Systematic procedure for going beyond the time-dependent Hartree-Fock approximation

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A systematic procedure that allows for corrections of arbitrary order to the time-dependent Hartree-Fock approach is presented and illustrated with reference to an exactly solvable U(3) model. Substantial improvements over the uncorrelated picture are obtained.

I. INTRODUCTION

The temporal evolution of an antisymmetrized uncorrelated many-body wave function in a nonlinear mean field has been the subject of careful study over many years, having engaged the attention of many nuclear theorists.[1] The time dependent Hartree-Fock method (TDHF) has thus been extensively (and rather successfully) applied to a variety of many fermion problems, yielding interesting insights into the intricacies of nuclear dynamics.[1-3]

Of course, several difficulties plague the TDHF approach that are inherent either to the single particle approximation or to a determinantal picture.[4-6] Comparisons of TDHF with exact Schrödinger solutions have been made that shed much light upon the inner workings of this popular technique.[7,8]

Attractive theoretical considerations regarding higher order approaches have also been formulated.[9,10] They deal with the inclusion of collisional kernels in the equations of motion and special relaxation time approximations.

An excellent review of mean field and higher order approaches is given in Ref. 11, where interesting new approximations are also developed from a general statistical viewpoint based on information theory and on sophisticated projection techniques (see also Ref. 12).

However, it is our intention here to attempt to go beyond the uncorrelated particle model by examining some critical aspects of the TDHF description that allow for a natural, tractable, and simple way of extending its scope, the central idea being to establish a connection between the temporal evolution of observables and the closure of some particular semialgebras. Numerical results are presented in an exact, but not trivial, solvable model.

The paper is organized as follows: Section II recasts the TDHF approach in a manner compatible with the considerations just outlined, which allow for a systematic way of introducing corrections to the single-particle picture. Application to a U(3) model is thoroughly discussed in Sec. III and some conclusions are drawn in Sec. IV.

II. FORMALISM

A. A TDHF review

Let $\hat{O}_\alpha$ $(\alpha=1,\ldots,q)$ be the operators representing the observables we are interested in. The time evolution of these relevant operators is given by Ehrenfest's theorem,

$$-i\hbar d\langle\hat{O}_\alpha\rangle_t/dt=\langle[\hat{H},\hat{O}_\alpha]\rangle_t\ , \tag{2.1}$$

where $\hat{H}$ stands for the Hamiltonian of the corresponding system. Assume now that the set $\{\hat{O}_\alpha\}$ closes a partial Lie algebra under commutation with $\hat{H}$,

$$[\hat{H},\hat{O}_\alpha]=i\hbar\sum_{\beta=0}^{q}\hat{O}_\beta b_{\beta\alpha}\ , \tag{2.2}$$

the $b_{\beta\alpha}$ being c numbers (structure constants). Recourse to (2.2) allows one to recast (2.1) as

$$d\langle\hat{O}_\alpha\rangle_t/dt=-\sum_{\beta=0}^{q}b_{\beta\alpha}\langle\hat{O}_\beta\rangle_t\ , \tag{2.3}$$

which provides us with a set of coupled (linear) differential equations that completely determine the time evolution of the relevant expectation values $\langle\hat{O}_\alpha\rangle_t$, provided one knows the corresponding initial values $\langle\hat{O}_\alpha\rangle_{t=0}$. The entire dynamics of the problem is embedded in the value of the structure factors $b_{\beta\alpha}$, as long as we confine our interest to the temporal evolution of the set $\{\langle\hat{O}_\alpha\rangle\}$.

The closure of such a partial Lie algebra of Eq. (2.2) is not, in most instances an attainable goal (in the case of a many-body system). Commutating an n-body operator with an m-body one yields, in general, $(n+m-1)$-body operators. In principle, we will succeed only in those situations for which the Hamiltonian is of single particle (s.p.) character. An approximate, self-consistent description is, however, always at hand if one restricts the relevant wave function (w.f.) to be, at all times, of a given prescribed form. A nonlinear closure results as a consequence (see below).

