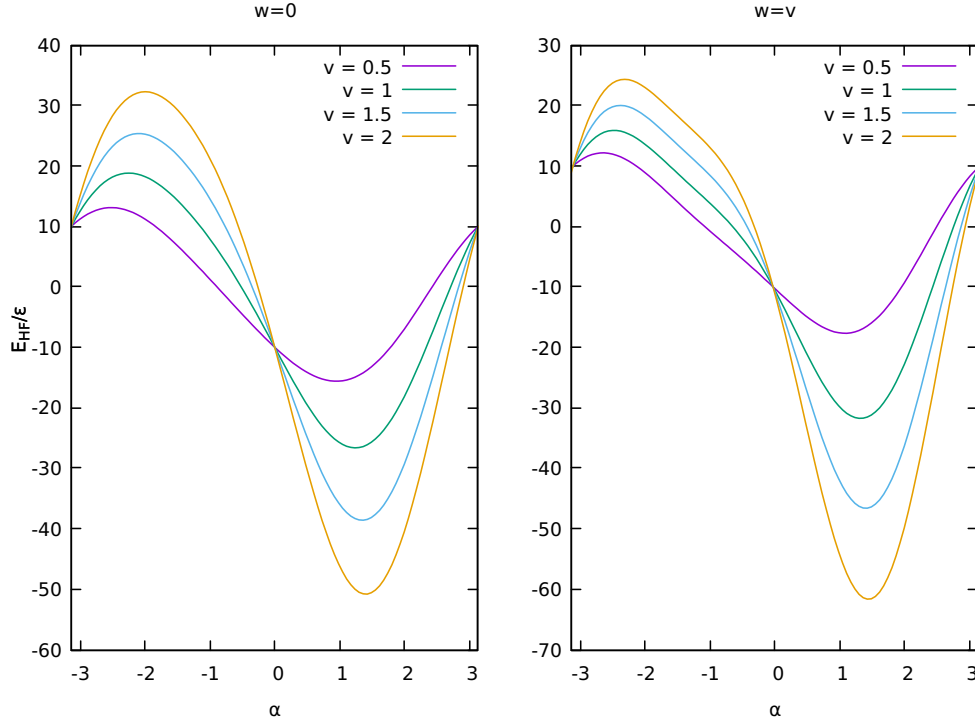


Figure 3.2: HF ground state energy as a function of α for different values of v , g and w .

3.3 Random phase approximation

In this section we will develop the RPA for the generalized LMG model. The derivation of the equation is completely equivalent to the previous case. Nevertheless, the new terms appearing in the HF Hamiltonian lead to different expressions for the RPA matrix elements. Since this Hamiltonian differs from the previous only by the terms proportional to g , we only need to calculate the matrix elements with these terms. The details of the calculations can be found in Appendix C.2; here we report the results:

$$\begin{aligned} A_{1,1} &= \epsilon \left(\cos \alpha - w + \frac{3}{2}(v+w) \sin^2 \alpha + 2g \sin \alpha \right) \\ B_{1,1} &= \epsilon \left(w - \frac{v+w}{2}(1 + \cos^2 \alpha) \right), \end{aligned} \quad (3.16)$$

where we now specify the subscript on both terms for later convenience in SRPA. The newly calculated RPA matrix elements differ only for the A matrix, which shows now an additional term proportional to g .

This has huge consequences on the RPA matrix. In Sec. 2.4 we discussed that for RPA to be effective the amplitude Y should be small compared to X . If Y is too strong, the replacement of the correlated ground state $|\text{RPA}\rangle$ by $|\text{HF}\rangle$ is not justified. In the

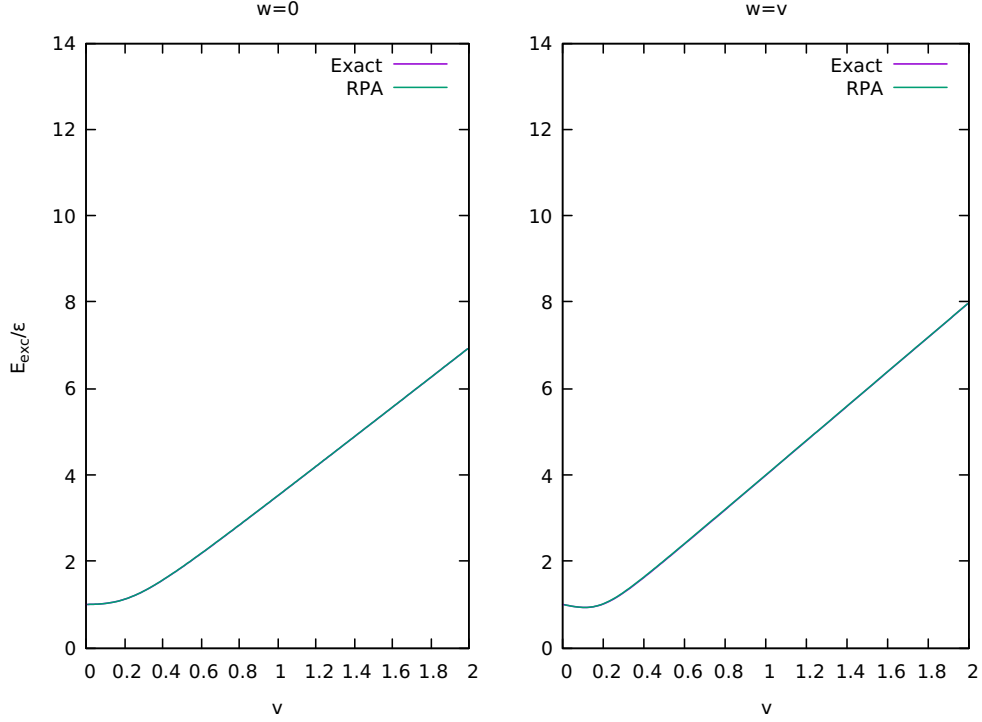
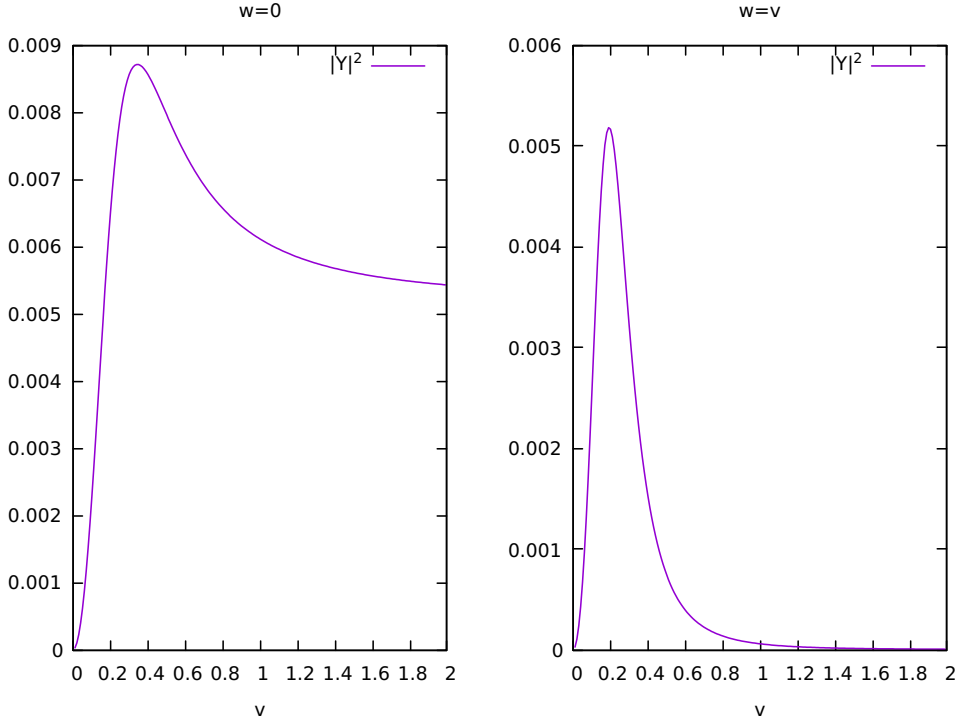


Figure 3.3: First excitation energy for RPA approximation and exact solution. The two curves are superimposed.

LMG model, for $\nu = 1$ and $w = 0$ or $\nu = w = 0.5$ both amplitudes diverge, and therefore the approximation fails. The presence of g in the generalized LMG model makes A and B terms different, and the breakdown for $\nu = 1$ and $w = 0$ or $\nu = w = 0.5$ of RPA is now solved.

The RPA matrix elements must be evaluated using the values for the variational parameter α obtained by the minimization condition (3.15). The excitation energy ω resulting by the matrix diagonalization is shown in Fig. 3.3 compared with the exact value. The accuracy of the RPA solution is now outstanding, both in the $w = 0$ and $w = v$ case.

In Fig. 3.4 we show the RPA Y amplitude. As can be seen, the squared modulus of the Y amplitude is always very small. This result reveals the new model as a weakly correlated system, which could also be described with good accuracy using TDA. Of course, this is true only for the chosen set of potentials, namely $g = v$. We will see, in the next chapters, that other choices could lead to more correlated systems.

Figure 3.4: Squared modulus of Y amplitude.

3.4 Second Random Phase Approximation

In this section we will derive the SRPA for the generalized LMG model. Unlike RPA, the presence of the terms proportional to g in the HF Hamiltonian lead to a change in the definition of the SRPA equations. Indeed, to retain hermiticity in the SRPA matrix we need to start from a more general equation of motion than (1.32), namely we need to use (1.33). This leads to the same set of matrix elements apart from the off-diagonal terms in $\mathcal{A}$, which are now defined as

$$\begin{aligned}
 A'_{1,2} &= \frac{1}{2} (\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle + \langle \text{HF} | [K_-, H], K_+^2 | \text{HF} \rangle) \\
 &= \frac{1}{2} (\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle + \langle \text{HF} | [K_+^2, [H, K_-]] | \text{HF} \rangle) \\
 &= \frac{1}{2} (A_{1,2} + A_{2,1}^*) \\
 A'_{2,1} &= \frac{1}{2} (\langle \text{HF} | [K_-^2, [H, K_+]] | \text{HF} \rangle + \langle \text{HF} | [K_-^2, H], K_+ | \text{HF} \rangle) \\
 &= \frac{1}{2} (\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle + \langle \text{HF} | [K_+, [H, K_-^2]] | \text{HF} \rangle) \\
 &= \frac{1}{2} (A_{2,1} + A_{1,2}^*)
 \end{aligned} \tag{3.17}$$

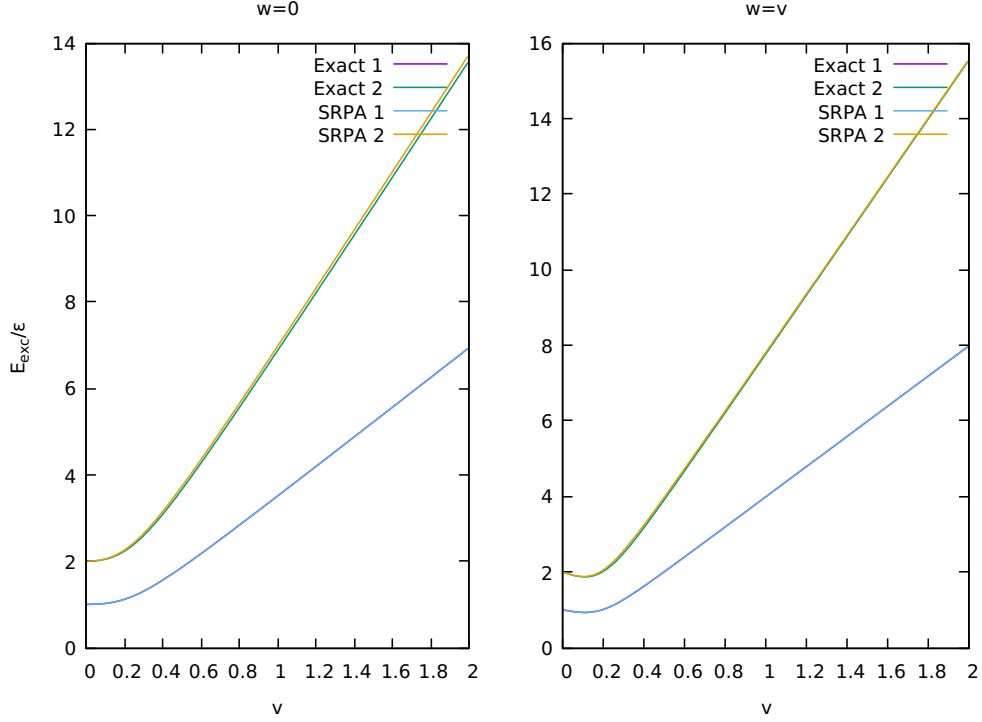


Figure 3.5: Excitation energies for SRPA approximation and the exact solution. The two curves are almost superimposed.

Since the matrix elements in our model are always real, this choice of the equation of motion indeed guarantees the SRPA matrix hermiticity:

$$A'_{1,2} = A'_{2,1} \quad (3.18)$$

Similar situation would occur in $\mathcal{B}$, but, as we have already discussed for the LMG model, due to the use of HF ground state $B_{1,2}$ and $B_{2,1}$ are 0. The SRPA matrix to solve is thus:

$$\begin{pmatrix} A_{1,1} & A'_{1,2} & B_{1,1} & 0 \\ A'_{1,2} & A_{2,2} & 0 & 0 \\ -B_{1,1} & 0 & -A_{1,1} & -A'_{1,2} \\ 0 & 0 & -A'_{1,2} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X_\nu \\ Z_\nu \\ Y_\nu \\ W_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X_\nu \\ Z_\nu \\ Y_\nu \\ W_\nu \end{pmatrix} \quad (3.19)$$

The terms $A_{1,1}$ and $B_{1,1}$ are the RPA matrix elements and they are given in (3.16). The calculation of $A_{1,2}$, $A_{2,1}$ and $A_{2,2}$ are reported in Appendix C.2; the results read

$$\begin{aligned} A'_{1,2} &= \frac{\epsilon}{2\sqrt{2(N-1)}} (\sin \alpha(N-1) - (v+w) \sin \alpha \cos \alpha(N-5) - 2g \cos \alpha(N-1)) \\ A_{2,2} &= \frac{\epsilon}{N-1} (2 \cos \alpha(N-1) - 2w(N-2) + 3(v+w) \sin^2 \alpha(N-2) + 4g \sin \alpha(N-1)). \end{aligned} \quad (3.20)$$

All the SRPA matrix elements must be evaluated using the value of α obtained by the minimization condition in (3.15). The excitation energies given by the solution of the eigenvalue problem are shown in (3.5) as function of v . They are compared with the exact result, showing the remarkable accuracy of the approximation, both in the first and in the second excited states and for $w = 0$ and $w = v$.

