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Approach to the Nuclear Many-Body Problem by Variationally Determined Transformation. II

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We present a generalization of the Hartree-Fock (HF) method incorporating two-body correlations. The correlations are introduced by means of a unitary operator e^{iF}, where F is a Hermitian one- and two-body operator to be determined by the variational principle. Assuming that the matrix elements of F are small so that powers of F higher than the second may be neglected, a set of linear equations determining F is obtained. The relation between our method and methods used to treat singular interactions is discussed. The method is applied to two recently suggested models and is compared with the HF method, second-order perturbation theory, and with the random-phase approximation. It is found that our method yields very good results within the range of validity of our approximations, which seems to call forth applications to more realistic problems. Possible applications to the study of collective phenomena in nuclei are indicated.

I. INTRODUCTION

In a previous introductory note some features of a new approximate treatment of the nuclear many-body problem were sketched.[1] In the present paper we would like
(a) to present and discuss this method in more detail;
(b) to present results of its application to two models which are more complicated and (hopefully) more realistic than the model employed in I;
(c) to comment on further possible applications of the method, particularly in regard to the study of collective phenomena in nuclei.

The nuclear Hamiltonian, being a Hermitian operator, may be diagonalized by a unitary transformation. This unitary transformation may be represented by the unitary operator e^{iF}, where F is a Hermitian many-body operator. In Sec. II we start by considering the Hartree-Fock (HF) method as a particular scheme for an approximate calculation of the operator F. The main virtue of these considerations is that this form of the HF method readily suggests both a generalization and a further approximation. These form the main subjects of that section. Our method is essentially based on the assumption that the interaction is nonsingular. At the end of Sec. II we discuss the relationship of our approach to methods used in treating singular interactions. It is seen that despite some outward formal similarities, the methods are basically different. The source of the difference lies (of course) in the different assumptions made about the interaction. The application of the method to two solvable models is dealt with in Sec. III. Both models may be regarded as generalizations of the two-level Lipkin model considered in I. One of them is a two-level model due to Abecasis, Faessler, and Plastino (AFP),[2] which has a nontrivial HF solution for any values of its parameters. The other model is a three-level model proposed by Li, Klein, and Dreizler (LKD)[3,4] (this model has nontrivial HF solutions only in the "strong-coupling" case, which is not considered in the present paper). The results of our approach are compared with the exact ones and with those of standard approximations, viz., the HF method, the random-phase approximation (RPA), and second-order perturbation theory. We regard these applications as an intermediate stage between the testing of the method by the Lipkin model[1] and the two-level pairing model[5] and an application to real nuclei. Indeed, the results obtained so far (in Refs. 1 and 5 and in the present paper) seem to warrant the application of the method to realistic problems, especially along the lines to be suggested in Sec. IV. The applications of the method to the solvable models suggest possible simplifications and variations of the method, which may be particularly suitable to treating collective phenomena in nuclei. These possibilities are discussed in the last section.

II. GENERALIZATION OF THE HARTREE-FOCK METHOD

We study an N-fermion system with a Hamiltonian H,

$$H=\sum_{\alpha\beta} t_{\alpha\beta}a_\alpha^\dagger a_\beta+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta} V^a_{\alpha\beta,\gamma\delta}a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma\,. \tag{2.1}$$

Here, $a_\alpha^\dagger$ is a creation operator for a single-fermion state, the index α represents all the relevant quantum numbers, and $V^a_{\alpha\beta\gamma\delta}$ is the antisymmetrized matrix element of the interaction. Let us start by a brief review of the HF method in a formulation which most naturally leads to our generalization. The HF method (see, e.g., the work of Villars[6] for a detailed discussion) is a variational principle for the determination of the best single-particle wave functions. Let the set $\{A_\alpha^\dagger\}$ represent single-particle creation operators which are a solution of the HF problem, and let $|\chi_0\rangle$ be the corresponding HF ground state, i.e.,

$$|\chi_0\rangle=\prod_{\mu=1}^{N} A_\mu^\dagger|0\rangle\,. \tag{2.2}$$

The variational principle applied to $|\chi_0\rangle$ leads immediately (see Ref. 6) to the "Brillouin condition" and to the HF equation, which is a nonlinear equation determining the set $\{A_\alpha^\dagger\}$. However, we may adopt a slightly different point of view.[7] Let $|\Phi_0\rangle$ be the Slater determinant representing the unperturbed ground state, i.e.,[8]

$$|\Phi_0\rangle=\prod_{\mu=1}^{N} a_\mu^\dagger|0\rangle\,. \tag{2.3}$$

The two single-particle sets $\{A_\alpha^\dagger\}$ and $\{a_\alpha^\dagger\}$ are related through a unitary transformation

$$A_\alpha^\dagger=e^{iF}a_\alpha^\dagger e^{-iF}\,, \tag{2.4}$$

and the two approximate ground states $|\Phi_0\rangle$ and $|\chi_0\rangle$ are related through

$$|\chi_0\rangle=e^{iF}|\Phi_0\rangle\,, \tag{2.5}$$

where F is a Hermitian single-particle operator. In general, the Hamiltonian may be diagonalized by a unitary transformation e^{iK} and the real ground state is related to $|\Phi_0\rangle$ by an equation similar to (2.5), where K is a Hermitian many-body operator. In the HF approach, one restricts K to be a single-particle operator, and a solution of the HF problem is equivalent to the determination of F [Eqs. (2.4), (2.5)] from the variational principle

$$\delta\langle\chi_0|H|\chi_0\rangle=\delta\langle\Phi_0|e^{-iF}He^{iF}|\Phi_0\rangle=0\,. \tag{2.6}$$

Obviously, the variation in Eq. (2.6) is with respect to the matrix elements of F, and, in general, it leads to a set of nonlinear equations (of infinite order) for these matrix elements. In this respect, this point of view of the HF method seems to be of no use as a means to an exact solution of the HF equation. However, this point of view does suggest a possible approximate solution of the equation for F. Suppose that the initial set $\{a_\alpha^\dagger\}$ is not too bad an approximation to the set $\{A_\alpha^\dagger\}$, and especially that $|\Phi_0\rangle$ is not too bad an approximation to $|\chi_0\rangle$. Under these assumptions it seems plausible that the matrix elements of F are small so that higher powers of F than the second may be neglected. Writing

$$F=\sum_{\sigma\mu} f_{\sigma\mu}a_\sigma^\dagger a_\mu+\text{H.c.}\,, \tag{2.7}$$

expanding $\langle\Phi_0|e^{-iF}He^{iF}|\Phi_0\rangle$ up to second order in F, and carrying out the variation, one obtains a set of linear equations for the matrix elements of F.[7]