The TDHF method can be viewed in this particular light. The w.f. here is restricted to be a Slater determinant, and expectation values of those relevant operators that do not belong to our semialgebra are evaluated by recourse to Wick's theorem. The time evolution of s.p. operators $\hat{O}_\alpha^{(1)}$ is thus given by

$$-i\hbar d\langle\hat{O}_\alpha^{(1)}\rangle/dt=\langle[\hat{H},\hat{O}_\alpha^{(1)}]\rangle_{\rm HF}\equiv\langle[\hat{h},\hat{O}_\alpha^{(1)}]\rangle\ , \tag{2.4}$$

where the subscript HF tells us that self-consistent expectation values, obtained by recourse to Wick's theorem, are being referred to. Of course, $\hat{h}$ is the mean field, effective s.p. Hamiltonian,

$$\hat{h}=\sum_{\alpha}(\partial\langle\hat{H}\rangle_{\mathrm{HF}}/\partial\langle\hat{O}_{\alpha}^{(1)}\rangle)\hat{O}_{\alpha}^{(1)}\ , \tag{2.5}$$

and it is quite obvious here that we are closing the $\hat{O}_{\alpha}^{(1)}$ algebra in a nonlinear way.

This renowned approach, that locally extremalizes the quantum action and is exact in the classical limit,[13] can be regarded, within the present context, as being characterized by two operational features. If we cast $\hat{H}$ in the usual fashion,

$$\hat{H}=\hat{H}_0+\hat{V}\ , \tag{2.6}$$

where $\hat{H}_0$ is of s.p. nature and $\hat{V}$ is (in most cases) the two-body interaction, the prescription (2.4) entails: (i) closing a semialgebra with $\hat{H}_0$, and (ii) including in it, in addition, all those s.p. operators that appear, via Wick's theorem, in $\langle[\hat{V},\hat{O}_{\alpha}^{(1)}]\rangle_{\mathrm{HF}}$.

The mean field treatment is the one that yields, at the (initial) time $t=0$, the correct first-order temporal derivative of the $\langle\hat{O}_{\alpha}^{(1)}\rangle$.

On the other hand, for two-body operators $\hat{O}_{\alpha}^{(2)}$ (nth body operators $\hat{O}_{\alpha}^{(n)}$), Ehrenfest's theorem does not, in general, hold within the mean-field framework,

$$-i\hbar d\langle\hat{O}_{\alpha}^{(n)}\rangle_{\mathrm{HF}}/dt\neq\langle[\hat{H},\hat{O}_{\alpha}^{(n)}]\rangle_{\mathrm{HF}}\ , \tag{2.7}$$

and, as a consequence, first-order temporal derivatives of the $\langle\hat{O}_{\alpha}^{(n)}\rangle$ are not the correct ones at $t=0$.

B. Going beyond the TDHF approach

We shall attempt to "improve" the mean field treatment by forcing $\langle\hat{O}_{\alpha}^{(n)}\rangle$ expectation values, $1\leq n<M$, to fulfill Ehrenfest's prescription. The two operational features (i) and (ii) of Sec. II A will be retained for $n=M$, and a nonlinear closure will be effected in which the relevant nth-body operators that arise out of the corresponding commutations with $\hat{V}$ will be included. Our proposal can be succinctly casted as follows:

$$-i\hbar d\langle\hat{O}_{\alpha}^{(j)}\rangle/dt=\langle[\hat{H},\hat{O}_{\alpha}^{(j)}]\rangle,\quad j=1,\ldots,M-1 \tag{2.8a}$$

$$-i\hbar d\langle\hat{O}_{\beta}^{(M)}\rangle/dt=\langle[\hat{H}_0,\hat{O}_{\beta}^{(M)}]\rangle+\langle[\hat{V},\hat{O}_{\alpha}^{(M)}]\rangle_{\mathrm{HF}}\ . \tag{2.8b}$$