In Fig. 3.7 and 3.8 we present the square of the amplitudes appearing in the excitation operator (2.47) for the first and the second excited states, respectively. We did not expect the situation to change with respect of the RPA case, which demonstrated very small correlations. Indeed, in both cases for the excitation energies only one amplitudes is huge compared to the others. The amplitudes which correspond to the first excitation are strongly dominated by X , which is consistent with idea that this state must be due primarily by the 1p-1h excitation term. For the second excited state, the high value of Z reveals the importance of the 2p-2h excitation process. In both case, the W term looks always negligible.

These results confirm the fact that RPA and SRPA are effective in describing the excitation of the new model Hamiltonian. The presence of g potential in the Hamiltonian is indeed the key of the success of these approximation methods.

3.4.1 RPA and SRPA comparison

It is interesting to compare the RPA and SRPA result for the first excitation energy. In principle, including correlations with 2p-2h configurations, SRPA is a more complete theory. Nevertheless, the approximation (1.60) which must be made to calculate the commutators here is deeply different than the QBA used in RPA. We present the result as the percentage deviation from the exact result for the excitation energy, namely

$$\%Error = \frac{Exc - Exact}{Exact} \times 100. \quad (3.21)$$

Fig. 3.6 shows the overall improvement of SRPA over RPA, especially for the $w = v$ case. It must be noted, though, that for very small values of the potential, RPA gives a slightly better result. These considerations are equivalent also for other choices of the potentials.

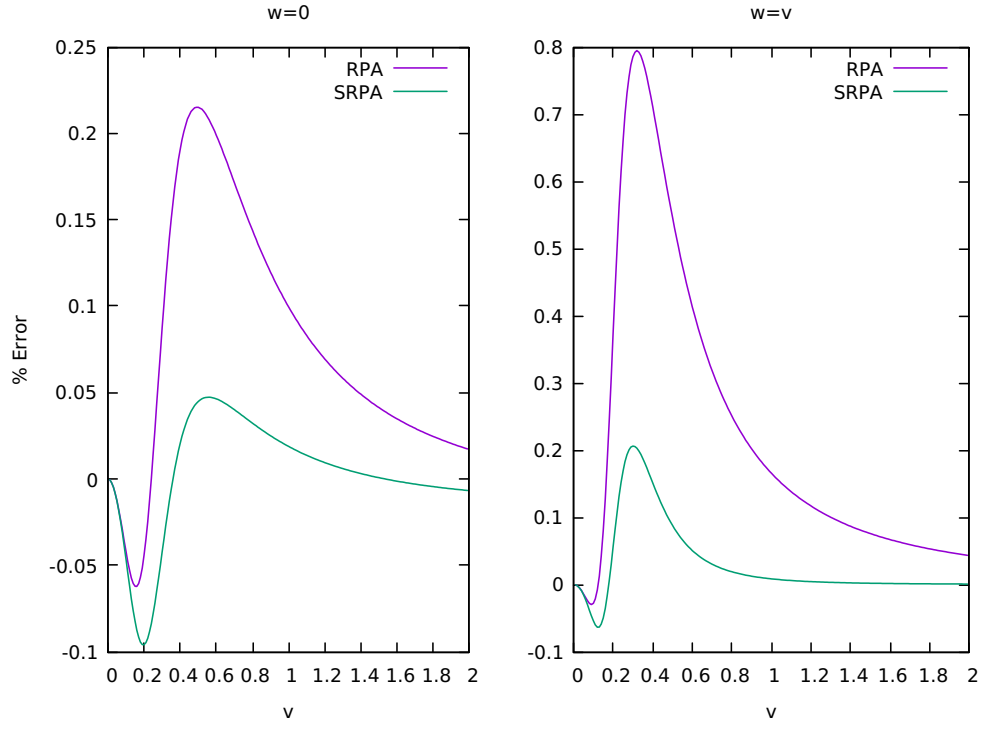


Figure 3.6: Percentage error for RPA and SRPA approximation compared with exact solution for the first excited state.

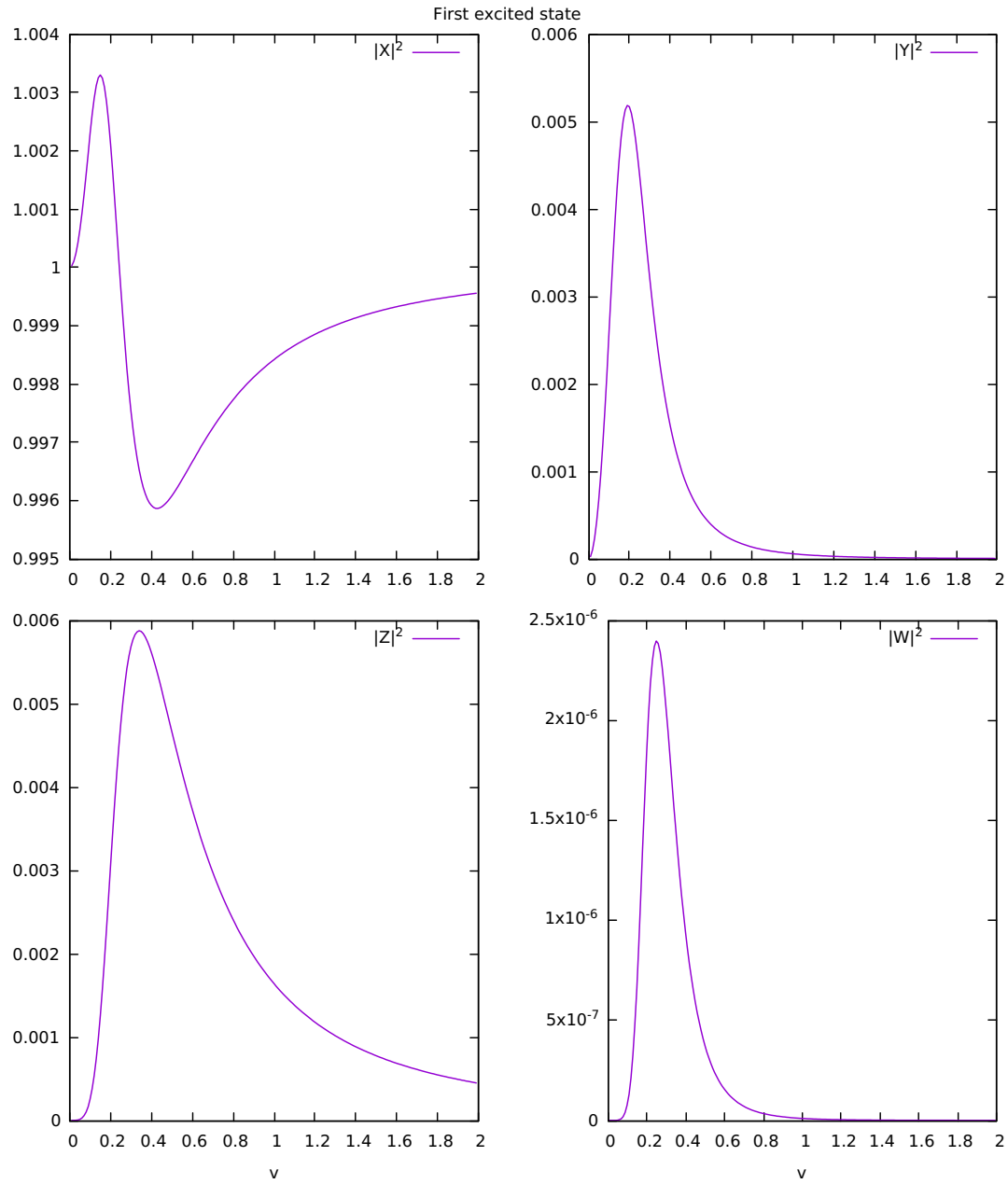


Figure 3.7: SRPA square amplitudes of the first excited state.

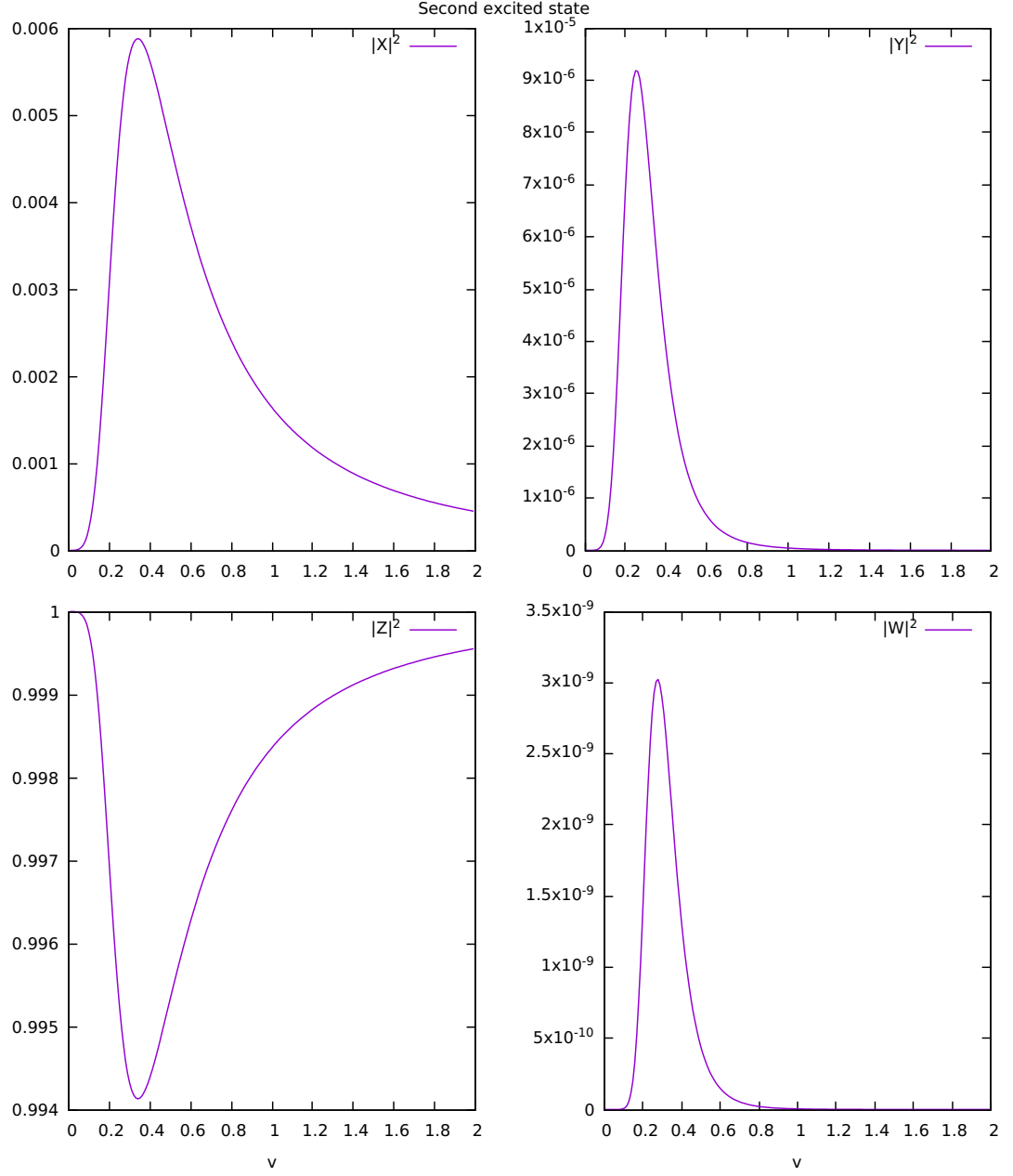


Figure 3.8: SRPA square amplitudes of the second excited state.

Chapter 4

Particle-Vibration Coupling

In this chapter we will develop the Particle-Vibration Coupling (PVC) theory for the LMG model. As the SRPA, this approximation represents a way of going beyond the RPA scheme. We will not go through the many aspects of the theory, for which we refer to [19–21].

4.1 Introduction

The spirit of PVC is to take into account the coupling between vibrations in nuclei and single-particle excitations. This is achieved including the phonon states along with pure particle states in the configuration space.

This approach can help in the evaluation of the spreading width of giant resonances. As we know, the SRPA tackles the problem by enlarging the model space with the subspace of 2p-2h states. On average, these configurations are higher in energy. Nevertheless, they introduce correlations which decrease the energy of the low lying states. PVC starts from the consideration that, as we know from the RPA, the phonon states have a lower energy than the single 1p-1h excitations. The idea of PVC in this context is thus to expand the RPA model space with the subspace containing 1p-1h states and phonon states. This allows to include the couplings among 1p-1h and phonon states, which are believed to describe with satisfactory detail the low energy spectra. Moreover, the formalism of PVC allows to reduce the configuration space choosing the most important phonons to be included, i.e. the low energy ones and the collective states. In this sense, the coupling between a phonon and a particle-hole are intended to describe the physical mechanism leading to the spreading of the collective modes [19].

In PVC theory the excitation operator has the following form:

$$Q_\nu^\dagger = \sum_{mi} \left(X_{mi}^\nu a_m^\dagger a_i - Y_{mi}^\nu a_i^\dagger a_m \right) + \sum_{mnkL} \left(Z_{mnkL}^\nu a_m^\dagger a_i Q_{kL}^\dagger - W_{mnkL}^\nu Q_{kL} a_i^\dagger a_m \right). \quad (4.1)$$

As was already explained, the underlying idea of PVC is to highlight the role of the phonon in the interaction with 1p-1h states. In this picture, the configuration space can

be taken as the product space of a subspace containing the ground and 1p-1h excitations and a subspace containing phonons, namely:

$$|\text{PVC}\rangle \equiv |\text{HF}\rangle \otimes |\text{RPA}\rangle. \quad (4.2)$$

For realistic calculations we refer to [28] and [29].