Now, the above form of the HF problem suggests an obvious generalization incorporating two-body correlations. In analogy to Eq. (2.4), let us now introduce new fermion operators $b_\alpha^\dagger$ via the unitary transformation

$$b_\alpha^\dagger=e^{iF}a_\alpha^\dagger e^{-iF}\,, \tag{2.8}$$

where now F is a one- and *two*-body Hermitian operator

$$F=\sum_{\sigma\mu} f_{\sigma\mu}a_\sigma^\dagger a_\mu+\sum_{\sigma\tau\mu\nu} f_{\sigma\tau,\mu\nu}a_\sigma^\dagger a_\tau^\dagger a_\mu a_\nu+\text{H.c.} \tag{2.9}$$

Formally, the $b^\dagger$ operators behave as single-particle fermion operators and, again in analogy to the HF problem, we may use the variational principle to determine the best ground state $|\psi_0\rangle$ which is a Slater determinant of the $b^\dagger$'s, i.e., it has the form

$$|\psi_0\rangle=\prod_{\mu=1}^{N} b_\mu^\dagger|0\rangle\,. \tag{2.10}$$

Obviously, $|\psi_0\rangle$ is related to the unperturbed ground state $|\Phi_0\rangle$ through

$$|\psi_0\rangle=e^{iF}|\Phi_0\rangle\,, \tag{2.11}$$

and the variational principle now consists in minimizing

$$E_g(F)\equiv\langle\psi_0|H|\psi_0\rangle=\langle\Phi_0|e^{-iF}He^{iF}|\Phi_0\rangle \tag{2.12}$$

with respect to the independent variational parameters $f_{\sigma\mu}$, $f_{\sigma\tau,\mu\nu}$, $f^*_{\sigma\mu}$, and $f^*_{\sigma\tau,\mu\nu}$. Clearly, this operator F [Eq. (2.9)] is expected to be a much better approximation to the operator K, which was mentioned previously, than the operator F [Eq. (2.7)] of the HF problem, and we expect the states formed by the $b^\dagger$ operators to be a much better approximation to the exact eigenstates of the system than the HF states. Of course, since F is determined from the variational principle for the

ground state, we may expect an improved description mostly for the low-lying states.

However, all these expectations depend to a large extent on the possibility of solving the variational problem exactly. But, even more than in the HF case, carrying out the exact variation of Eq. (2.12) to all orders in F will not yield any tractable set of equations. Still, in analogy to the approximate treatment of the HF problem,[7] we may attempt an approximate treatment of the variational problem. Let us note that within the framework of the shell model, the low-lying unperturbed states usually furnish a rather satisfactory description of the single-particle properties of nuclei, and this is especially true for the shell-model ground state. In addition, the single-particle shell-model Hamiltonian with a residual (rather weak) interaction is successful even at explaining collective phenomena in nuclei.[9] Under these circumstances it seems reasonable to assume (cf. the work of da Providência[10]) that the matrix elements $f_{\sigma\mu}$ and $f_{\sigma\tau,\mu\nu}$ are small enough so that an expansion in powers of F may be terminated after the second power. The validity of this assumption and of the whole approach should, of course, be checked separately for every case to be considered. But, at least the *internal consistency* of our method is easily checked, since once we have solved the equations determining F we can immediately observe whether our assumption comes true and the matrix elements of F are indeed small.

Let us now return to the problem of the variation of Eq. (2.12). Up to second order in F, the expression to be varied reads

$$E_g(F)=\langle\Phi_0|H|\Phi_0\rangle+i\langle\Phi_0|[H,F]|\Phi_0\rangle +\tfrac{1}{2}i^2\langle\Phi_0|[[H,F],F]|\Phi_0\rangle\,. \tag{2.13}$$

Before proceeding further, we find it convenient to introduce a more compact notation (cf. the work of Rowe[11]). This will facilitate both the writing of the set of equations obtained from the variation and the discussion in Sec. IV. Denote the set of one- and two-body operators $\{a_\sigma^\dagger a_\mu,\ a_\sigma^\dagger a_\tau^\dagger a_\mu a_\nu\}$ by the set $\{A_i^\dagger\}$, and denote the set of matrix elements $\{f_{\sigma\mu}, f_{\sigma\tau,\mu\nu}\}$ by $\{f_i\}$. In this notation the operator F reads

$$F=\sum_i f_i A_i^\dagger+\text{H.c.} \tag{2.14}$$

Define now the matrices k and w as follows:

$$k_{ij}\equiv\tfrac{1}{2}(\langle\Phi_0|[A_i,[H,A_j^\dagger]]|\Phi_0\rangle+\langle\Phi_0|[[A_i,H],A_j^\dagger]|\Phi_0\rangle), \tag{2.15}$$

$$w_{ij}\equiv\tfrac{1}{2}(\langle\Phi_0|[A_i,[A_j,H]]|\Phi_0\rangle+\langle\Phi_0|[[H,A_i],A_j]|\Phi_0\rangle)\,. \tag{2.16}$$

Also define[12]

$$V_i\equiv\langle\Phi_0|[H,A_i]|\Phi_0\rangle\,. \tag{2.17}$$

Using the above definitions, the set of equations obtained after varying Eq. (2.13) with respect to the f's and f^*'s reads

$$\begin{pmatrix}k & w\\ w^* & k^*\end{pmatrix}\begin{pmatrix}f\\ -f^*\end{pmatrix}=-i\begin{pmatrix}V\\ V^*\end{pmatrix}. \tag{2.18}$$

From Eq. (2.18) it is clear that for the case when the residual interaction is not too strong, the assumption that the matrix elements of F are small is likely to be valid.