Starting with the observables of interest, the semialgebra with $\hat{H}$ is exactly closed up to $(M-1)$ body operators, while in the last step prescriptions (i) and (ii) are used to attain an approximate closure. One can appreciate the fact that up to $(M-1)$ correlations are taken into account within this scheme. Moreover, correct Mth-order temporal derivatives of the $\langle\hat{O}_{\alpha}^{(1)}\rangle$ are obtained at $t=0$ [indeed, correct $(M-n+1)$th-order temporal derivatives at $t=0$ are attained for nth-body operators]. The TDHF approximation is recovered for $M=1$.

Of special interest is, of course, the case $M=2$, and we shall restrict our attention to this particular case, so that our equations will read

$$-i\hbar d\langle\hat{O}_{\alpha}^{(1)}\rangle/dt=\langle[\hat{H},\hat{O}_{\alpha}^{(1)}]\rangle\ , \tag{2.8c}$$

$$-i\hbar d\langle\hat{O}_{\beta}^{(2)}\rangle/dt=\langle[\hat{H}_0,\hat{O}_{\beta}^{(2)}]\rangle+\langle[\hat{V},\hat{O}_{\beta}^{(2)}]\rangle_{\mathrm{HF}}\ , \tag{2.8d}$$

where the $\hat{O}_{\beta}^{(2)}$ belong to the set $\{[\hat{V},\hat{O}_{\alpha}^{(1)}]\}$. Notice that Wick's theorem is employed only in the last commutator on the right-hand side (rhs) of (2.8d). As a consequence, the unperturbed temporal evolution of two-body operators is not affected. More explicitly, if

$$\hat{H}_0=\sum_{i}\epsilon_i c_i^{\dagger}c_i \tag{2.9}$$

and

$$\hat{O}_{\beta}^{(2)}=O_{i_1i_2i_4i_3}c_{i_1}^{\dagger}c_{i_2}^{\dagger}c_{i_3}c_{i_4}\ , \tag{2.10}$$

we have

$$[\hat{H}_0,\hat{O}_{\beta}^{(2)}]=w_{\beta}\hat{O}_{\beta}^{(2)} \tag{2.11}$$

and

$$-i\hbar d\langle\hat{O}_{\beta}^{\prime(2)}\rangle/dt=\langle[\hat{V},\hat{O}_{\beta}^{\prime(2)}]\rangle_{\mathrm{HF}}\ , \tag{2.12a}$$

where $w_{\beta}=\epsilon_{i_1}+\epsilon_{i_2}-(\epsilon_{i_3}+\epsilon_{i_4})$ and

$$\hat{O}_{\beta}^{\prime(2)}=\exp[-(i/\hbar)w_{\beta}t]\hat{O}_{\beta}^{(2)}\ , \tag{2.12b}$$

so that the Wick's theorem evaluation is applied only to the "perturbed" temporal evolution. The nonlinear character of the closure is a consequence of the term $\langle[\hat{V},\hat{O}_{\beta}^{(2)}]\rangle_{\mathrm{HF}}$.

The most suitable s.p. unperturbed Hamiltonian [to be employed in (2.6)] is the static Hartree-Fock Hamiltonian obtained via (2.5) using stationary mean values $\langle\hat{O}_{\alpha}^{(1)}\rangle$. In this way, $\hat{V}$ becomes the (static) residual interaction, without s.p. contributions.

The TDHF evolution takes our system along trajectories that lie on surfaces of constant Hartree-Fock energy $\langle\hat{H}\rangle_{\mathrm{HF}}$ and occupation numbers. The approach we are putting forward here, instead, yields s.p. trajectories that, as in the exact picture, are not constrained in such a fashion.

It goes without saying that the present approach is not restricted by the necessity of starting, at $t=0$, with a Slater determinant (a pure state), and can thus accommodate initial conditions that require a "mixed" s.p. state for its description.