4.2 The generalized Lipkin model case

As we have seen, excitations in PVC theory are build as 1p-1h or 1p-1h and a phonon. For the LMG model, we have already remarked the fact that there exists only one possible kind of 1p-1h excitation. Similarly, also the phonon is unique. This allows us to pull the amplitudes out from the sum and write, for the excitation operator of the system:

$$Q_\nu^\dagger = \frac{1}{\sqrt{N}} \left(X'_\nu K_+ - Y'_\nu K_- + Z'_\nu K_+ Q_{\text{RPA}}^\dagger - W'_\nu Q_{\text{RPA}} K_- \right), \quad (4.3)$$

where $Q_{\text{RPA}}^\dagger$ is the usual RPA excitation operator

$$Q_{\text{RPA}}^\dagger = \frac{1}{\sqrt{N}} (X K_+ - Y K_-). \quad (4.4)$$

The term $1/\sqrt{N}$ in the excitation operator $Q_\nu^\dagger$ has been added for the normalization of the amplitudes, which reads, as in SRPA:

$$|X'|^2 - |Y'|^2 + |Z'|^2 - |W'|^2 = 1. \quad (4.5)$$

The derivation of the PVC equations can be done in an analogous way of RPA or SRPA. In realistic nuclear calculations is often useful to use a more effective formulation, which involves the diagonalization of a smaller matrix. This procedure can be found in Appendix ???. In our case, starting from the equation of motion (1.33), we write the set of 4 equations:

$$\begin{aligned} \langle 0 | [K_-, H, Q_\nu^\dagger] | 0 \rangle &= \omega_\nu \langle 0 | [K_-, Q_\nu^\dagger] | 0 \rangle \\ \langle 0 | [Q_{\text{RPA}} K_-, H, Q_\nu^\dagger] | 0 \rangle &= \omega_\nu \langle 0 | [Q_{\text{RPA}} K_-, Q_\nu^\dagger] | 0 \rangle \\ \langle 0 | [K_+, H, Q_\nu^\dagger] | 0 \rangle &= \omega_\nu \langle 0 | [K_+, Q_\nu^\dagger] | 0 \rangle \\ \langle 0 | [K_+ Q_{\text{RPA}}^\dagger, H, Q_\nu^\dagger] | 0 \rangle &= \omega_\nu \langle 0 | [K_+ Q_{\text{RPA}}^\dagger, Q_\nu^\dagger] | 0 \rangle, \end{aligned} \quad (4.6)$$

where we call $|0\rangle$ the state $|\text{PVC}\rangle$ for simplicity of notation. The commutators can be evaluated with the choice for the ground state made in (4.2). We can start with the terms on r.h.s.: as an example, we write down the calculations for the term on the second line

(the first one is trivial since it is the same that appears in RPA equations):

$$\begin{aligned}
\langle 0 | [Q_{\text{RPA}} K_-, Q_\nu^\dagger] | 0 \rangle &\approx \langle \text{RPA} | \langle \text{HF} | [Q_{\text{RPA}} K_-, Q_\nu^\dagger] | \text{HF} \rangle | \text{RPA} \rangle \\
&= \frac{1}{\sqrt{N}} \langle \text{RPA} | \langle \text{HF} | Q_{\text{RPA}} K_- K_+ Q_{\text{RPA}}^\dagger | \text{HF} \rangle | \text{RPA} \rangle \\
&= \frac{1}{\sqrt{N}} \langle \text{HF} | K_- K_+ | \text{HF} \rangle \langle \text{RPA} | Q_{\text{RPA}} Q_{\text{RPA}}^\dagger | \text{RPA} \rangle \\
&= \sqrt{N},
\end{aligned} \tag{4.7}$$

where the last step follows for the normalization of RPA phonon. Same result is obtained for all commutators on RHS, so that we can write our equations in matrix notation:

$$\begin{pmatrix} A_{1,1} & A'_{1,2} & B_{1,1} & B'_{1,2} \\ A'_{1,2} & A_{2,2} & B'_{1,2} & B_{2,2} \\ -B_{1,1} & -B'_{1,2} & -A_{1,1} & -A'_{1,2} \\ -B'_{1,2} & -B_{2,2} & -A'_{1,2} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix}, \tag{4.8}$$

where we have defined:

$$\begin{aligned}
A_{1,1} &= \frac{\langle 0 | [K_-, [H, K_+]] | 0 \rangle}{N} \\
A_{1,2} &= \frac{\langle 0 | [K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | 0 \rangle}{N} \\
A_{2,1} &= \frac{\langle 0 | [Q_{\text{RPA}} K_-, [H, K_+]] | 0 \rangle}{N} \\
A_{2,2} &= \frac{\langle 0 | [Q_{\text{RPA}} K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | 0 \rangle}{N},
\end{aligned} \tag{4.9}$$

and

$$\begin{aligned}
B_{1,1} &= -\frac{\langle 0 | [K_-, [H, K_-]] | 0 \rangle}{N} \\
B_{1,2} &= -\frac{\langle 0 | [K_-, [H, Q_{\text{RPA}} K_-]] | 0 \rangle}{N} \\
B_{2,1} &= -\frac{\langle 0 | [Q_{\text{RPA}} K_-, [H, K_-]] | 0 \rangle}{N} \\
B_{2,2} &= -\frac{\langle 0 | [Q_{\text{RPA}} K_-, [H, Q_{\text{RPA}} K_-]] | 0 \rangle}{N}.
\end{aligned} \tag{4.10}$$

Also, we have:

$$\begin{aligned}
A'_{1,2} &= \frac{1}{2} (A_{1,2} + A_{2,1}) \\
B'_{1,2} &= \frac{1}{2} (B_{1,2} + B_{2,1}),
\end{aligned} \tag{4.11}$$

to retain hermiticity of the matrix. The terms $A_{1,1}$ and $B_{1,1}$ are the same of RPA, and have already been calculated in sec. 3.3. It is also easy to check that

$$B_{1,2} = B_{2,1} = B_{2,2} = 0, \tag{4.12}$$

so that the PVC matrix looks alike the SRPA one:

$$\begin{pmatrix} A_{1,1} & A'_{1,2} & B_{1,1} & 0 \\ A'_{1,2} & A_{2,2} & 0 & 0 \\ -B_{1,1} & 0 & -A_{1,1} & -A'_{1,2} \\ 0 & 0 & -A'_{1,2} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix}. \quad (4.13)$$

4.2.1 PVC matrix elements

In this section we will evaluate the matrix elements of the PVC matrix. We start with the off-diagonal term $A_{1,2}$, whose expectation value in the numerator is:

$$\begin{aligned} \langle 0[K_-[H, K_+Q_{\text{RPA}}^\dagger]]0 \rangle &\approx \langle \text{HF} | \langle \text{RPA} | [K_-[H, K_+Q_{\text{RPA}}^\dagger]] | \text{RPA} \rangle | \text{HF} \rangle \\ &= \langle \text{HF} | \langle \text{RPA} | K_- H K_+ Q_{\text{RPA}}^\dagger | \text{RPA} \rangle | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_+ | \text{HF} \rangle \langle \text{RPA} | H Q_{\text{RPA}}^\dagger | \text{RPA} \rangle \\ &= N \langle \text{RPA} | [H, Q_{\text{RPA}}^\dagger] | \text{RPA} \rangle \\ &= N \langle \text{HF} | [H, Q_{\text{RPA}}^\dagger] | \text{HF} \rangle. \end{aligned} \quad (4.14)$$

The steps are carried out taking care the fact that $K_\pm$ and Q_{RPA} acts on different subspaces, and therefore expliciting the only non-zero results. We can then write down the phonon by means of operator K_+ and K_- , and find the expectation value in HF state:

$$\begin{aligned} &= \sqrt{N} (X \langle \text{HF} | [H, K_+] | \text{HF} \rangle + Y \langle \text{HF} | [K_-, H] | \text{HF} \rangle) \\ &= \sqrt{N} (X + Y) \langle \text{HF} | H K_+ | \text{HF} \rangle, \end{aligned} \quad (4.15)$$

where in the last step we used the property that the matrix elements are all real (the complex conjugate is obtained changing $-$ to $+$). We end up with:

$$\begin{aligned} A_{1,2} &= \frac{X + Y}{\sqrt{N}} \langle \text{HF} | H K_+ | \text{HF} \rangle \\ &= \epsilon \sqrt{N} (X + Y) \left(\frac{\sin \alpha}{2} - g \cos \alpha - \frac{v + w}{4} \sin(2\alpha) \right), \end{aligned} \quad (4.16)$$

where we used the explicit form the HF Hamiltonian (3.14) to evaluate the expectation value. In this expression, only the terms proportional to K_- needed to be evaluated. With similar steps, one obtains $A_{2,1} = 0$. We proceed with the calculation of the $A_{2,2}$ term, whose numerator reads:

$$\begin{aligned} \langle 0[Q_{\text{RPA}} K_- [H, K_+ Q_{\text{RPA}}^\dagger]]0 \rangle &\approx \langle \text{HF} | \langle \text{RPA} | [Q_{\text{RPA}} K_- [H, K_+ Q_{\text{RPA}}^\dagger]] | \text{RPA} \rangle | \text{HF} \rangle \\ &= \langle \text{HF} | \langle \text{RPA} | Q_{\text{RPA}} K_- H K_+ Q_{\text{RPA}}^\dagger - \\ &\quad Q_{\text{RPA}} K_- K_+ Q_{\text{RPA}}^\dagger H | \text{RPA} \rangle | \text{HF} \rangle \\ &= \langle \text{HF} | K_- H K_+ | \text{HF} \rangle + N \langle \text{RPA} | Q H Q_{\text{RPA}}^\dagger | \text{RPA} \rangle \\ &\quad - N \langle \text{RPA} | Q Q_{\text{RPA}}^\dagger H | \text{RPA} \rangle - \langle \text{HF} | K_- K_+ H | \text{HF} \rangle \\ &= \langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle + N \langle \text{RPA} | Q, [H, Q_{\text{RPA}}^\dagger] | \text{RPA} \rangle. \end{aligned} \quad (4.17)$$

The second term of the last sum can be expanded writing explicitly the phonon, and switching to the HF ground state by means of the commutator:

$$\begin{aligned}
\langle \text{RPA} | Q, [H, Q_{\text{RPA}}^\dagger] | \text{RPA} \rangle &\approx \langle \text{HF} | [Q, [H, Q_{\text{RPA}}^\dagger]] | \text{HF} \rangle \\
&= N^{-1} \left(X^2 \langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle - XY \langle \text{HF} | [K_-, [H, K_-]] | \text{RPA} \rangle \right. \\
&\quad \left. - YX \langle \text{HF} | [K_+, [H, K_+]] | \text{HF} \rangle + Y^2 \langle \text{HF} | [K_+, [H, K_-]] | \text{HF} \rangle \right) \\
&= N^{-1} (X^2 + Y^2) \langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle + \\
&\quad 2N^{-1} XY \langle \text{HF} | [K_+, [H, K_+]] | \text{HF} \rangle.
\end{aligned} \tag{4.18}$$

Coming back to the previous expression, we get

$$\begin{aligned}
\langle 0 | Q_{\text{RPA}} K_- [H, K_+ Q_{\text{RPA}}^\dagger] | 0 \rangle &= 2X^2 \langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle - 2XY \langle \text{HF} | [K_+, [H, K_+]] | \text{HF} \rangle \\
&= 2NX(XA_{1,1} - YB_{1,1}),
\end{aligned} \tag{4.19}$$

where we used of the normalization relation of the RPA amplitudes and wrote the result with the definition of the RPA matrix elements. We report the full result using RPA expressions (3.16):

$$\begin{aligned}
A_{2,2} &= 2X(XA_{1,1} - YB_{1,1}) \\
&= \epsilon 2X \left(X \left(\cos \alpha - w + \frac{3}{2}(v+w) \sin^2 \alpha + 2g \sin \alpha \right) + \right. \\
&\quad \left. Y \left(w - \frac{v+w}{2}(1 + \cos^2 \alpha) \right) \right).
\end{aligned} \tag{4.20}$$

4.2.2 Results

The eigenvalue problem in (4.13) can be solved numerically and four excitation energies are found. First, we compare the result for the first excitation energy with the RPA solution (see Fig. 4.1 above). With the usual choice of potential, namely $g = v$ and $w = 0$ or $w = v$, we observe that the two results are completely identical. Further studies with different values of the parameters shows a slightly, yet almost invisible, improvement of the PVC solution. These results suggest that for a simple Hamiltonian like the generalized LMG, the correlation introduced in the PVC scheme are non important.

We present the result for the excitation energy of the second state as the deviation with the exact, compared with SRPA, in Fig. (4.1). As can be seen from the plot, the error of PVC is about twice that of SRPA. Nevertheless, the error for both approximations is about few percentage points. It must be emphasized that, unlike SRPA, PVC calculations involves only one-particle operators inside the commutators. In this perspective, PVC has the advantage of offering good results with small computational efforts.

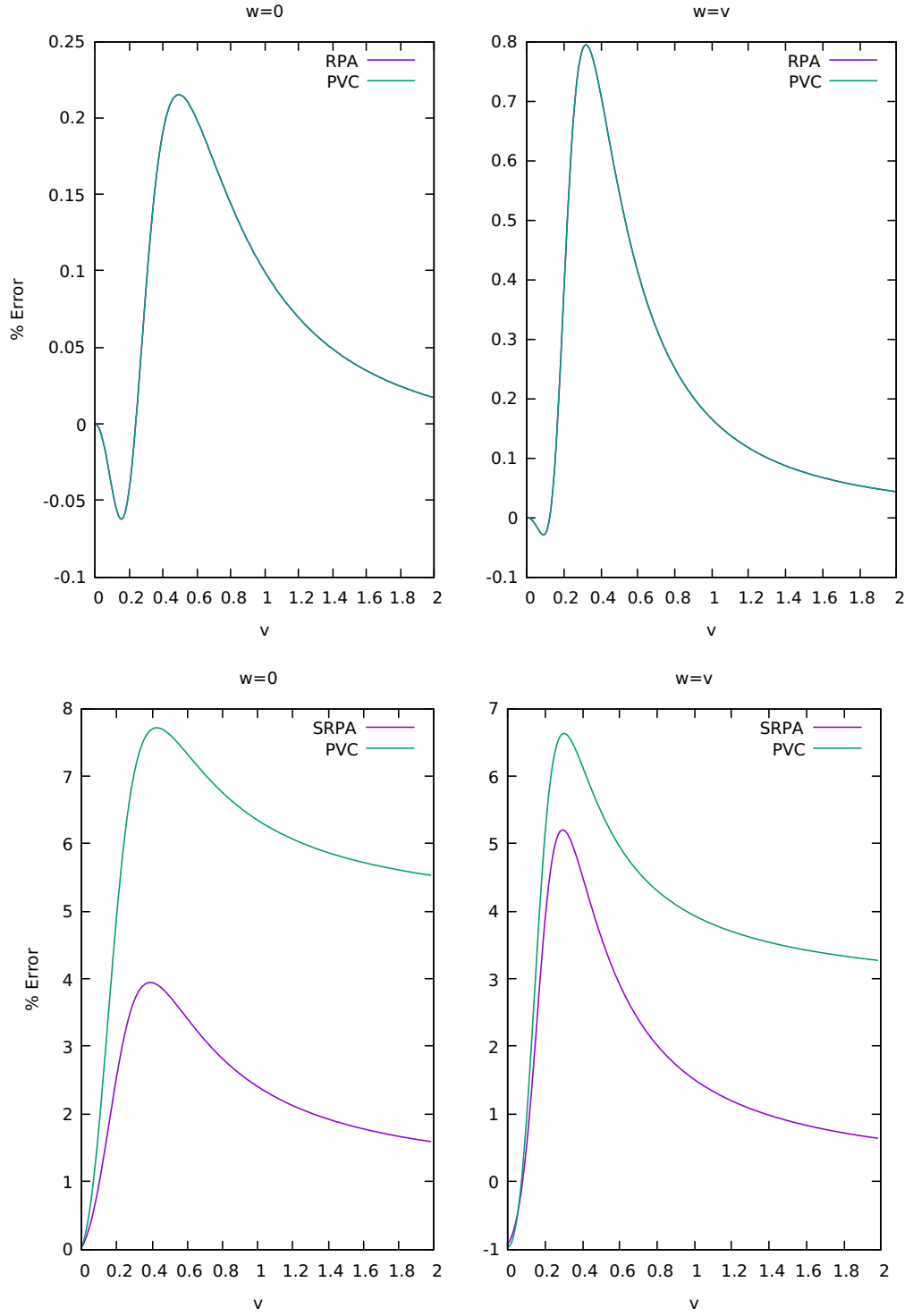


Figure 4.1: PVC and RPA comparison for the first excitation (above) and PVC and SRPA comparison for the second excitation energy (below).