Once the equations determining F have been solved, we may follow either of two possibilities which are completely equivalent. One possibility is as follows: The transformation (2.8) can be inverted to yield the $a^\dagger$'s in terms of the $b^\dagger$'s,

$$a_\alpha^\dagger=e^{-iF}b_\alpha^\dagger e^{iF}\,. \tag{2.19}$$

It is easily verified that in terms of the b operators F reads[13]

$$F=\sum_{\sigma\mu}f_{\sigma\mu}b_\sigma^\dagger b_\mu+\sum_{\sigma\tau\mu\nu}f_{\sigma\tau,\mu\nu}b_\sigma^\dagger b_\tau^\dagger b_\mu b_\nu+\text{H.c.} \tag{2.20}$$

Using Eqs. (2.19) and (2.20) we can express H in terms of the $b^\dagger$ operators, and the $b^\dagger$'s now play the role of single-particle creation operators, completely similar to the role of the $A_\alpha^\dagger$'s (representing the solution of the HF problem) in HF theory. Since the operator F defining the $b^\dagger$ operators [Eq. (2.8)] includes a genuinely essential two-body part (whereas, in the HF case F is strictly a single-particle operator), it is obvious that H expressed by means of the b operators is a many-body operator (while in the HF case expressing H in terms of the A_α's leaves us again with a two-body operator). This drawback is offset by the fact that as a consequence of our fundamental assumption we ought to express H in terms of the b's only up to second order in F, and this means that the expression of H in terms of the b's is at the most a four-body operator. The second possibility[14] is, once we have obtained F, to use (as in I) the unitary operator e^{iF} to define a new Hamiltonian H':

$$H'\equiv e^{-iF}He^{iF}\,, \tag{2.21}$$

which has, of course, the same spectrum as H and its eigenfunctions are related to those of H via the transformation e^{iF}. To the extent that we have succeeded in including in F important two-body correlations, these very same correlations will be absent in H' and, to that extent, H' describes "dressed particles" interacting more weakly than the "bare particles" described by H.[15] The unperturbed states corresponding to these "dressed par-

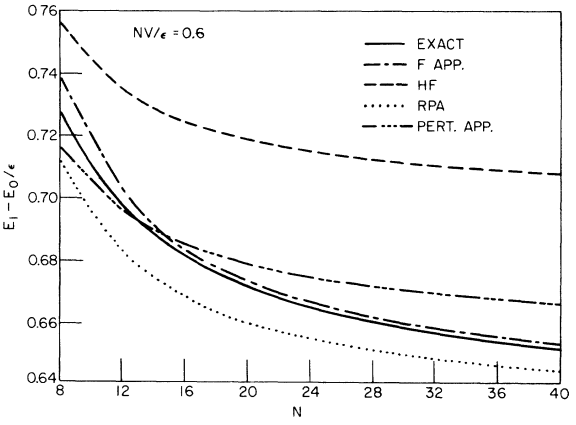

FIG. 1. Comparison of exact and approximate results for the AFP model. Excitation energy of the first excited state versus the number of particles for a fixed interaction strength $NV/\epsilon = 0.6$. (The results of our approximation are denoted by F.)

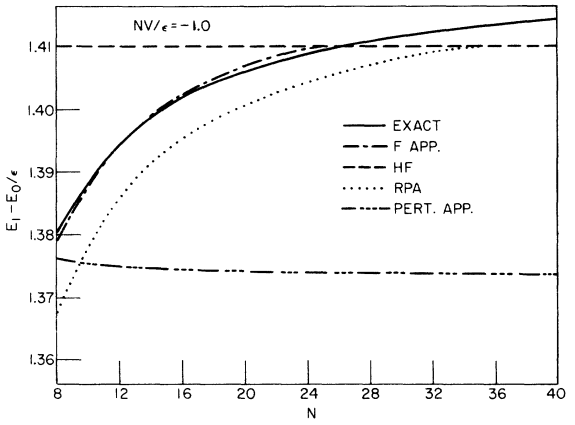

FIG. 3. The same as Fig. 1 for fixed interaction strength $NV/\epsilon = -1.0$ (for $N > 24$ the F approximation practically coincides with the HF approximation).

ticles" are expected to be a better zero-order description of the system than the corresponding states of the "bare particles" and in the same vein it is expected that any approximation method which could have been applied to H would yield even better results when applied to H'. In practice, we hope that already the diagonal matrix elements of H' (i.e., first-order perturbation theory applied to H') are sufficient to provide a rather accurate description of the low-lying energy levels of the system.

At this point, it seems worthwhile to comment on the relation between our method and methods devised to cope with singular interactions. Our method is appropriate for dealing with relatively weak interactions. This is indeed the case when one considers the shell-model Hamiltonian with a residual interaction, and the usual microscopic descriptions of collective states in nuclei are based on this kind of Hamiltonian.[9,16] On the other hand, the interaction between free nucleons (as determined from nucleon-nucleon scattering) is usually considered to include a short-range hard-core component. Methods which are suitable to deal with a weak long-range force[17] seem by their very nature to be unfit for dealing with strong short-range forces, and vice versa. Indeed, in terms of Feynman diagrams one deals with a weak long-range force by summing diagrams which differ in the number of interacting particles they contain, while the case of short-range forces is treated by summing diagrams grouped together according to the number of interacting particles they contain. In the latter case, in any given term the significant factor is the number of interacting particles rather than the number of interactions.[18] This means that the theory for dealing with strong

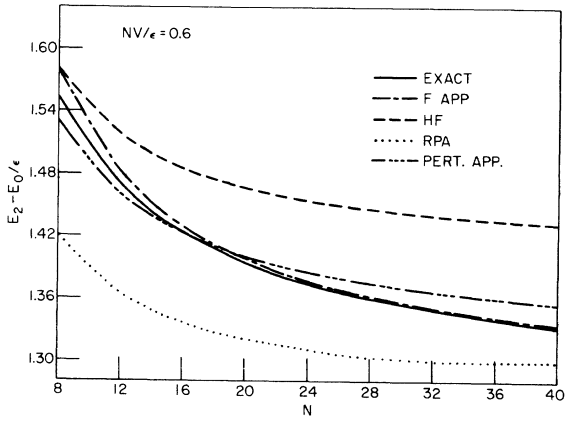

FIG. 2. The same as Fig. 1 for the excitation energy of the second excited state.