C. Alternative closures

The approach introduced in the preceding subsection has as its recurring theme the (nonlinear) closure of a semialgebra in a rather peculiar fashion. By analysis of alternative ways of closing the corresponding algebra, one can hope to shed some additional light on the problem discussed here.

A possibility is to replace the full Hamiltonian by a suitable, effective s.p. Hamiltonian at a given step [a given j in Eq. (2.8a)]. The simplest thing to do, in this vein, is to discard $\hat{V}$ along the way, namely, to work with the system

$$-i\hbar d\langle \hat{O}_\alpha^{(j)} \rangle /dt = \langle [\hat{H}, \hat{O}_\alpha^{(j)}] \rangle, \quad j = 1, \ldots, M-1 \tag{2.13a}$$

$$-i\hbar d\langle \hat{O}_\beta^{(M)} \rangle /dt = \langle [\hat{H}_0, \hat{O}_\beta^{(M)}] \rangle \ , \tag{2.13b}$$

which entails omitting the mean-field evaluation of $[\hat{V}, \hat{O}_\beta^{(M)}]$. This procedure is seen to be equivalent to a series expansion in $\hat{V}$; that is, we discard, in evaluating the time evolution of $\langle \hat{O}_\alpha^{(1)} \rangle$, the Mth power of the operator $\hat{V}$. The method is a linear one, but one needs to go up to $M = n+1$ (nth order) in order to get the right nth-order temporal derivative of $\langle \hat{O}_\alpha^{(1)} \rangle$ at $t = 0$.

Still a different way of closing our partial Lie algebra is to replace $\hat{H}_0$ by the dynamic mean field s.p. Hamiltonian $\hat{h}$ on the rhs of (2.13b). This is tantamount to working with a series expansion in the residual interaction $\hat{V}_{\rm res} = \hat{H} - \hat{h}$ and yields, once more, a nonlinear problem.

In this case the $M = 2$ situation is still equivalent to the TDHF one if no correlations are present in the initial state (i.e., when this is a pure state). This property, which ultimately refers to the stationary character of the TDHF trajectories, can be straightforwardly derived as follows. We write the expectation value of a two-body operator in the fashion

$$\langle \hat{O}_\beta^{(2)} \rangle = \langle \hat{O}_\beta^{(2)} \rangle_{\rm HF} + \langle \hat{O}_\beta^{(2)} \rangle_c \ , \tag{2.14}$$

where the subscript c denotes correlations, and evaluate the temporal evolution of the first term on the rhs,

$$-i\hbar d\langle \hat{O}_\beta^{(2)} \rangle_{\rm HF} /dt = \langle [\hat{h}, \hat{O}_\beta^{(2)}] \rangle_{\rm HF} + \Delta_\beta \ , \tag{2.15}$$

with

$$\Delta_\beta = \sum_\alpha \langle [\hat{H}, \hat{O}_\alpha^{(1)}] \rangle_c \partial \langle \hat{O}_\beta^{(2)} \rangle_{\rm HF} / \partial \langle O_\alpha^{(1)} \rangle \ . \tag{2.16}$$

By inspection of (2.13b) (with $\hat{H}_0$ replaced by $\hat{h}$) it follows that

$$-i\hbar d\langle \hat{O}_\beta^{(2)} \rangle_c /dt = \langle [\hat{h}, \hat{O}_\beta^{(2)}] \rangle_c - \Delta_\beta \ , \tag{2.17}$$

so that, if no correlations are present at $t = 0$, they will vanish for all t.

The idea of replacing $\hat{H}_0$ with $\hat{h}$ thus seems to be particularly suited for dealing with those situations in which correlations are initially present, and are thus not amenable to a TDHF treatment.