4.3 Extended Particle-Vibration Coupling

In PVC approach the basis state for all configurations is the product space of HF and RPA. As we have explained before, this choice is motivated by the observed coupling between the resonance states with the compound nuclear states. Nevertheless, it may also seem unphysical to distinguish the basis state of the system into two separated subspaces.

In this section, we want to brake this fundamental assumption in order to take into accounts the couplings between 1p-1h excitations and the single 1p-1h excitations which constitute the phonon. The excitation operator should be as in PVC (4.3):

$$Q_\nu^\dagger = \frac{1}{\sqrt{N}} (X'_\nu K_+ - Y'_\nu K_-) + \frac{1}{X\sqrt{2(N-1)}} (Z'_\nu K_+ Q_{\text{RPA}}^\dagger - W'_\nu Q_{\text{RPA}} K_-). \quad (4.21)$$

All the constant factors have been added to get the normalization of the amplitudes as in SRPA or in PVC. Note that the X term on the denominator of PVC excitation operator is the amplitude associated with the RPA phonon (4.5).

From a mathematical point of view, this is the natural generalization of the SRPA excitation operator, which now includes mixed terms like $K_+ K_-$ or $K_- K_+$, here weighted by the RPA amplitudes. Of course, the most general operator should introduce also new amplitudes for every additional terms. Nonetheless, this goes beyond the scope of this section.

Our aim is to build the equations starting from the equation of motion (1.33). This can be done along the line already discussed in previous sections. The set of equations read, in matrix form:

$$\begin{pmatrix} A_{1,1} & A'_{1,2} & B_{1,1} & B'_{1,2} \\ A'_{1,2} & A_{2,2} & B'_{1,2} & B_{2,2} \\ -B_{1,1} & -B'_{1,2} & -A_{1,1} & -A'_{1,2} \\ -B'_{1,2} & -B_{2,2} & -A'_{1,2} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X'_\nu \\ Z'_\nu \\ Y'_\nu \\ W'_\nu \end{pmatrix}, \quad (4.22)$$

where

$$\begin{aligned} A_{1,1} &= \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N} \\ A_{1,2} &= \frac{\langle \text{HF} | [K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | \text{HF} \rangle}{X\sqrt{2N(N-1)}} \\ A_{2,1} &= \frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_+]] | \text{HF} \rangle}{X\sqrt{2N(N-1)}} \\ A_{2,2} &= \frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | \text{HF} \rangle}{2X^2(N-1)}, \end{aligned} \quad (4.23)$$

and

$$\begin{aligned}
B_{1,1} &= -\frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N} \\
B_{1,2} &= -\frac{\langle \text{HF} | [K_-, [H, Q_{\text{RPA}} K_-]] | \text{HF} \rangle}{X \sqrt{2N(N-1)}} \\
B_{2,1} &= -\frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_-]] | \text{HF} \rangle}{X \sqrt{2N(N-1)}} \\
B_{2,2} &= -\frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_- Q_{\text{RPA}}]] | \text{HF} \rangle}{2X^2(N-1)}.
\end{aligned} \tag{4.24}$$

The evaluation of the matrix elements are reported in Appendix C.3. We find out that $B_{1,2}$, $B_{2,1}$ and $B_{2,2}$ are non-zero because of the presence of mixed terms like $K_+ K_-$ or $K_- K_+$ due to the phonon. We report the results:

$$\begin{aligned}
\frac{A'_{1,2}}{\epsilon} &= \sqrt{\frac{1}{8(N-1)}} (\sin \alpha(N-1) - (v+w) \sin \alpha \cos \alpha(N-3) - 2g \cos \alpha(N-1)) \\
&\quad - \frac{Y}{X \sqrt{2(N-1)}} N (-\sin \alpha(N-1) - (v+w) \sin \alpha \cos \alpha + 2g \cos \alpha) \\
&\quad + \frac{1}{\sqrt{8(N-1)}} (v+w) \sin(2\alpha), \\
\frac{A_{2,2}}{\epsilon} &= \frac{1}{N-1} (2 \cos \alpha(N-1) - 2w(N-2) + 3(v+w) \sin^2 \alpha(N-2) + 4g \sin \alpha(N-1)) + \\
&\quad + \frac{Y}{X} \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right),
\end{aligned} \tag{4.25}$$

and

$$\begin{aligned}
\frac{B'_{1,2}}{\epsilon} &= \frac{Y}{2X \sqrt{2(N-1)}} N \left(-\sin \alpha + \frac{v+w}{2} \sin(2\alpha) + 2g \cos \alpha \right), \\
\frac{B_{2,2}}{\epsilon} &= -\frac{Y}{X} \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right).
\end{aligned} \tag{4.26}$$

Evaluated all the results using α_{HF} , we can solve numerically the eigenvalue problem (4.22). The results for the excitation energy is compared with the SRPA solution as the deviation from the exact solution in Fig. 4.2. The extended PVC results shows better agreement with the exact result, especially for the second excited state, where the improvement is consistent.

The comparison with PVC highlights the great improvement made within this extension. Nevertheless, it must be emphasized the fact that the amount of calculations rose due to the presence of non-zero $B_{1,2}$, $B_{2,1}$ and $B_{2,2}$ terms. This eigenvalue problem might lead to formidable computational efforts, therefore discouraging real nuclei applications.

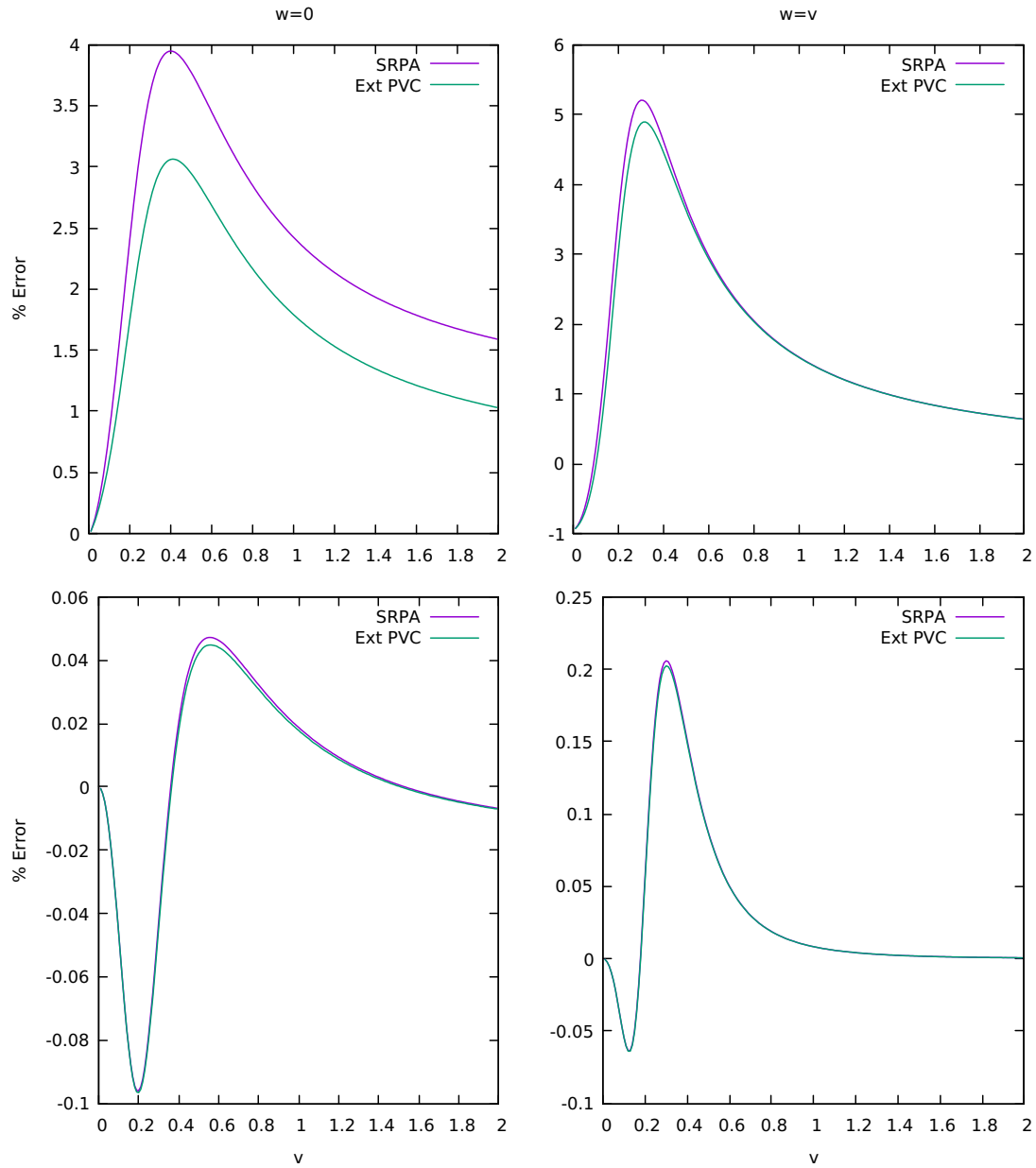


Figure 4.2: Percentage error for extended PVC and SRPA compared with exact solution for the first (below) and the second (above) excitation energy.

Chapter 5

Sensitivity to the potential parameters

In this chapter we want to offer insights on some specific features of the generalized LMG model. Up to now, the model has been used to test the approximation theories. We restricted our studies to specific choices of the potentials to allow the comparison among the various models and with previous results in literature. However, it is worth to have a glance of the new model in a more general fashion. The generalized LMG model is found to exhibit interesting properties, some of which are in contrast with the old model, and deserve to be presented.

5.1 Excited states

In this section the generalized LMG Hamiltonian will be studied choosing $v = 0$ (to ignore the pairing effects) and letting w and g to assume different values. To do that, 3D plot will be used to visualize the results.

In Fig. 5.1 the first two excited states of a 20-particles generalized LMG model are drawn. As can be seen, the energy is a smooth function of both potentials and is always increasing with g . When $g \rightarrow 0$, the energy of both the first and the second excited state are decreasing with w , but they do not tend to zero. The behavior of the model in this case is interesting, and deserves to be studied in detail. Consider, for simplicity, the 3-particles generalized LMG Hamiltonian:

$$\frac{H_3}{\epsilon} = \begin{pmatrix} -\frac{3}{2} - \frac{3}{4}w & 0 & 0 & 0 \\ 0 & -\frac{1}{2} - \frac{7}{4}w & 0 & 0 \\ 0 & 0 & \frac{1}{2} - \frac{7}{4}w & 0 \\ 0 & 0 & 0 & \frac{3}{2} - \frac{3}{4}w \end{pmatrix} \quad (5.1)$$

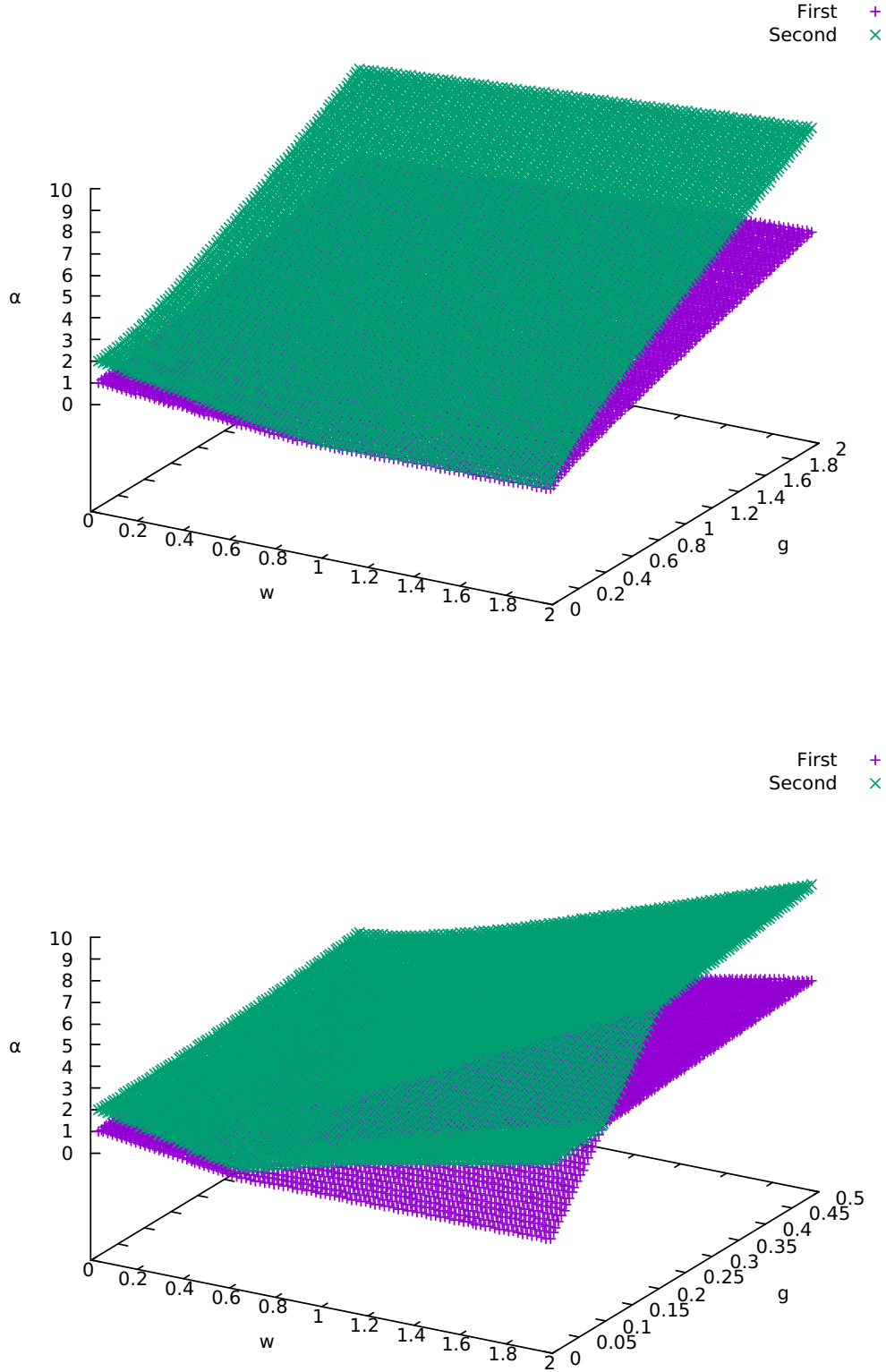
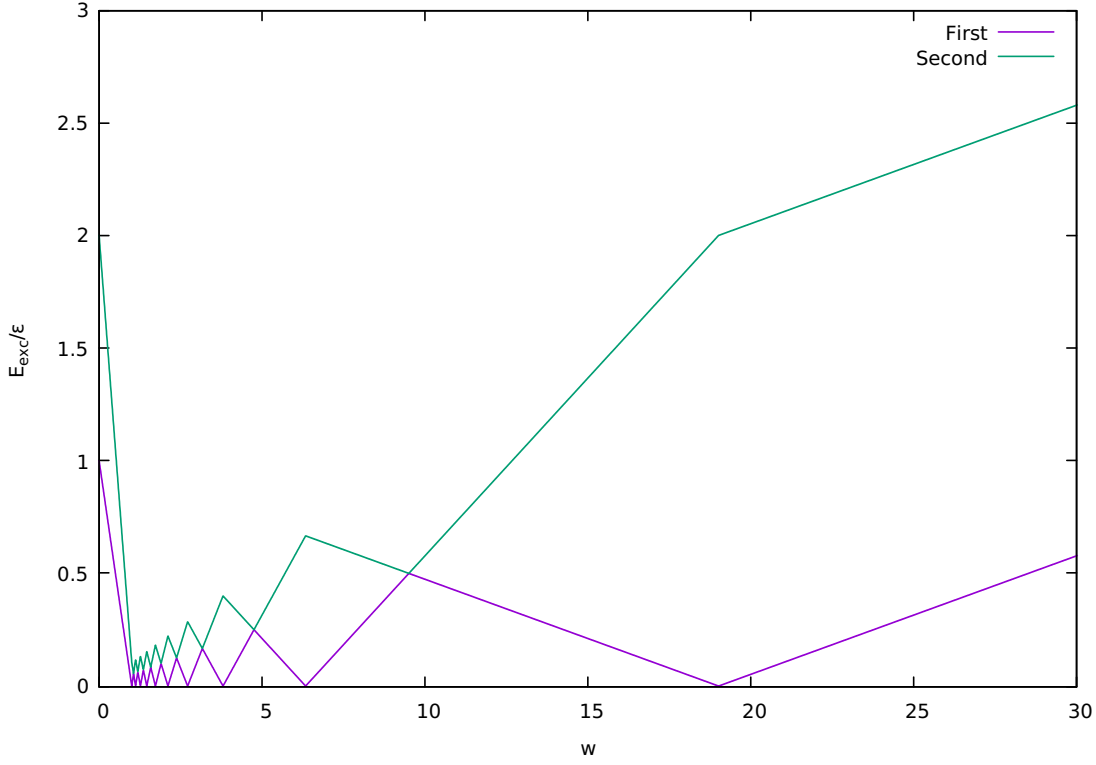