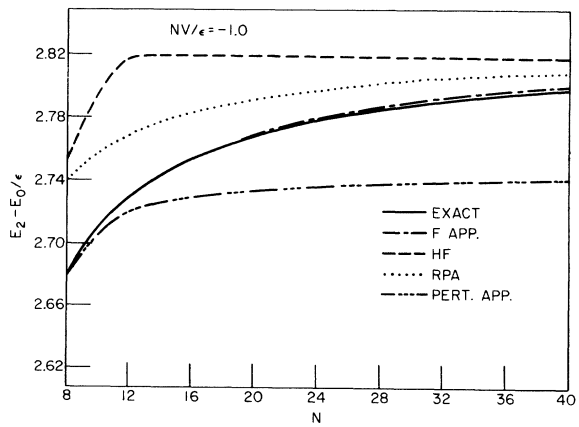

FIG. 4. The same as Fig. 3 for the excitation energy of the second excited state.

short-range correlations is essentially a cluster theory,[18] and indeed the more recent developments of the Brueckner method (see, e.g., Refs. 9 and 18), as well as the Jastrow method[19] and the Villar's unitary-model-operator approach,[6,20,21] all resort to some version of a cluster expansion.

To see how the different assumptions concerning the nature of the interaction lead to different formalisms, let us return to the expression of H in terms of the b operators (or, alternatively, return to H'). H as a functional of the b operators (or H' as a functional of the $a^\dagger$'s) is an infinite power series in the matrix elements of F. In our approach we have assumed that these matrix elements are small so that the series may be truncated at the second power of F. This assumption seems to hold when the interaction is not too strong [see Eq. (2.18)]. However, for an interaction containing a hard core this assumption is certainly wrong and one has to perform partial summations in order to obtain nondivergent results. One natural way of performing these summations is to express H as a sum of a one-body operator, two-body operator, etc.[6] in terms of the b operators, i.e.,

$$H=\sum_{\alpha\beta} t_{\alpha\beta} b_\alpha^\dagger b_\beta + \sum_{\alpha\beta\gamma\delta} u^{(2)}_{\alpha\beta,\gamma\delta} b_\alpha^\dagger b_\beta^\dagger b_\delta b_\gamma + \cdots , \tag{2.22}$$

where[6,21]

$$u^{(2)}_{\alpha\beta,\gamma\delta}=\langle\alpha\beta|\, e^{-iF_{12}}(t_1+t_2+v_{12})e^{iF_{12}}-(t_1+t_2)\,|\gamma\delta\rangle \ . \tag{2.23}$$

Here, $e^{iF_{12}}$ defines the action of e^{iF} in the space of two-particle wave functions, and $|\alpha\beta\rangle \equiv a_\alpha^\dagger a_\beta^\dagger|0\rangle$. A general procedure for computing the many-body terms implicit in Eq. (2.22) is discussed in Ref. 21. Equation (2.22) is the starting point of the unitary-model-operator approach.[6,20] It represents a particular method of summing the infinite power series in F and constitutes a cluster expansion of H [or of H', if we substitute the a operators for the b operators in (2.22)]. This seems to be the proper treatment of a strong short-range interaction, while for a weak long-range interaction our approach seems appropriate.

Finally, let us point out an essential difference between the approximate solution of the HF problem (Ref. 7) and the approximate treatment of the Hamiltonian suggested in the present paper. The method of Ref. 7 is, *at best*, merely an approximate solution of the HF equations. It can be considered as a good approximation to the low-lying states of the system only insofar as two conditions are satisfied, namely, that it is a good approximation to the HF problem, *and* the HF states furnish a good description of the low-lying states. On the other hand, the method of the present paper does not depend on the HF solution being a good one. In fact, in the next section we shall see that our method is a much better approximation to the exact solution than the HF method.

III. APPLICATIONS

In the present section we apply the method proposed in I and in the previous section to two solvable models[2,3] which simulate the nuclear shell

TABLE I. Comparison of exact and approximate results for the first five excitation energies in the LKD model.

Values of the parameters		$\frac{E_1-E_0}{\epsilon_2-\epsilon_1}$	$\frac{E_2-E_0}{\epsilon_2-\epsilon_1}$	$\frac{E_3-E_0}{\epsilon_2-\epsilon_1}$	$\frac{E_4-E_0}{\epsilon_2-\epsilon_1}$	$\frac{E_5-E_0}{\epsilon_2-\epsilon_1}$
$N=6$ $\epsilon=1.8$	Exact	1.900	2.299	3.577	4.200	4.785
$y=z=0.5$ $x=1.0$	F appr.	1.833	2.227	3.667	4.117	4.616
$NW_{12}=0.8$	Pert.	1.625	2.369	4.007	4.225	5.034
$NW_{13}=0.4$	RPA	1.633	1.958	3.591	5.224	5.549
$NW_{23}=0.2$						
$N=6$ $\epsilon=1.8$	Exact	2.007	2.326	3.728	4.199	4.647
$x=-0.8$ $y=0.4$ $z=0$	F appr.	1.988	2.292	3.803	4.190	4.610
$NW_{12}=0.8$	Pert.	1.880	2.404	4.064	4.312	4.890
$NW_{13}=0.4$	RPA	1.915	2.155	4.070	4.310	5.745
$NW_{23}=0.2$						
As above except	Exact	1.925	2.190	3.742	4.248	4.852
for $x=y=z=0.8$	F appr.	1.682	2.109	4.037	4.081	4.182
	Pert.	1.731	1.978	4.139	4.395	4.732
	RPA	0.570	1.787	3.507	4.067	4.637
$N=20$ $\epsilon=1.8$	Exact	0.839	1.094	1.738	2.093	2.595
$x=0.4$	F appr.	0.800	1.104	1.680	2.037	2.446
$y=z=0.5$	Pert.	0.784	1.088	1.651	1.980	2.421
$NW_{ij}=0$	RPA	0.562	0.649	1.124	1.773	2.047

model with a residual interaction. These models were suggested recently for testing new approximation methods in the nuclear many-body problem. Both models are more complicated than the Lipkin model[22] employed in I, and therefore may be expected to be more realistic than the Lipkin model. We study the excitation energies of states which may be reached from the ground state by the application of one- and two-particle operators. These are the states which are usually studied within the RPA.