As a final remark, we conclude this section by mentioning that if we replace $\hat{H}_0$ by $\hat{h}$ in Eq. (2.8d) one obtains the relationship

$$-i\hbar d\langle \hat{O}_\beta^{(2)} \rangle_c /dt = \langle [\hat{h}, \hat{O}_\beta^{(2)}] \rangle_c - \Delta_\beta + \langle [\hat{V}_{\rm res}, \hat{O}_\beta^{(2)}] \rangle_{\rm HF} \ , \tag{2.18}$$

which is to be compared to the corresponding result that one would find in the preceding subsection, namely

$$-i\hbar d\langle \hat{O}_\beta^{(2)} \rangle_c /dt = \langle [\hat{H}_0, \hat{O}_\beta^{(2)}] \rangle_c - \Delta_\beta + \langle [\hat{H}_0 - \hat{h}, \hat{O}_\beta^{(2)}] \rangle_{\rm HF} + \langle [\hat{V}, \hat{O}_\beta^{(2)}] \rangle_{\rm HF} \ , \tag{2.19}$$

In both instances one clearly appreciates the fact that correlations possess a nonvanishing initial derivative.

III. APPLICATION

A. The model

We shall illustrate the techniques introduced in Sec. II with reference to a well-known, exactly solvable model.[14] N fermions are distributed among three 2Ω-fold degenerate s.p. levels and, for the sake of simplicity, we shall take $N = 2\Omega$. The ket $|p,i\rangle$ denotes the s.p. states with $1 \le p \le 2\Omega$ and $1 \le i \le 3$.

The s.p. operators

$$\hat{G}_{ij} = \sum_{p=1}^{2\Omega} c_{Pi}^\dagger c_{Pj}, \quad i,j = 1,2,3 \tag{3.1}$$

obey U(3) commutation rules,

$$[\hat{G}_{ij}, \hat{G}_{kl}] = \hat{G}_{il}\delta_{jk} - \hat{G}_{kj}\delta_{il} \ , \tag{3.2}$$

and with them we shall construct our Hamiltonian,[15] with a monopole interaction term

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_i \epsilon_i \hat{G}_{ii} + \tfrac{1}{2} \sum_{i \ne j} V_{ij} \hat{G}_{ij}^{\,2} \ , \tag{3.3}$$

with $\epsilon_1 \le \epsilon_2 \le \epsilon_3$ and $V_{ij} = V_{ji}^*$. This model represents a very simplified scheme of a nucleus, with two different collective modes of excitation that interact with each other and with the ground state.

With the help of Wick's theorem, one easily finds, with the definitions

$$g_{ij} = \langle \hat{G}_{ij} \rangle / N \ , \qquad v_{ij} = V_{ij}(N-1) \ , \tag{3.4}$$

the results

$$\langle \hat{H} \rangle = N \left[\sum_i \epsilon_i g_{ii} + \tfrac{1}{2} \sum_{i \ne j} v_{ij} g_{ij}^2 \right] \tag{3.5}$$

and

$$\hat{h} = \sum_i \epsilon_i \hat{G}_{ii} + \sum_{i \ne j} v_{ij} g_{ij} \hat{G}_{ij} \ . \tag{3.6}$$

A given Slater determinant (SD) built up with the help of the generators $\hat{G}_{ij}$ belongs to the completely symmetric representation of U(3), namely $(N,0,0)$. Its basic states are

$$|n_2,n_3\rangle=(n_1!/N!n_2!n_3!)^{1/2}\hat{G}_{21}^{n_2}\hat{G}_{31}^{n_3}|0\rangle\ , \tag{3.7}$$

where

$$\begin{aligned}&0\le n_2+n_3\le N\ ,\\&n_1+n_2+n_3=N\end{aligned} \tag{3.8}$$

are the requirements which the occupation numbers n_i obviously fulfill and $|0\rangle$ is the unperturbed ground state (u.g.s.) for which $n_1=N$ and $n_2=n_3=0$. The exact ground state (g.s.) of $\hat{H}$ belongs to this representation, within which any SD can be written as