Figure 5.1: First two excited states for the generalized LMG model for $v = 0$ (above) and $v = w$ (below).

Figure 5.2: First and second excitation energy for $v = g = 0$.

The matrix is already diagonalized and we can read the eigenvalues directly. For small values of w , the ground state is clearly given by the value on the first column. When $w = 1$, though, the minimum energy state became the one with the eigenvalue on the second column. Thus, this Hamiltonian exhibit level crossing. In calculating the excitation energy, one needs to be careful on which state is assumed to be the ground. In this case, depending on how strong is the potential the first excitation energy has a different expression:

$$E_{exc} = \begin{cases} w - \frac{1}{2}, & \text{for } w < 1 \\ \frac{1}{2} - w, & \text{for } w > 1 \end{cases} \quad (5.2)$$

The number of times the ground state changes is related to the dimension of the matrix, and thus to the number of particles. In Fig. 5.2 we show this behavior for the first two excitation energies of the 20-particle generalized LMG model. The ground state (and so the excitation energy) here need to change 9 times as the potential increases. In the plot, the excitation energies are saw-shaped due to the “moving” of both the ground state and the excited state in the 20-particles Hamiltonian.

As it can be seen from the plot, there exists values for the potentials where the energy of the first and the second excited states are equal. This degeneracy of excited states

suggests the existence of a quantum phase transition.

5.2 Correlations

All the considerations about the effectiveness of the approximations methods in the last chapters have been obtained sticking to the case $g = v$. In this section, we want to generalize the discussion we made in Sec. 3.2 for a broader choices of potentials.

Quasi-particle ground state

The first step is to analyze the HF minimization condition (3.15). We recall for the reader the meaning of α as the parameter which define the unitary transformation (2.21). The values of α which minimize the HF energy now depend on both w and g . The resulting surface is drawn in Fig. 5.3. As can be seen, apart from small values of w and g , it is almost constant. Indeed, for high values of both potentials, α tend to $\pi/2 \approx 1.57$, which correspond to the limiting case when the unitary transformation of the single-particle operators is 0 on the diagonal and 1 off-diagonal.

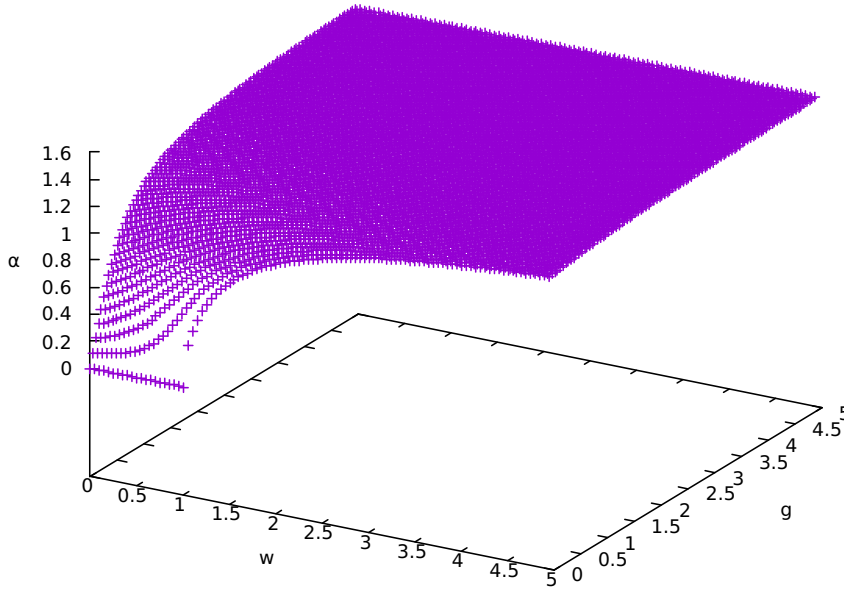
It is worthwhile to note the limiting case of the LMG model which is find when $g \rightarrow 0$: it is evident from the plot that the value of α changes discontinuously from 0 ($0 < w < 1$) to a complex function of w ($w > 1$). Since we know that in the LMG model w appears paired with v as $v + w$ in the minimization condition, the dependece of α in this case must be $\arccos(1/w)$ (see (2.28)). When g is turned on, the graph shows that the discontinuity of α is solved. Nevertheless, $\alpha \neq 0$ for all values of g and w : this means that a non-trivial unitary transformation (2.21) is always needed to ensure to find a minimum of the HF energy.

RPA amplitudes

We want now apply the RPA theory to the generalized LMG model to study the behavior of the amplitudes X and Y with various values of the potentials. This is interesting, since it gives a measure of the correlations between the 1p-1h excitations. On top of Fig. 5.4 we show the $|Y|^2$ for the case $v = g$: it is just the 3D extension of the plot 2.8, which includes now g . As it was predicted in Sec. 3.3, when g is turned on the divergence of $|Y|^2$ disappears.

Nevertheless, the $g = v$ case of the generalized LMG model demonstrated very small correlations, as it was clear looking Fig. 3.4. A system like that can be adequately described even by TDA theory. We wonder now if the situation changes with different choices of the potentials. In Fig. 5.4 $|Y|^2$ is now drawn for $v = 0$. In this case, correlations appear to be very strong when g is small and w is large. This can be understood looking at the expressions of A and B in the RPA matrix:

$$\begin{aligned} A_{1,1} &= \frac{\epsilon w}{2} (1 - 3 \cos^2 \alpha) + \epsilon (\cos \alpha + 2g \sin \alpha) \\ B_{1,1} &= \frac{\epsilon w}{2} (1 - \cos^2 \alpha), \end{aligned} \tag{5.3}$$

Figure 5.3: The result of the variational procedure for $v = 0$.

When $g = 0$, the variational parameter must be taken as (2.28), leading to

$$\begin{aligned} A_{1,1} &= \frac{\epsilon w}{2} \left(1 - \frac{3}{w} \right) + \epsilon \cos \alpha \\ B_{1,1} &= \frac{\epsilon w}{2} \left(1 - \frac{1}{w} \right), \end{aligned} \tag{5.4}$$

The two terms gets closer when w increases, and this lead to $A \approx B$, as it was in the LMG model when $w = 0$ and $v = 1$ or $w = v = 0.5$. The approximations fails only when the potentials are very strong. Nevertheless, the issue is solved if g is dependent by w : in this situation, the RPA matrix elements are never equal, and the approximation works for every values of the potentials.

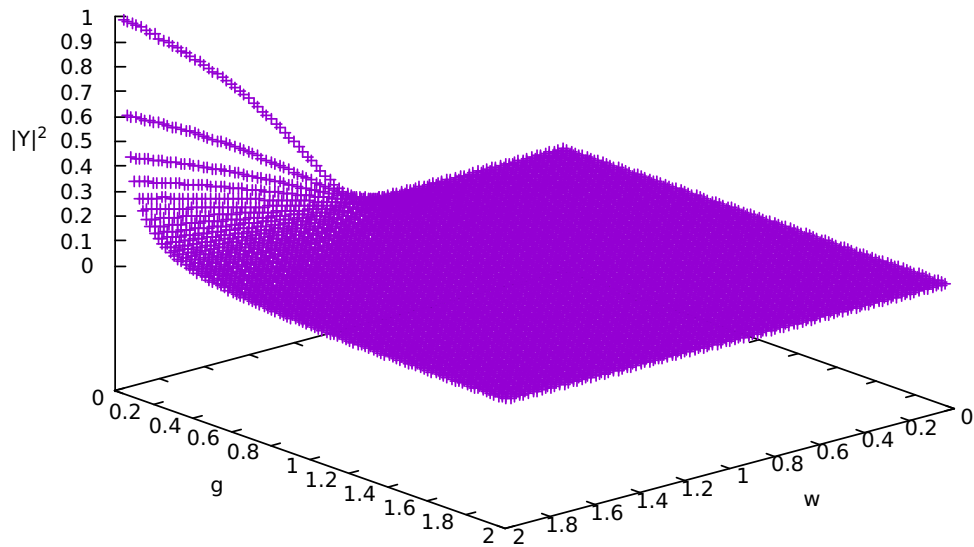
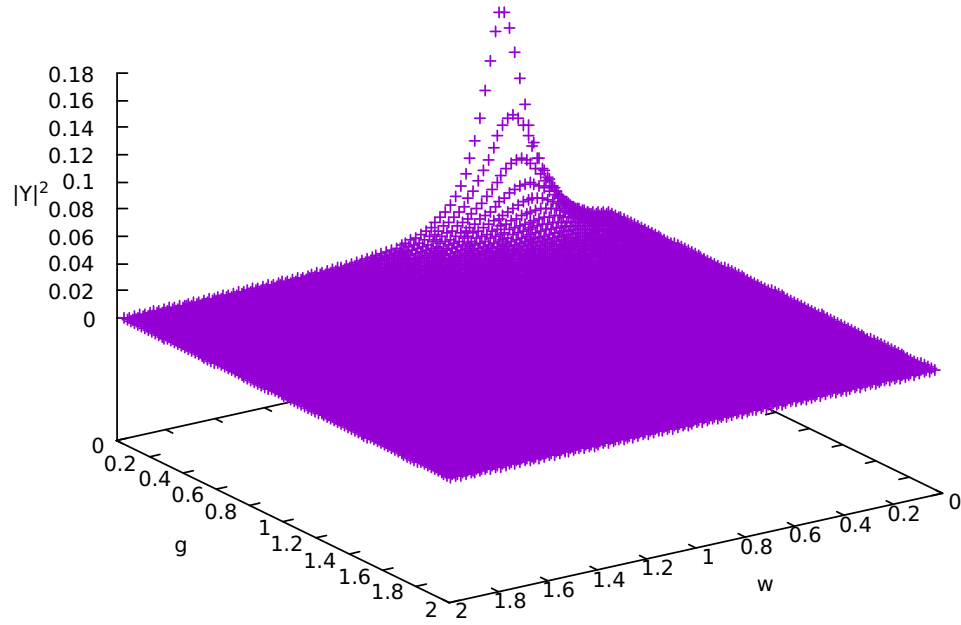


Figure 5.4: $|Y|^2$ for the case $v = w$ (above) and $v = 0$ (below) as function of g and w .

5.3 Full spectrum

In this section we want to compare the shape of the spectrum of the LMG model with the one of its generalized version. In order to have many eigenvalues, this time we consider 50-particle models. For simplicity, we decide to draw only the first 20 eigenvalues. They can be found in Fig. 5.5 as a function of v . In the LMG model case, we adopted $w = v$, while for the generalized LMG model we used $w = g = v$.

The main difference between the two plots is the presence of different states with the same energy in the LMG model. Indeed, when the potentials are large enough, in the LMG model the first 20 eigenvalues merge in pairs, leading to a degeneracy among the excited states. This happens at around $0.4 < v < 0.6$. Moreover, it is interesting to note that in this same region the eigenvalues of the LMG model shrink together. This was already noted in [5], where this feature is said to be related to a quantum phase transition.

The generalized LMG model do not present these features. As it can be seen from the figure, the difference in energy among the eigenvalues is almost always constant when the potentials are small, and slowly increasing for strong interactions.