A. AFP Model (Ref. 2)

The feature of this model which makes it more realistic than the Lipkin model is that it yields a nontrivial HF solution for all values of the interaction strength. The model consists of N fermions distributed between two single-particle energy levels. The two levels are separated by an energy difference ϵ, and each level is N-fold degenerate. The creation operators for the single-particle states are denoted by $a^\dagger_{p\alpha}$, where $\alpha = +1\ (-1)$ denotes the upper (lower) level, and $p = 1, \ldots, N$ denotes all the other quantum numbers. The Hamiltonian for the system is

$$H = \tfrac{1}{2}\epsilon \sum_{p\alpha} \alpha a^\dagger_{p\alpha} a_{p\alpha} + \tfrac{1}{4} V \sum_{p\alpha\beta} \beta a^\dagger_{p\alpha} a_{p\beta} \sum_{q\gamma\delta} \gamma a^\dagger_{q\gamma} a_{q\delta} \,. \tag{3.1}$$

Introducing the quasispin operators

$$J_+ \equiv J_-^\dagger \equiv \sum_p a^\dagger_{p,+1} a_{p,-1} \,, \tag{3.2}$$

$$J_z \equiv \tfrac{1}{2} \sum_{p\alpha} \alpha a^\dagger_{p\alpha} a_{p\alpha} \,, \tag{3.3}$$

$$J_x \equiv \tfrac{1}{2}(J_+ + J_-) \,, \tag{3.4}$$

$$J^2 \equiv \tfrac{1}{2}(J_+ J_- + J_- J_+) + J_z^{\,2} \,, \tag{3.5}$$

the Hamiltonian may be expressed in terms of these quasispins,[2,7]

$$H = \epsilon J_z + V J_x + V J^2 - V J_x^{\,2} \,. \tag{3.6}$$

The unperturbed ground state is obviously

$$|\Phi_0\rangle = \prod_{p=1}^{N} a^\dagger_{p,-1} |0\rangle \tag{3.7}$$

and in the quasispin representation it belongs to the irreducible multiplet with $J = \frac{1}{2}N$, and is an eigenstate of J_z with $m = -\frac{1}{2}N$. The unperturbed

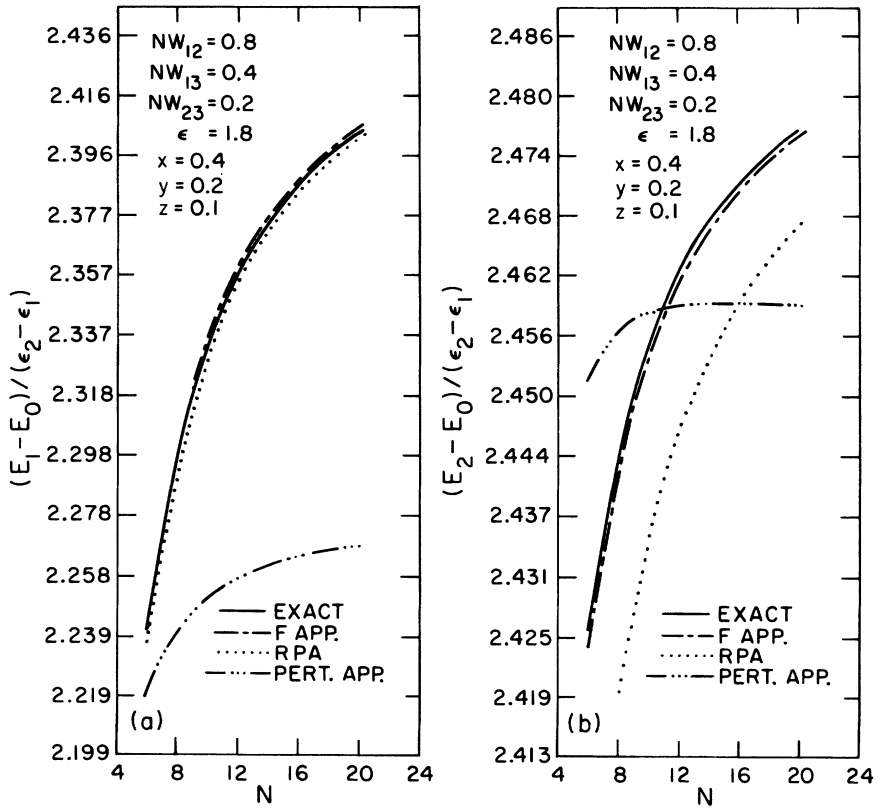

FIG. 5. Comparison of exact and approximate results for the two lowest excitation energies in the LKD model as functions of the number of particles N: (a) excitation energy of the first excited state, (b) excitation energy of the second excited state.

states in this ground-state multiplet are denoted by $|\frac{1}{2}N, m\rangle$, $m = -\frac{1}{2}N, \ldots, \frac{1}{2}N$. For this model, our operator F reads

$$F = f_1 J_+ + f_2 J_+^2 + \text{H.c.} \tag{3.8}$$

Calculating $E_g(F) \equiv \langle \Phi_0 | e^{-iF} H e^{iF} | \Phi_0 \rangle$ up to second order in the f's and minimizing, we get

$$f_1 = \frac{iV[8\epsilon - 3(N-1)V]}{8[\epsilon - (N-1)V][2\epsilon - (N-1)V] - (N-1)V^2}, \tag{3.9}$$

$$f_2 = -\frac{iV[2\epsilon - (2N-3)V]}{8[\epsilon - (N-1)V][2\epsilon - (N-1)V] - (N-1)V^2}. \tag{3.10}$$

The simplest procedure is to approximate the eigenenergies of the system by the expectation values of $H' = e^{-iF} H e^{iF}$ (up to second order in the f's). From the expressions (3.9) and (3.10) it is clear that our approximation will break down when the interaction strength NV is too big (i.e., of order ϵ) since in this case the f's become too big. This furnishes an immediate criterion for the region where our method is applicable.

In Figs. 1–4 we compare the results of our method with the exact results, with the HF results,[2,7] with second-order perturbation theory, and with the RPA. The results of the RPA in the figures have been calculated using the HF basis. We have checked and found out that (as may be expected) this provides an improvement over an RPA calculation with respect to the unperturbed basis $\{a^\dagger_{p\alpha}\}$. As the HF energies we took the expectation values of the Hamiltonian in the appropriate HF eigenstates. The calculations of perturbation theory were done with respect to the unperturbed basis $\{a^\dagger_{p\alpha}\}$. From the figures it is obvious that the results of our method are very good. Similar results have been obtained for other values of NV/ϵ and also for the excitation energies as functions of the interaction strength NV/ϵ for fixed values of N, as long as the basic condition for the validity of our method (i.e., small f's) is fulfilled. Finally, we should point out that although the results of our method are better than those of the other approximations, this does not imply that the other approximations are really bad. Indeed, a mere glance at the fine scale used in the figures is sufficient to convince us that although our method yields better results, the other approximations are not too far off.

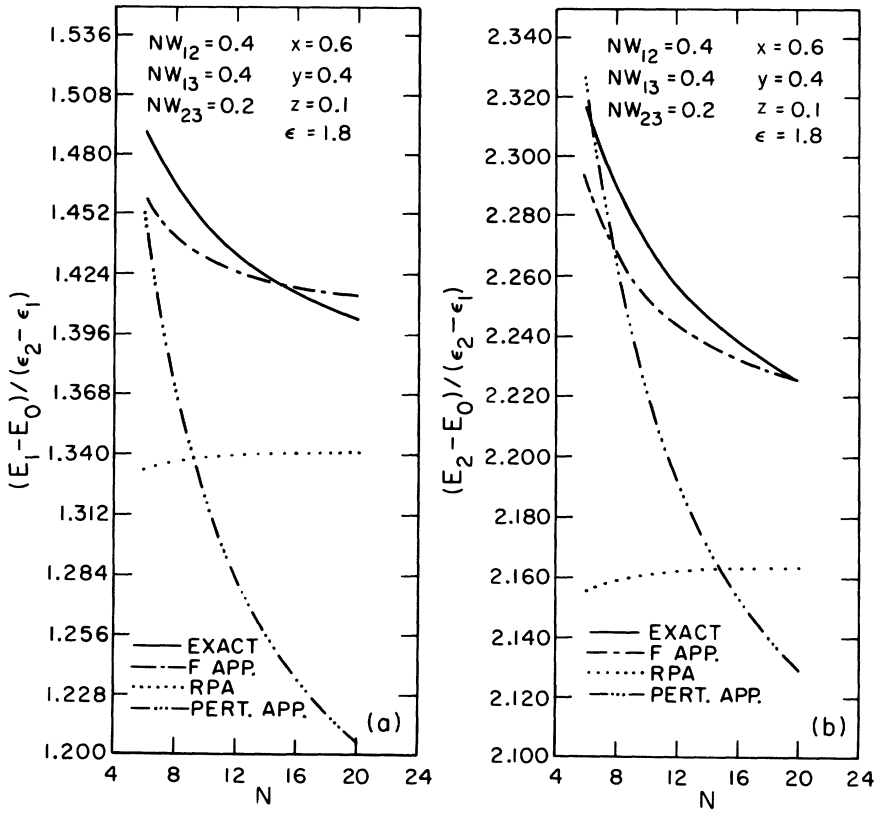

FIG. 6. The same as in Fig. 5 for different values of the parameters: (a) excitation energy of the first excited state, (b) excitation energy of the second excited state.

B. LKD Model (Ref. 3)

This model (see Ref. 3 for a more complete discussion of the model) is a three-level generalization of the two-level Lipkin model. The LKD model consists of N fermions distributed among three N-fold degenerate single-particle levels with energies $\epsilon_1 < \epsilon_2 < \epsilon_3$. A single-particle state is specified by the quantum numbers m and α, where $m = 1, 2, \ldots, N$ numbers the substates within a level, and $\alpha = 1, 2, 3$ designates the different levels. A two-body interaction of the monopole-monopole type is assumed between the levels. This interaction scatters particles between the levels without changing the value of m. The Hamiltonian for the system is therefore taken as[23]

$$H = \sum_{m\alpha} \epsilon_\alpha a^\dagger_{m\alpha} a_{m\alpha} + V_{12} \sum_{mm'} (a^\dagger_{m2} a^\dagger_{m'1} a_{m'2} a_{m1} + \text{H.c.}) + V_{13} \sum_{mm'} (a^\dagger_{m3} a^\dagger_{m'1} a_{m'3} a_{m1} + \text{H.c.}) + V_{23} \sum_{mm'} (a^\dagger_{m3} a^\dagger_{m'2} a_{m'3} a_{m2} + \text{H.c.})$$
$$+ W_{12} \sum_{mm'} (a^\dagger_{m2} a^\dagger_{m'1} a_{m'2} a_{m1} + \text{H.c.}) + W_{13} \sum_{mm'} (a^\dagger_{m3} a^\dagger_{m'1} a_{m'3} a_{m1} + \text{H.c.}) + W_{23} \sum_{mm'} (a^\dagger_{m3} a^\dagger_{m'2} a_{m'3} a_{m2} + \text{H.c.}) \,. \tag{3.11}$$

The unperturbed ground state for the model is $|\Phi_0\rangle$,

$$|\Phi_0\rangle = \prod_{m=1}^{N} a^\dagger_{m1} |0\rangle \,. \tag{3.12}$$

As in the Lipkin and AFP models, the Hamiltonian is immensely simplified by using its symmetries. Define the nine operators[3]

$$G_{\alpha\alpha'} = \sum_m a^\dagger_{m\alpha} a_{m\alpha'}; \quad \alpha, \alpha' = 1, 2, 3 \,. \tag{3.13}$$

These operators satisfy the commutation relations

$$[G_{\alpha\beta}, G_{\gamma\delta}] = \delta_{\beta\gamma} G_{\alpha\delta} - \delta_{\alpha\delta} G_{\gamma\beta} \,, \tag{3.14}$$

and are therefore the generators of a U(3) algebra. This becomes an SU(3) algebra upon imposing particle number conservation, which means that the particle number operator $\sum_{\alpha=1}^{3} G_{\alpha\alpha}$ has the fixed eigenvalue N. In terms of N and of the SU(3) generators, H reads

$$H = \sum_{\alpha=1}^{3} \epsilon_\alpha G_{\alpha\alpha} + V_{12}(G_{12}^2 + G_{21}^2) + V_{13}(G_{13}^2 + G_{31}^2) + V_{23}(G_{23}^2 + G_{32}^2) + W_{12}(G_{12}G_{21} + G_{21}G_{12} + G_{33} - N)$$
$$+ W_{13}(G_{13}G_{31} + G_{31}G_{13} + G_{22} - N) + W_{23}(G_{23}G_{32} + G_{32}G_{23} + G_{11} - N) \,. \tag{3.15}$$

We restrict ourselves to the ground-state band, consisting of the irreducible SU(3) multiplet containing $|\Phi_0\rangle$ and the states which may be reached from it by the application of the SU(3) generators. The Hamiltonian has no matrix elements between a state belonging to this multiplet and a state outside this multiplet. The unperturbed states in the ground-state band may be represented in the form[3]

$$|p, q\rangle = \left[\frac{(N-p-q)!}{N!\,p!\,q!}\right]^{1/2} (G_{21})^p (G_{31})^q |\Phi_0\rangle \,, \tag{3.16}$$

which stands for a normalized state with p particles in the second level, q particles in the third level, and $N-p-q$ particles in the first level.