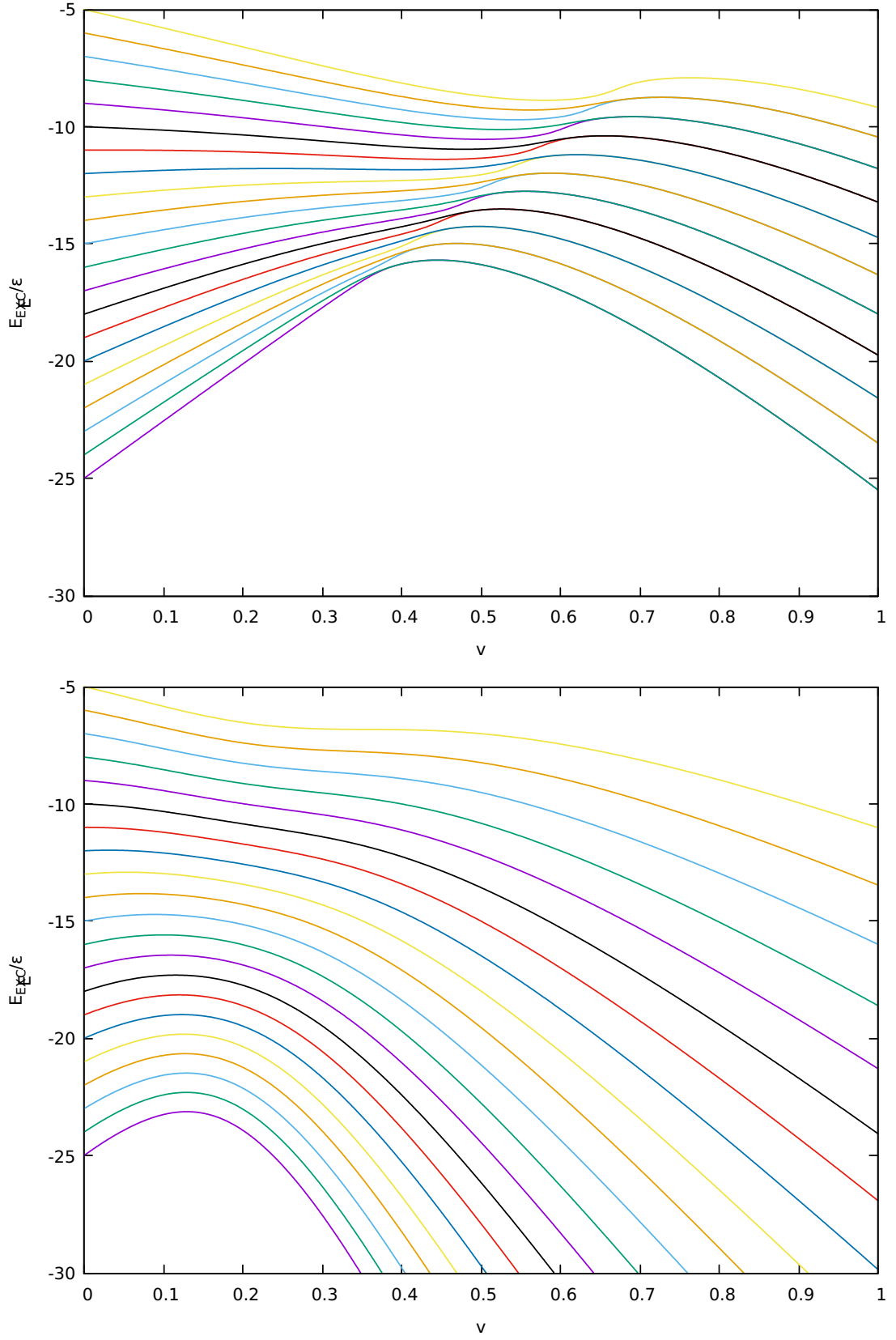


Figure 5.5: First 20 eigenvalues for a 50-particles LMG model (above) and generalized LMG model (below).

Conclusion

In nuclear physics, simple solvable models can be an important tool to test many-body techniques. The goodness of a theory can be estimated by its direct comparison with the exact results of the model. One of the most used models in literature [1] is the Lipkin-Mechov-Glick (LMG) model [4], which is an ideal system composed by two energy levels where the many-body Schrödinger equation for the interacting particles can be solved without approximations.

The literature related to the application of Hartree-Fock (HF) and Random-Phase Approximation (RPA) theories to the LMG model is extensive. It is known since the original formulation of the model that for a specific region of the parameter space the HF state is not able to reproduce the energy of the ground state [4]. This problem affects also the RPA, since its equations are calculated starting from the HF state. Nonetheless, these troubles can be solved adopting a quasi-particles Slater determinant for these specific values of the parameters. Then, the results for the ground state energy of the HF and the RPA are in good agreement with the exact solutions, especially when the number of particles is large [13].

Up to now, no attempts have been made to test the approximation methods which go beyond the RPA on the LMG model. The aim of this work has been to fill this gap using in particular the Second RPA (SRPA) and Particle-Vibration Coupling (PVC).

Our first discussions have been devoted to the application of HF and RPA theories to the LMG model. In these sections, we confirmed the results already present in literature. Nevertheless, the evaluation of the first excitation energy in RPA revealed the failure of this method to predict correct results for some values of the parameters of the potential. The problems arise in the region where HF is unable to describe the system and a different Slater determinant must be used. This breakdown might be due to intrinsic limitations of the mean-field theories when they are applied on such a simple Hamiltonian.

Using the LMG model, the SRPA theory allows to get the energy of the second excited state. Unfortunately, the application of this technique on the model revealed the same issues we have already found in RPA. In the SRPA case, both excitations energies disagree with the exact results where also the RPA failed. This suggests that the bad behavior of RPA in some regions cannot be solved by extending the model space. Furthermore, we have realized that the SRPA scheme does not improve much the results since the terms in the equations which account for the couplings between the 1p-1h and 2p-2h subspaces are all zero. This is due to the lack of terms in the Hamiltonian which allow to include these

couplings, and therefore it is a consequence of the simplicity of the LMG Hamiltonian.

This inadequacy of the LMG model has led us to propose an extended version of the model. Starting from the most general two-body interaction, we derived a model Hamiltonian for our two-level system which now comprises two more terms that are proportional to a part of the interaction which was before neglected. We believe that this is the most general Hamiltonian for a two-level system which satisfies the symmetries of the LMG Hamiltonian. In the last part of this thesis we offered insights on some specific features of the generalized LMG model with various choices for the parameters of the potential.

The application of the HF theory on this model evidenced the need to use a quasi-particles Slater determinant for all the values of the parameters. Nevertheless, the RPA solution for the first excitation energy is now remarkably close to the exact for all the values of the parameters. Also, the application of the SRPA to the new model gives very good solutions for both the excitation energies and in every region of the parameter space. These results highlight the good behavior of RPA and SRPA in describing the excitations of the new model: the presence of the new terms in the Hamiltonian is the key of their success.

With the new model, a comparison between the RPA and the SRPA solutions has been possible: the SRPA gives results which are on average 4 times closer to the exact than RPA. Still, the deviation from the exact is on the order of less than one percent for both the approximation methods. This is a consequence of the small correlations which the model exhibits with the adopted values for the parameters.

In chapter 4, the PVC theory has been developed for the generalized LMG model. Interestingly, the first excitation energy resulted almost identical to the one obtained using the RPA. The PVC allows to obtain also the second excitation energy of our model. Compared with the SRPA solution, it shows less agreement with the exact result. This suggests that for a simple Hamiltonian like the generalized LMG, a full calculation in SRPA is preferable than the PVC. In the last section of the chapter we tried to break the fundamental assumption of the PVC concerning the separation of 1p-1h and phonons subspaces. The results show the improved accuracy of the theory: the excitation energies are much closer to the exact, even than the SRPA solutions. Nevertheless, the increase of precision is at the expense of the calculational efforts: the presence of many non-zero terms in the Hamiltonian of this theory compared with SRPA might discourage real applications in nuclei.

Appendix A

Particle-hole representation

For some purposes it is convenient to redefine the zero of energy to the Fermi level, and to take the filled fermi sea (the $|\text{HF}\rangle$ ground state) as a vacuum state. This leads the introduction of a set of creation and annihilation operators b and $b^\dagger$ such that, for states under the fermi level:

$$\begin{aligned} b_i &= -a_i^\dagger \\ b_i^\dagger &= -a_i, \end{aligned} \tag{A.1}$$

while for levels above the fermi sea they are unchanged:

$$\begin{aligned} b_m &= a_m \\ b_m^\dagger &= a_m^\dagger \end{aligned} \tag{A.2}$$

The transformation preserves the usual fermion anti-commutation relations. In particular, for states under Fermi it can be easily proven that

$$\begin{aligned} \{b_i, b_j^\dagger\} &= \delta_{ij} \\ \{b_i, b_j\} &= \{b_i^\dagger, b_j^\dagger\} = 0. \end{aligned} \tag{A.3}$$

These new particles, or *quasi-particles*, are still fermions, but they are now called *particles* for above, and *holes* for below the Fermi surface. The ground state for the particles is the “vacuum” state for the quasi-particles. To understand the meaning of the minus sign in the transformation consider a single particle operator (which can be, for example, a background potential):

$$H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \tag{A.4}$$

In quasi-particle representation, we write

$$\begin{aligned} H &= \sum_m \epsilon_m b_m^{\dagger} b_m + \sum_i \epsilon_i b_i b_i^{\dagger} \\ &= \sum_m \epsilon_m b_m^{\dagger} b_m - \sum_i \epsilon_i b_i^{\dagger} b_i + \sum_i \epsilon_i \end{aligned} \tag{A.5}$$

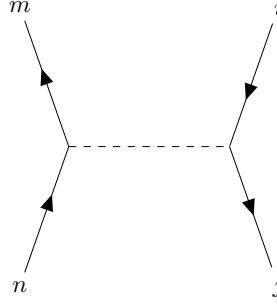


Figure A.1: Graphical representation of the interaction in (A.6)

so that, counting relative to the Fermi surface, the particle states refer to additive ϵ_m , while the hole states refer to subtractive ϵ_i , and there is a constant energy attached to the Hamiltonian given by the filled Fermi sea.

A two body interaction which couples particles and holes will have a different form with respect to the quasi-particles space. For example, the matrix element for the interaction which characterize the A matrix comes from the operator:

$$V = v_{mjin} a_m^\dagger a_j^\dagger a_n a_i \quad (\text{A.6})$$

In quasi-particle representation, we have:

$$V = v_{mjin} b_m^\dagger b_i^\dagger b_j b_n \quad (\text{A.7})$$

In a graphic representation of the interaction, particle lines are represented as directed lines, while hole lines are represented by downward-directed line. If we imagine a time scale perpendicular to the line denoting the interaction, the quasi-particles which are created by the interaction must stay on the top of the representation, while the destroyed quasi-particles stay below the interaction. In Fig. A.1 the graphical representation of the operator (A.7) is shown. This representation also illustrates the nature of the hole in switching sides of a matrix element when one use transformed operators.

Appendix B

QBA and SRPA

In this Appendix we want to describe in more detail the approximations used in RPA and SRPA theories to calculate the commutators present in the equations. We would like to provide a clear view on which terms are lost when switching to the HF ground state in the equations of motions.

Let us begin with the quasi-boson approximation given in (1.48). Using fermion commutation relations, the commutator of two one-body operators reads

$$[a_i^\dagger a_m, a_n^\dagger a_j] = \delta_{ij} \delta_{mn} - a_j a_i^\dagger \delta_{mn} - a_n^\dagger a_m \delta_{ij}. \quad (\text{B.1})$$

Consequently, the expectation value in the RPA ground state is

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{RPA} \rangle &= \delta_{ij} \delta_{mn} - \langle \text{RPA} | a_j a_i^\dagger | \text{RPA} \rangle \delta_{mn} \\ &\quad - \langle \text{RPA} | a_n^\dagger a_m | \text{RPA} \rangle \delta_{ij}. \end{aligned} \quad (\text{B.2})$$

The approximation which is done in RPA consists in taking the expectation value in the HF ground state. Due to the form of this state and the Pauli principle, we get

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{RPA} \rangle &\approx \langle \text{HF} | [a_i^\dagger a_m, a_n^\dagger a_j] | \text{HF} \rangle \\ &= \delta_{ij} \delta_{mn}. \end{aligned} \quad (\text{B.3})$$

Taking the HF expectation value instead of the RPA state is equivalent to approximate the one-body operators to boson operators. Indeed, each fermion pair operator $a_m^\dagger a_i$ can be expanded as a series of boson operators. This procedure is well described in [1]. The approximation we make consists in retaining the first term of the series. We define

$$\begin{aligned} B_{mi}^\dagger &= a_m^\dagger a_i \\ B_{mi} &= a_i^\dagger a_m, \end{aligned} \quad (\text{B.4})$$

where B is taken to satisfy boson commutation relations:

$$\begin{aligned} [B_{mi}, B_{nj}^\dagger] &= \delta_{mn} \delta_{ij} \\ [B_{mi}, B_{nj}] &= [B_{mi}^\dagger, B_{nj}^\dagger] = 0. \end{aligned} \quad (\text{B.5})$$

The expectation value in the RPA ground state is thus:

$$\langle \text{RPA} | [B_{mi}, B_{nj}^\dagger] | \text{RPA} \rangle = \delta_{ij} \delta_{mn}, \quad (\text{B.6})$$

which is equivalent if calculated in HF ground state. In RPA, the QBA is valid when the coefficients X are of the same order of magnitude, that is when the excitation is collective: in this case each single 1p-1h excitations have a small probability of being excited, and the violation of Pauli principle which follow from the approximation can be neglected [1].

In SRPA, we have to deal with the commutators of two-body operators. Using fermion commutation relations we get the following result:

$$\begin{aligned} [a_i^\dagger a_j^\dagger a_m a_n, a_p^\dagger a_q^\dagger a_k a_l] = & a(kl)a(pq)\delta_{il}\delta_{jk}\delta_{mq}\delta_{np} + \\ & + a(mn) \left(\delta_{np}\delta_{mq}\delta_{ik}a_l a_j^\dagger + \delta_{mp}\delta_{nq}\delta_{jk}a_l a_i^\dagger + \delta_{np}\delta_{mq}a_k a_i^\dagger a_j^\dagger a_l \right) \\ & + a(pq) \left(a_i^\dagger a_j^\dagger a_p^\dagger a_m a_k a_l \delta_{nq} + a_i^\dagger a_j^\dagger a_q^\dagger a_k a_l a_n \delta_{mn} \right) \\ & + a(ij) \left(a_p^\dagger a_q^\dagger a_i^\dagger a_l a_m a_n \delta_{jk} + a_p^\dagger a_q^\dagger a_k a_i^\dagger a_m a_n \delta_{jl} \right) \end{aligned} \quad (\text{B.7})$$

The approximation made in SRPA is to take the expectation value in the HF state. As can be seen, all the terms vanishes except for the first one:

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_j^\dagger a_m a_n, a_p^\dagger a_q^\dagger a_k a_l] | \text{RPA} \rangle & \approx \langle \text{HF} | [a_i^\dagger a_j^\dagger a_m a_n, a_p^\dagger a_q^\dagger a_k a_l] | \text{HF} \rangle \\ & = a(kl)a(pq)\delta_{il}\delta_{jk}\delta_{mq}\delta_{np} \end{aligned} \quad (\text{B.8})$$

As we did before, we can write the two-body operators appearing inside the commutator as the product of two boson operators. Nevertheless, the commutator of four boson operators gives only terms containing at most two boson operators. It follows that this is not the QBA approximation, since ¹:

$$\langle \text{RPA} | [B_{mi} B_{nj}, B_{pk}^\dagger B_{ql}^\dagger] | \text{RPA} \rangle \neq \langle \text{HF} | [B_{mi} B_{nj}, B_{pk}^\dagger B_{ql}^\dagger] | \text{HF} \rangle. \quad (\text{B.9})$$

¹To obtain QBA in SRPA one might need to extend the definition of B to higher terms of the boson expansion. This has not be checked here.