For the present model our operator F reads

$$F = f_1 G_{21} + f_2 G_{31} + f_3 G_{21}^2 + f_4 G_{31}^2 + f_5 G_{21} G_{31} + \text{H.c.} \tag{3.17}$$

The coefficients $f_1, \ldots, f_5$ are determined by expanding $\langle \Phi_0 | e^{-iF} H e^{iF} | \Phi_0 \rangle$ up to second order in the f's and minimizing, to get[24]

$$f_1 = f_2 = f_5 = 0 \,, \tag{3.18}$$

$$f_3 = \tfrac{1}{2} i \frac{V_{13}V_{23} - V_{12}[\epsilon_3 - \epsilon_1 + 2(N-2)W_{13}]}{V_{23}^2 - [\epsilon_2 - \epsilon_1 + 2(N-2)W_{12}][\epsilon_3 - \epsilon_1 + 2(N-2)W_{13}]} \,, \tag{3.19a}$$

$$f_4 = \tfrac{1}{2} i \frac{V_{12}V_{23} - V_{13}[\epsilon_2 - \epsilon_1 + 2(N-2)W_{12}]}{V_{23}^2 - [\epsilon_2 - \epsilon_1 + 2(N-2)W_{12}][\epsilon_3 - \epsilon_1 + 2(N-2)W_{13}]} \,. \tag{3.19b}$$

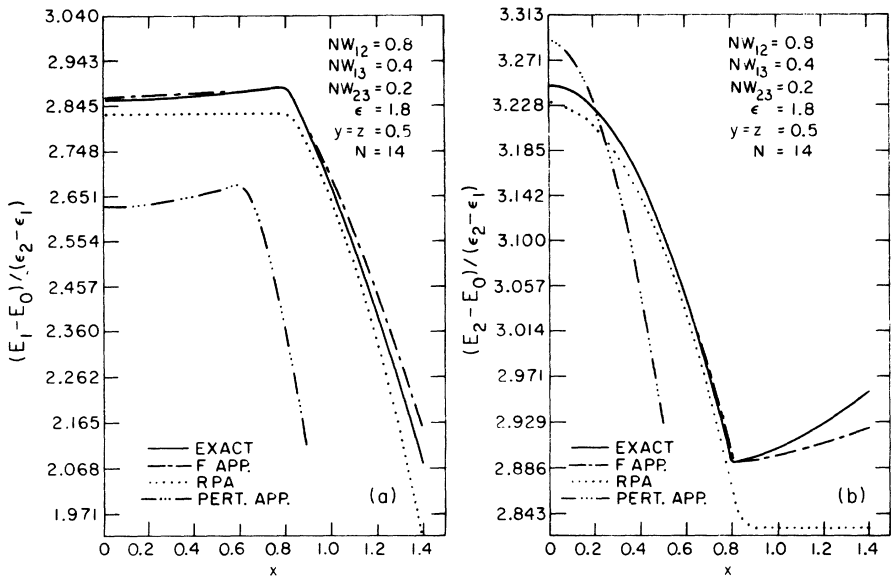

FIG. 7. Comparison of exact and approximate results for the two lowest excitation energies in the LKD model as functions of the interaction strength x [see Eq. (3.22)]: (a) excitation energy of the first excited state, (b) excitation energy of the second excited state.

Again, in our approximation we take the eigen energies of the system to be the diagonal matrix elements of H', i.e.,

$$E_F(p, q) = \langle p, q | e^{-iF} H e^{iF} | p, q \rangle . \tag{3.20}$$

The results of our approximation were compared with the exact ones, with the RPA and with second-order perturbation theory. It should be noticed that in this model there are two levels which may be considered as representing one-particle–one-hole excitations, i.e., the states $|1, 0\rangle$ and $|0, 1\rangle$, and three levels which may be considered as two-particle–two-hole excitations, i.e., $|2, 0\rangle$; $|0, 2\rangle$; $|1, 1\rangle$. Therefore in Table I we present a sample of characteristic results for the *first five* excitation energies. Following Ref. 3 we have used the

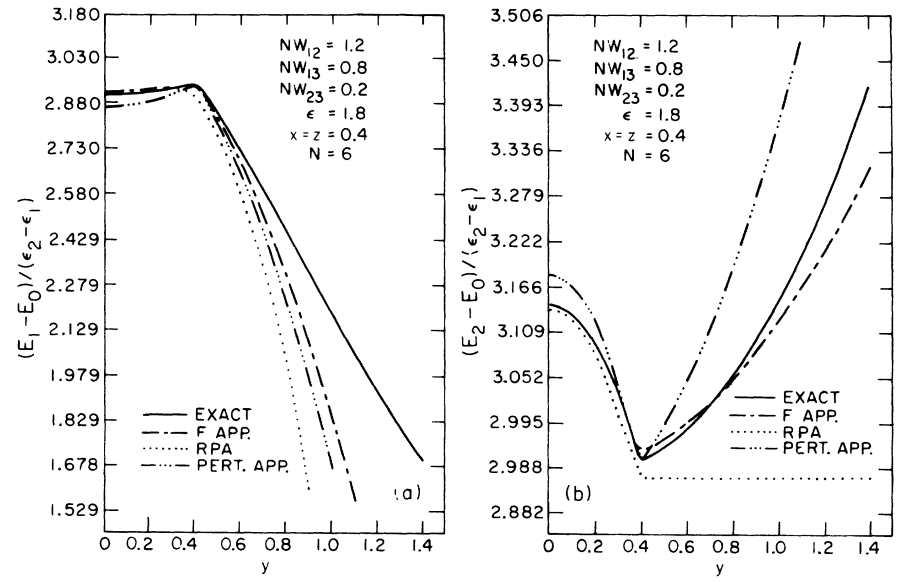

FIG. 8. Comparison of exact and approximate results for the two lowest excitation energies in the LKD model as functions of the interaction strength y [see Eq. (3.22)]: (a) excitation energy of the first excited state, (b) excitation energy of the second excited state.

following conventions for the parameters of the model:

$$\epsilon_1 \equiv 0; \quad \epsilon_2 - \epsilon_1 \equiv 1; \quad \frac{\epsilon_3 - \epsilon_1}{\epsilon_2 - \epsilon_1} \equiv \epsilon > 1, \tag{3.21}$$

$$x \equiv \frac{NV_{12}}{\epsilon_2 - \epsilon_1}; \quad y \equiv \frac{NV_{13}}{\epsilon}; \quad z \equiv \frac{NV_{23}}{\epsilon_2 - \epsilon_1}. \tag{3.22}$$

In Figs. 5–8 we present characteristic results for the two lowest excitation energies as functions of N and of x and y. Similar results were obtained for negative values of x and y. The dependence of the energy levels on z was found out to be very weak. All the results obtained show that on the average our method yields very good results. It sometimes happens that for particular values of the parameters and for a particular excitation energy the RPA or second-order perturbation theory yields a slightly better result than our approximation. But, this does not hold for the other excitation energies at the same values of the parameters, and the over-all results of our approximation are much better than those of the other approximations. As we have pointed out for the case of the AFP model, this does not mean that the RPA and second-order perturbation theory are really bad approximations. As is obvious from the figures, although the RPA and second-order perturbation theory seem sometimes far away from the exact results, in many cases this is due merely to the fine scale we are using in the figures.

IV. DISCUSSION

In the former sections and in I we have proposed a method for dealing with two-body correlations in nuclear systems and have applied it rather successfully to several solvable models. One of the important assumptions that we have made is that one may truncate the expression in powers of F at the second power. This leads to a set of linear[25] equations which for the cases of the models considered (in the present paper, in I and in Ref. 5) is very easily solved. However, for more realistic cases, taking into account the two-particle–two-hole states induced by the two-body part of F may well yield in Eq. (2.18) a matrix of such enormous dimensions as to make its inversion impractical in many interesting cases. Obviously, to make the method work for real nuclei, the dimensions of the matrices involved have somehow to be drastically reduced. As a matter of fact, we have clear-cut examples of such a reduction in all the cases of the models considered (in the present paper, in I, and in Ref. 5). It should be realized that in principle in all those cases we should have had to invert matrices which are approximately of the order of $N^4 \times N^4$, where N is the degeneracy of each of the levels in the models. However, by using the symmetries of the models we were left with (at the most) 2×2 matrices. In the cases of the models this enormous reduction is exact, due to the symmetries. Now, when we investigate how this reduction has been formally achieved, we find out that it is done through the use of the "collective" operators J_+, G_{21}, G_{31} (in the present paper and in I) and L_+S_-.[5] We employed these operators to define the operator F, instead of employing the general one-particle–one-hole and two-particle–two-hole operators $a_\sigma^\dagger a_\mu$ and $a_\sigma^\dagger a_\tau^\dagger a_\mu a_\nu$. Those "collective" operators (and their powers) acting on the unperturbed ground state generate the ground-state band which is the set of "collective" states in which we are interested. For the solvable models this ground-state band is exactly separable from any other set of states, and therefore restricting ourselves merely to the "collective" operators is exact. But, this treatment naturally suggests a similar approach to more complicated systems, i.e., restricting oneself to a few collective operators (which should somehow be analogous to J_+, G_{21}, G_{31}, or L_+S_-) instead of dealing with the far too numerous general one-particle–one-hole and two-particle–two-hole operators. In this connection, let us recall that the experiments tell us that usually the low-lying excited states of nuclei do *not* coincide with the enormous number of one-particle–one-hole or two-particle–two-hole states. In fact, the lowest-lying excited states consist usually of a very small number of collective states that are described fairly well (at least to lowest order) by a *coherent combination* of one-particle–one-hole states or two-particle–two-hole states. These states often form, together with the ground state, some kind of a collective "multiplet." The matrix elements of the Hamiltonian between states belonging to this "multiplet" and states outside the "multiplet" are relatively small and electromagnetic transition probabilities are especially enhanced between particular members of that multiplet. These observations point to a possible modification of our method which may perhaps be considered more phenomenological than the original form (as put forward in Sec. II and in I), but may be quite easy to handle in practice. This version is easily formulated by using the form of F in Eq. (2.14),

$$F = \sum_i f_i A_i^\dagger + \text{H.c.}$$

In this equation we now consider the set $\{A_i^\dagger\}$ not as representing the set $\{a_\sigma^\dagger a_\mu, a_\sigma^\dagger a_\tau^\dagger a_\mu a_\nu\}$ but rather as representing a small number of collective one-body and two-body operators (analogous to the collective operators J_+, J_+^2, G_{21}, G_{31}, G_{21}^2, G_{31}^2,

$G_{21}G_{31}$, and L_+S_- of the solvable models). The system of equations resulting from the variation is formally the same as Eq. (2.18), but its dimensions will be incomparably smaller.

Possible choices of both the one-particle–one-hole and two-particle–two-hole collective operators for this modified version of our method are the one-particle–one-hole and two-particle–two-hole creation parts of the one- and two-phonon operators of the RPA or of the Tamm-Dancoff (TD) approximation. By means of such a choice we may presumably take into account the interaction between the one- and two-phonon states of the RPA and thus account for the well-known anharmonicities discovered over the recent years in the spectra of even-even nuclei. It should be noted that our treatment of the solvable models followed that prescription. Indeed the operators J_+, G_{21}, G_{31}, J_+^2, G_{21}^2, G_{31}^2, $G_{21}G_{31}$ are the one-particle–one-hole and two-particle–two-hole creation parts of the RPA (TD) one- and two-phonon operators.

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[13]This is obvious, since the matrix elements of a transformation matrix are the same in the old and in the new representation and therefore F has the same matrix elements with respect to the $b^\dagger$ operators as it has with respect to the $a^\dagger$ operators.

[14]This possibility is of course completely equivalent to the first one, but it seems to us more convenient from a practical (i.e., computational) point of view.

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[24]The vanishing of the f_1, f_2, and f_5 is obviously due to the symmetries of the model.

[25]To be contrasted with the *non*linear set of equations which is obtained in general and seems impossible to solve even for the solvable models.