Appendix C

Details on the calculations of the matrix elements

C.1 LMG Hamiltonian

We start from HF Hamiltonian (2.23), which is obtained by a unitary transformation of the operator that appear in the LMG Hamiltonian

$$\begin{aligned} \tilde{H} = & \frac{\epsilon}{2} \left[2 \cos \alpha \tilde{K}_0 + \sin \alpha (\tilde{K}_+ + \tilde{K}_-) \right] + \frac{W}{2} \left[\tilde{K}_+^2 + \tilde{K}_-^2 - \{\tilde{K}_+, \tilde{K}_-\} \right] \\ & - \frac{V+W}{4} \left[\sin^2 \alpha \left(4\tilde{K}_0^2 - \{\tilde{K}_+, \tilde{K}_-\} \right) - \sin 2\alpha \left(\{\tilde{K}_0, \tilde{K}_+\} + \{\tilde{K}_0, \tilde{K}_-\} \right) \right. \\ & \left. + (1 + \cos^2 \alpha)(\tilde{K}_+^2 + \tilde{K}_-^2) \right] \end{aligned} \quad (\text{C.1})$$

In our model, the HF ground state is the state where all the particles stay in the lower level. Using the angular momentum basis, the ground state correspond to (2.24):

$$|\text{HF}\rangle = |N/2, -N/2\rangle, \quad (\text{C.2})$$

The action of the operators involved in the Hamiltonian follows from the usual angular momentum relations (2.13), and are written in (2.25). In the following, we will need to evaluate these operators with states obtained by *ph* production. Using the angular momentum relations, we find

$$\begin{aligned} K_0 |N/2, -N/2 + 1\rangle &= \left(-\frac{N}{2} + 1 \right) |N/2, -N/2 + 1\rangle \\ K_+ |N/2, -N/2 + 1\rangle &= \sqrt{2(N-1)} |N/2, -N/2 + 2\rangle \\ K_- |N/2, -N/2 + 2\rangle &= \sqrt{2(N-1)} |N/2, -N/2 + 1\rangle \\ K_0 |N/2, -N/2 + 2\rangle &= \left(-\frac{N}{2} + 2 \right) |N/2, -N/2 + 2\rangle \\ K_+ |N/2, -N/2 + 2\rangle &= \sqrt{3(N-2)} |N/2, -N/2 + 3\rangle \\ K_- |N/2, -N/2 + 3\rangle &= \sqrt{3(N-2)} |N/2, -N/2 + 2\rangle. \end{aligned} \quad (\text{C.3})$$

Calculation of RPA matrices

We start with the calculation of the matrix elements appearing within RPA equations. The results of these calculations can also be found in [13].

$$A_{1,1} = \frac{\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle}{N}. \quad (\text{C.4})$$

Many terms of the Hamiltonian don't contribute to the expectation value with respect to the HF ground state. For this reason, we are left with the effective Hamiltonian

$$H_{\text{eff}} = \epsilon \cos \alpha K_0 - \frac{W}{2} \{K_+, K_-\} - \frac{V+W}{4} \sin^2 \alpha (4K_0^2 - \{K_+, K_-\}). \quad (\text{C.5})$$

Let's consider separately the contributions of the operators inside the effective Hamiltonian to the expectation value in the numerator:

$$\begin{aligned} \langle \text{HF} | [K_-, [K_0, K_+]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_0 K_+ - K_+ K_0] | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_0 K_+ - K_- K_+ K_0 | \text{HF} \rangle \\ &= N. \end{aligned} \quad (\text{C.6})$$

$$\begin{aligned} \langle \text{HF} | [K_-, [\{K_+, K_-\}, K_+]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_+ K_- K_+ + K_- K_+ K_+ - K_+ K_- K_+] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_+^2 | \text{HF} \rangle \\ &= 2N(N-1). \end{aligned} \quad (\text{C.7})$$

$$\begin{aligned} \langle \text{HF} | [K_-, [K_0^2, K_+]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_0^2 K_+ - K_+ K_0^2] | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_0^2 K_+ - K_- K_+ K_0^2 | \text{HF} \rangle \\ &= N(-N+1). \end{aligned} \quad (\text{C.8})$$

Using the definition of the potential v and w as in (2.17) we get the expectation value:

$$\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle = \epsilon N \left(\cos \alpha - w + \frac{3}{2}(v+w) \sin^2 \alpha \right), \quad (\text{C.9})$$

By which we get the RPA A matrix element:

$$A_{1,1} = \epsilon \left(\cos \alpha - w + \frac{3}{2}(v+w) \sin^2 \alpha \right). \quad (\text{C.10})$$

We consider now

$$B_{1,1} = -\frac{\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle}{N} \quad (\text{C.11})$$

Again, we are left with the effective Hamiltonian

$$H_{\text{eff}} = \left(\frac{W}{2} - \frac{V+W}{4} (1 + \cos^2 \alpha) \right) K_+^2. \quad (\text{C.12})$$

The contribution of the operator K_+^2 to the expectation value is

$$\begin{aligned}\langle \text{HF} | [K_-, [K_+^2, K_-]] | \text{HF} \rangle &= -\langle \text{HF} | [K_-, K_- K_+^2] | \text{HF} \rangle \\ &= -\langle \text{HF} | K_-^2 K_+^2 | \text{HF} \rangle \\ &= -2N(N-1).\end{aligned}\tag{C.13}$$

Using the definition of the potential v and w as in (2.17) we get:

$$\langle \text{HF} | [K_-, [H, K_-]] | \text{HF} \rangle = -\epsilon N \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right).\tag{C.14}$$

By which we get the RPA B matrix element:

$$B_{1,1} = \epsilon \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right).\tag{C.15}$$

Calculation of SRPA matrices

Calculation of $A_{1,2}$

$$A_{1,2} = \frac{\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle}{N\sqrt{2(N-1)}}\tag{C.16}$$

As before, we are left with the effective Hamiltonian

$$H_{\text{eff}} = \frac{\epsilon}{2} \sin \alpha K_- + \frac{V+W}{4} \sin 2\alpha \{K_0, K_-\}.\tag{C.17}$$

We consider separately the contributions of operators K_- and $\{K_0, K_-\}$ to the expectation value:

$$\begin{aligned}\langle \text{HF} | [K_-, [K_-, K_+^2]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_- K_+^2 - K_+^2 K_-] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_+^2 | \text{HF} \rangle \\ &= 2N(N-1).\end{aligned}\tag{C.18}$$

$$\begin{aligned}\langle \text{HF} | [K_-, [\{K_0, K_-\}, K_+^2]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_0 K_- K_+^2 + K_- K_0 K_+^2] | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_0 K_- K_+^2 + K_-^2 K_0 K_+^2 | \text{HF} \rangle \\ &= -2N(N-1)(N-3).\end{aligned}\tag{C.19}$$

Using the definition of the potential v and w as in (2.17) we get:

$$\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle = \epsilon N \sin \alpha (N-1 - (v+w) \cos \alpha (N-3)).\tag{C.20}$$

By which we get the matrix element:

$$A_{1,2} = \frac{\epsilon \sin \alpha}{\sqrt{2(N-1)}} (N-1 - (v+w) \cos \alpha (N-3)).\tag{C.21}$$

Calculation of $A_{2,1}$

$$A_{2,1} = \frac{\langle \text{HF} | [K_-^2, [H, K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} \quad (\text{C.22})$$

As before, we are left with the effective Hamiltonian

$$H_{\text{eff}} = \frac{\epsilon}{2} \sin \alpha K_+ + \frac{V+W}{4} \sin 2\alpha \{K_0, K_+\}. \quad (\text{C.23})$$

We consider separately the contributions of operators K_+ and $\{K_0, K_+\}$ to the expectation value:

$$\langle \text{HF} | [K_-^2, [K_+, K_+]] | \text{HF} \rangle = 0, \quad (\text{C.24})$$

and

$$\begin{aligned} \langle \text{HF} | [K_-^2, [\{K_0, K_+\}, K_+]] | \text{HF} \rangle &= \langle \text{HF} | [K_-^2, [K_0 K_+ + K_+ K_0, K_+]] | \text{HF} \rangle \\ &= \langle \text{HF} | [K_-^2, K_0 K_+^2 + K_+ K_0 K_+ \\ &\quad - K_+ K_0 K_+ - K_+ K_+ K_0] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_0 K_+^2 + K_-^2 K_+ K_0 K_+ \\ &\quad - K_-^2 K_+ K_0 K_+ - K_-^2 K_+^2 K_0 | \text{HF} \rangle \\ &= 4N(N-1) \end{aligned} \quad (\text{C.25})$$

Using the definition of the potential v and w as in (2.17) we get:

$$\langle \text{HF} | [K_-^2, [H, K_+]] | \text{HF} \rangle = \epsilon N 2(v+w) \cos \alpha \sin \alpha. \quad (\text{C.26})$$

By which we get the matrix element:

$$A_{2,1} = \frac{\epsilon}{\sqrt{2(N-1)}} 2(v+w) \cos \alpha \sin \alpha. \quad (\text{C.27})$$

As can be seen, in principle $A_{2,1} \neq A_{1,2}$. Nevertheless, when using α_{HF} , the two expression became equivalent, so that hermiticity of the SRPA equation is preserved.

Calculation of $A_{2,2}$

$$A_{2,2} = \frac{\langle \text{HF} | [K_-^2, [H, K_+^2]] | \text{HF} \rangle}{2N(N-1)} \quad (\text{C.28})$$

The effective Hamiltonian is now

$$H_{\text{eff}} = \epsilon \cos \alpha K_0 - \frac{W}{2} \{K_+, K_-\} - \frac{V+W}{4} \sin^2 \alpha (4K_0^2 - \{K_+, K_-\}). \quad (\text{C.29})$$

Let's consider again separately the various contributions to the expectation value of the numerator:

$$\begin{aligned}\langle \text{HF} | [K_-^2, [K_0, K_+^2]] | \text{HF} \rangle &= \langle \text{HF} | [K_-^2, K_0 K_+^2 - K_+^2 K_0] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_0 K_+^2 - K_-^2 K_+^2 K_0 | \text{HF} \rangle \\ &= 4N(N-1).\end{aligned}\tag{C.30}$$

$$\begin{aligned}\langle \text{HF} | [K_-^2, [\{K_+ K_-\}, K_+^2]] | \text{HF} \rangle &= \langle \text{HF} | [K_-^2, [K_+ K_- + K_- K_+, K_+^2]] | \text{HF} \rangle \\ &= \langle \text{HF} | [K_-^2, K_+ K_- K_+^2 + K_- K_+^3 - K_+^2 K_- K_+] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_+ K_- K_+^2 + K_-^3 K_+^3 - K_-^2 K_+^2 K_- K_+ | \text{HF} \rangle \\ &= 8N(N-1)(N-2).\end{aligned}\tag{C.31}$$

$$\begin{aligned}\langle \text{HF} | [K_-^2, [K_0^2, K_+^2]] | \text{HF} \rangle &= \langle \text{HF} | [K_-^2, K_0^2 K_+^2 - K_+^2 K_0^2] | \text{HF} \rangle \\ &= \langle \text{HF} | K_-^2 K_0^2 K_+^2 - K_-^2 K_+^2 K_0^2 | \text{HF} \rangle \\ &= -4N(N-1)(N-2).\end{aligned}\tag{C.32}$$

Using the definition of the potential v and w as in (2.17) we get:

$$\langle \text{HF} | [K_-^2, [H, K_+^2]] | \text{HF} \rangle = \epsilon 2N (2 \cos \alpha (N-1) - 2w(N-2) + 3(v+w) \sin^2 \alpha (N-2))\tag{C.33}$$

By which we get the matrix element:

$$A_{2,2} = \frac{\epsilon}{N-1} (2 \cos \alpha (N-1) - 2w(N-2) + 3(v+w) \sin^2 \alpha (N-2))\tag{C.34}$$

C.2 Extended LMG Hamiltonian

The generalized HF LMG Hamiltonian reads:

$$\begin{aligned}\tilde{H} &= \frac{\epsilon}{2} \left[2 \cos \alpha \tilde{K}_0 + \sin \alpha (\tilde{K}_+ + \tilde{K}_-) \right] + \frac{W}{2} \left[\tilde{K}_+^2 + \tilde{K}_-^2 - \{\tilde{K}_+, \tilde{K}_-\} \right] \\ &\quad - \frac{V+W}{4} \left[\sin^2 \alpha (4\tilde{K}_0^2 - \{\tilde{K}_+, \tilde{K}_-\}) - \sin 2\alpha (\{\tilde{K}_0, \tilde{K}_+\} + \{\tilde{K}_0, \tilde{K}_-\}) \right. \\ &\quad \left. + (1 + \cos^2 \alpha)(\tilde{K}_+^2 + \tilde{K}_-^2) \right] - G \left(\cos \alpha (\tilde{K}_+ + \tilde{K}_-) - 2 \sin \alpha \tilde{K}_0 \right) (N-1)\end{aligned}\tag{C.35}$$

The Hamiltonian is equal to the old one except for the term:

$$H' = -G \left(\cos \alpha (\tilde{K}_+ + \tilde{K}_-) - 2 \sin \alpha \tilde{K}_0 \right) (N-1).\tag{C.36}$$

In order to correct the previous result of the LMG case, we only need to evaluate this term.

Calculation of $A_{1,1}$

We need to evaluate:

$$H'_{\text{eff}} = 2G(N-1)\sin\alpha K_0. \quad (\text{C.37})$$

Using the result of the previous section, we get:

$$\langle \text{HF} | [K_-, [H'_{\text{eff}}, K_+]] | \text{HF} \rangle = \epsilon 2Ng \sin\alpha \quad (\text{C.38})$$

So that the full expectation value results:

$$\langle \text{HF} | [K_-, [H, K_+]] | \text{HF} \rangle = \epsilon N \left(\cos\alpha - w + \frac{3}{2}(v+w)\sin^2\alpha + 2g\sin\alpha \right), \quad (\text{C.39})$$

and the matrix element is:

$$A_{1,1} = \epsilon \left(\cos\alpha - w + \frac{3}{2}(v+w)\sin^2\alpha + 2g\sin\alpha \right). \quad (\text{C.40})$$

Calculation of $A_{1,2}$

The effective Hamiltonian here results:

$$H'_{\text{eff}} = -G\cos\alpha(N-1)K_- \quad (\text{C.41})$$

Which gives

$$\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle = -\epsilon 2Ng\cos\alpha(N-1) \quad (\text{C.42})$$

So that the full expectation value results:

$$\begin{aligned} \langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle &= \epsilon N (\sin\alpha(N-1) - (v+w)\sin\alpha\cos\alpha(N-3) \\ &\quad - 2g\cos\alpha(N-1)). \end{aligned} \quad (\text{C.43})$$

So that the full matrix element results:

$$A_{1,2} = \frac{\epsilon}{\sqrt{2(N-1)}} (\sin\alpha(N-1) - (v+w)\sin\alpha\cos\alpha(N-3) - 2g\cos\alpha(N-1)) \quad (\text{C.44})$$

Calculation of $A_{2,1}$

The effective Hamiltonian here results:

$$H'_{\text{eff}} = -G\cos\alpha(N-1)K_+ \quad (\text{C.45})$$

Which gives

$$\langle \text{HF} | [K_-^2, [H'_{\text{eff}}, K_+^2]] | \text{HF} \rangle = 0. \quad (\text{C.46})$$

So that the full matrix element is the same as before, namely:

$$A_{2,1} = \frac{\epsilon}{\sqrt{2(N-1)}} 2(v+w)\cos\alpha\sin\alpha. \quad (\text{C.47})$$

Calculation of $A_{2,2}$

The effective Hamiltonian here results:

$$H'_{\text{eff}} = 2G \sin \alpha (N - 1) K_0 \quad (\text{C.48})$$

We need to calculate:

$$\langle \text{HF} | [K_-^2, [H'_{\text{eff}}, K_+^2]] | \text{HF} \rangle = \epsilon 8Ng \sin \alpha (N - 1) \quad (\text{C.49})$$

So that the full expectation value results:

$$\begin{aligned} \langle \text{HF} | [K_-^2, [H, K_+^2]] | \text{HF} \rangle &= \epsilon 2N (2 \cos \alpha (N - 1) - 2w(N - 2) + \\ &\quad 3(v + w) \sin^2 \alpha (N - 2) + 4g \sin \alpha (N - 1)) \end{aligned} \quad (\text{C.50})$$

So that the full matrix element results:

$$A_{2,2} = \frac{\epsilon}{N - 1} (2 \cos \alpha (N - 1) - 2w(N - 2) + 3(v + w) \sin^2 \alpha (N - 2) + 4g \sin \alpha (N - 1)) \quad (\text{C.51})$$

C.3 PVC matrix element calculation**Calculation of $A_{1,2}$**

$$\begin{aligned} A_{1,2} &= \frac{\langle \text{HF} | [K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | \text{HF} \rangle}{X \sqrt{2N(N - 1)}} \\ &= \frac{\langle \text{HF} | [K_-, [H, K_+^2]] | \text{HF} \rangle}{N \sqrt{2(N - 1)}} - \frac{Y \langle \text{HF} | [K_-, [H, K_+ K_-]] | \text{HF} \rangle}{X N \sqrt{2(N - 1)}} \end{aligned} \quad (\text{C.52})$$

The first term has already been evaluated in (C.43). For the second term, the effective Hamiltonian results:

$$H_{\text{eff}} = \left(\frac{\epsilon}{2} \sin \alpha - G \cos \alpha (N - 1) \right) K_+ + \frac{V + W}{4} \sin 2\alpha \{K_0, K_+\}. \quad (\text{C.53})$$

The contributions to the expectation value of the numerator are

$$\begin{aligned} \langle \text{HF} | [K_-, [K_+, K_+ K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_+^2 K_- - K_+ K_- K_+] | \text{HF} \rangle \\ &= - \langle \text{HF} | K_- K_+ K_- K_+ | \text{HF} \rangle \\ &= -N^2. \end{aligned} \quad (\text{C.54})$$

and

$$\begin{aligned} \langle \text{HF} | [K_-, [\{K_0, K_+\}, K_+ K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, [K_0 K_+ + K_+ K_0, K_+ K_-]] | \text{HF} \rangle \\ &= \langle \text{HF} | [K_-, K_0 K_+^2 K_- + K_+ K_0 K_+ K_- \\ &\quad - K_+ K_- K_0 K_+ - K_+ K_- K_+ K_0] | \text{HF} \rangle \\ &= - \langle \text{HF} | K_- K_+ K_- K_0 K_+ + K_- K_+ K_- K_+ K_0 | \text{HF} \rangle \\ &= N^2 (N - 1). \end{aligned} \quad (\text{C.55})$$

$$\langle \text{HF} | [K_-, [H, K_+ K_-]] | \text{HF} \rangle = \epsilon N^2 \left(-\frac{\sin \alpha}{2} (N-1) - \frac{v+w}{2} \sin \alpha \cos \alpha + g \cos \alpha \right). \quad (\text{C.56})$$

Coming back to the matrix element and inserting the definition of the potentials v , w and g , we get:

$$\begin{aligned} A_{1,2} = & \sqrt{\frac{1}{2(N-1)}} (\sin \alpha (N-1) - (v+w) \sin \alpha \cos \alpha (N-3) - 2g \cos \alpha (N-1)) + \\ & - \frac{Y}{2X\sqrt{2(N-1)}} N (-\sin \alpha (N-1) - (v+w) \sin \alpha \cos \alpha + 2g \cos \alpha). \end{aligned} \quad (\text{C.57})$$

Calculation of $A_{2,1}$

$$\begin{aligned} A_{2,1} &= \frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_+]] | \text{HF} \rangle}{X\sqrt{2N(N-1)}} \\ &= \frac{\langle \text{HF} | [K_-^2, [H, K_+]] | \text{HF} \rangle}{N\sqrt{2(N-1)}} - \frac{Y \langle \text{HF} | [K_+ K_-, [H, K_+]] | \text{HF} \rangle}{NX\sqrt{2(N-1)}} \end{aligned} \quad (\text{C.58})$$

The first term has already been evaluated in (C.26). For the second term, the effective Hamiltonian is:

$$H_{\text{eff}} = \left(\frac{\epsilon}{2} \sin \alpha - G \cos \alpha (N-1) \right) K_- + \frac{V+W}{4} \sin 2\alpha \{K_0, K_-\}. \quad (\text{C.59})$$

The contribution to the expectation value is

$$\langle \text{HF} | [K_+ K_-, [H, K_+]] | \text{HF} \rangle = 0. \quad (\text{C.60})$$

So that we are left with

$$A_{2,1} = \frac{\epsilon}{\sqrt{2(N-1)}} (v+w) \sin(2\alpha). \quad (\text{C.61})$$

Calculation of $A_{2,2}$

$$\begin{aligned} A_{2,2} &= \frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_+ Q_{\text{RPA}}^\dagger]] | \text{HF} \rangle}{2X^2(N-1)} \\ &= \frac{1}{2X^2N(N-1)} (X^2 \langle \text{HF} | [K_-^2, [H, K_+^2]] | \text{HF} \rangle \\ &\quad - XY \langle \text{HF} | [K_-^2, [H, K_+ K_-]] | \text{HF} \rangle \\ &\quad - YX \langle \text{HF} | [K_+ K_-, [H, K_+^2]] | \text{HF} \rangle \\ &\quad + Y^2 \langle \text{HF} | [K_+ K_-, [H, K_+ K_-]] | \text{HF} \rangle) \end{aligned} \quad (\text{C.62})$$

The first term has already been evaluated in (C.50). Since it's easy to demonstrate that

$$\begin{aligned}\langle \text{HF} | [K_+ K_-, [H, K_+^2]] | \text{HF} \rangle &= 0 \\ \langle \text{HF} | [K_+ K_-, [H, K_+ K_-]] | \text{HF} \rangle &= 0\end{aligned}\quad (\text{C.63})$$

So that we are left with

$$A_{2,2} = \frac{\langle \text{HF} | [K_-^2, [H, K_+^2]] | \text{HF} \rangle}{2N^2(N-1)} - \frac{Y \langle \text{HF} | [K_-^2, [H, K_+ K_-]] | \text{HF} \rangle}{2N^2 X(N-1)} \quad (\text{C.64})$$

For the second term, the effective Hamiltonian is

$$H_{\text{eff}} = \left(\frac{W}{2} - \frac{V+W}{4} (1 + \cos^2 \alpha) \right) K_+^2. \quad (\text{C.65})$$

The contribution to the expectation value is

$$\begin{aligned}\langle \text{HF} | [K_-^2, [K_+^2, K_+ K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_-^2, K_+^2 K_+ K_- - K_+ K_- K_+^2] | \text{HF} \rangle \\ &= -\langle \text{HF} | K_-^2 K_+ K_- K_+^2 | \text{HF} \rangle \\ &= -4N(N-1)^2\end{aligned}\quad (\text{C.66})$$

Using the definition of the potential v and w as in (2.17) we get:

$$\langle \text{HF} | [K_-^2, [H, K_+ K_-]] | \text{HF} \rangle = -\epsilon 2N(N-1) \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right) \quad (\text{C.67})$$

Coming back to the matrix element, we get:

$$\begin{aligned}A_{2,2} &= \epsilon \frac{1}{N-1} (2 \cos \alpha (N-1) - 2w(N-2) + 3(v+w) \sin^2 \alpha (N-2) + 4g \sin \alpha (N-1)) + \\ &\quad + \epsilon \frac{Y}{X} \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right)\end{aligned}\quad (\text{C.68})$$

Calculation of $B_{1,2}$

$$\begin{aligned}B_{1,2} &= -\frac{\langle \text{HF} | [K_-, [H, Q_{\text{RPA}} K_-]] | \text{HF} \rangle}{X \sqrt{2N(N-1)}} \\ &= \frac{Y \langle \text{HF} | [K_-, [H, K_+ K_-]] | \text{HF} \rangle}{NX \sqrt{2(N-1)}}\end{aligned}\quad (\text{C.69})$$

In this case, the effective Hamiltonian results:

$$H_{\text{eff}} = \left(\frac{\epsilon}{2} \sin \alpha - G \cos \alpha (N-1) \right) K_+ + \frac{V+W}{4} \sin 2\alpha \{K_0, K_+\}. \quad (\text{C.70})$$

The contributions to the expectation value of the numerator are

$$\begin{aligned}\langle \text{HF} | [K_-, [K_+, K_+ K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, K_+^2 K_- - K_+ K_- K_+] | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_+^2 K_- - K_- K_+ K_- K_+ | \text{HF} \rangle \\ &= -N^2.\end{aligned}\quad (\text{C.71})$$

and

$$\begin{aligned}\langle \text{HF} | [K_-, [\{K_0, K_+\}, K_+ K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_-, [K_0 K_+ + K_+ K_0, K_+ K_-]] | \text{HF} \rangle \\ &= \langle \text{HF} | [K_-, K_0 K_+ K_+ K_- + K_+ K_0 K_+ K_- \\ &\quad - K_+ K_- K_0 K_+ - K_+ K_- K_+ K_0] | \text{HF} \rangle \\ &= \langle \text{HF} | K_- K_0 K_+ K_+ K_- + K_- K_+ K_0 K_+ K_- \\ &\quad - K_- K_+ K_- K_0 K_+ - K_- K_+ K_- K_+ K_0 | \text{HF} \rangle \\ &= N^2(N-1).\end{aligned}\quad (\text{C.72})$$

The contribution to the expectation value with the definition of the potentials v , w and g is

$$\langle \text{HF} | [K_-, [H, K_+ K_-]] | \text{HF} \rangle = \epsilon \frac{N^2}{2} \left(-\sin \alpha + \frac{v+w}{2} \sin(2\alpha) + 2g \cos \alpha \right) \quad (\text{C.73})$$

Coming back to the matrix element, we get:

$$B_{1,2} = \frac{\epsilon Y}{2X \sqrt{2(N-1)}} N \left(-\sin \alpha + \frac{v+w}{2} \sin(2\alpha) + 2g \cos \alpha \right). \quad (\text{C.74})$$

Calculation of $B_{2,1}$

$$\begin{aligned}B_{2,1} &= -\frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, K_-]] | \text{HF} \rangle}{X \sqrt{2N(N-1)}} \\ &= \frac{Y \langle \text{HF} | [K_+ K_-, [H, K_-]] | \text{HF} \rangle}{NX \sqrt{2(N-1)}}\end{aligned}\quad (\text{C.75})$$

In this case, the effective Hamiltonian results:

$$H_{\text{eff}} = \left(\frac{\epsilon}{2} \sin \alpha - G \cos \alpha (N-1) \right) K_+ + \frac{V+W}{4} \sin 2\alpha \{K_0, K_+\}. \quad (\text{C.76})$$

The contributions to the expectation value of the numerator are

$$\begin{aligned}\langle \text{HF} | [K_+ K_-, [K_+, K_-]] | \text{HF} \rangle &= 2 \langle \text{HF} | [K_+ K_-, K_0] | \text{HF} \rangle \\ &= 0.\end{aligned}\quad (\text{C.77})$$

and

$$\begin{aligned}
\langle \text{HF} | [K_+ K_-, [\{K_0, K_+\}, K_-]] | \text{HF} \rangle &= \langle \text{HF} | [K_+ K_-, [K_0 K_+ + K_+ K_0, K_-]] | \text{HF} \rangle \\
&= \langle \text{HF} | [K_+ K_-, K_0 [K_+, K_-] + [K_+, K_-] K_0] | \text{HF} \rangle \\
&= 4 \langle \text{HF} | [K_+ K_-, K_0^2] | \text{HF} \rangle \\
&= 0.
\end{aligned} \tag{C.78}$$

We conclude that:

$$B_{2,1} = 0. \tag{C.79}$$

Calculation of $B_{2,2}$

$$\begin{aligned}
B_{1,2} &= -\frac{\langle \text{HF} | [Q_{\text{RPA}} K_-, [H, Q_{\text{RPA}} K_-]] | \text{HF} \rangle}{2X^2(N-1)} \\
&= -\frac{1}{2NX^2(N-1)} (X^2 \langle \text{HF} | [K_-^2, [H, K_-^2]] | \text{HF} \rangle \\
&\quad - XY \langle \text{HF} | [K_-^2, [H, K_+ K_-]] | \text{HF} \rangle \\
&\quad - YX \langle \text{HF} | [K_+ K_-, [H, K_-^2]] | \text{HF} \rangle \\
&\quad + Y^2 \langle \text{HF} | [K_+ K_-, [H, K_+ K_-]] | \text{HF} \rangle)
\end{aligned} \tag{C.80}$$

Since it's easy to demonstrate that

$$\begin{aligned}
\langle \text{HF} | [K_-^2, [H, K_-^2]] | \text{HF} \rangle &= 0 \\
\langle \text{HF} | [K_+ K_-, [H, K_-^2]] | \text{HF} \rangle &= 0 \\
\langle \text{HF} | [K_+ K_-, [H, K_+ K_-]] | \text{HF} \rangle &= 0
\end{aligned} \tag{C.81}$$

we are left with

$$B_{2,2} = \frac{Y}{2NX(N-1)} \langle \text{HF} | [K_-^2, [H, K_+ K_-]] | \text{HF} \rangle \tag{C.82}$$

The matrix element has already been evaluated in (C.67). So the matrix element is

$$B_{2,2} = -\epsilon \frac{Y}{X} \left(w - \frac{v+w}{2} (1 + \cos^2 \alpha) \right) \tag{C.83}$$

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