$$\begin{aligned}|\Psi\rangle&=(x_1)^N\exp(h_1\hat{G}_{21}+h_2\hat{G}_{31})|0\rangle\\&=\sum_{n_2,n_3}(N!/n_1!n_2!n_3!)^{1/2}x_1^{n_1}x_2^{n_2}x_3^{n_3}|n_2,n_3\rangle\\&=\sum_{n_2,n_3}C_{n_2n_3}(0)|n_2,n_3\rangle\equiv|\Psi(0)\rangle\ ,\end{aligned} \tag{3.9}$$

with

$$\begin{aligned}&h_1=x_2/x_1,\quad h_2=x_3/x_1\ ,\\&|x_1|^2+|x_2|^2+|x_3|^2=1\ .\end{aligned} \tag{3.10}$$

The s.p. density matrix can be easily shown to be

$$\rho_{p_jq_i}=\langle c_{qi}^\dagger c_{pj}\rangle=\delta_{pq}N^{-1}\langle\hat{G}_{ij}\rangle=x_i^*x_j\ , \tag{3.11}$$

while the exact time dependent evolution of (3.9) is found by diagonalizing $\hat{H}$ in the basis $|n_2,n_3\rangle$ [$(N+2)(N+1)/2$ is the dimension of the corresponding energy matrix which can be blocked in four submatrices due to the particular structure of the interaction in (3.3)]. The relevant matrix elements read

$$\hat{G}_{ii}|n_in_jn_k\rangle=n_i|n_in_jn_k\rangle,\quad n_i+n_j+n_k=N \tag{3.12a}$$

$$\hat{G}_{ij}|n_in_jn_k\rangle=[n_j(n_i+1)]^{1/2}|n_i+1,n_j-1,n_k\rangle\ , \tag{3.12b}$$

where for the sake of clarity the redundant quantum number n_1 has been explicitly cited.

The w.f. (3.9) at time t will be given by

$$\begin{aligned}|\Psi(t)\rangle&=\exp[-(i/\hbar)\hat{H}t]|\Psi(0)\rangle\\&=\sum_{n_2,n_3}C_{n_2n_3}(t)|n_2,n_3\rangle\ ,\end{aligned} \tag{3.13}$$

with

$$\begin{aligned}C_{n_2n_3}(t)=\sum_L\sum_{m_2,m_3}&A^L_{n_2n_3}A^{L*}_{m_2m_3}\\&\times\exp[-(i/\hbar)E_Lt]C_{m_2m_3}(0)\ .\end{aligned} \tag{3.14}$$

The matrix $A^L_{n_2n_3}$ in (3.14) connects the eigenstates $|L\rangle$ of $\hat{H}$ [$1\le L\le\binom{n+2}{2}$] with the basic states $|n_2,n_3\rangle$ of the $(N,0,0)$ representation

$$A^L_{n_2n_3}=\langle n_2n_3|L\rangle\ , \tag{3.15}$$

while E_L are the corresponding eigenvalues

$$\hat{H}|L\rangle=E_L|L\rangle \tag{3.16}$$

[the coefficients $C_{n_2n_3}(0)$ have been defined in (3.9)].

The exact expectation values, evaluated at the time t, of the generators $\hat{G}_{ij}$, are easily computed with the help of (3.12). As an example we have

$$\begin{aligned}\langle\hat{G}_{ij}\rangle_t&=\sum_{n_i,n_j}[n_j(n_i+1)]^{1/2}\\&\quad\times C^*_{n_i+1,n_j-1,n_k}(t)C_{n_in_jn_k}(t),\quad i\ne j\\\langle\hat{G}_{ii}\rangle_t&=\sum_{n_2,n_3}n_i|C_{n_2n_3}(t)|^2\ ,\end{aligned} \tag{3.17}$$

in self-explanatory notation.

B. TDHF treatment

Within the present context, the TDHF equations of motion read

$$\begin{aligned}-i\hbar\,dg_{ij}/dt&=(1/N)\langle[\hat{h},\hat{G}_{ij}]\rangle\\&=(\epsilon_i-\epsilon_j)g_{ij}+v_{ji}g_{ji}(g_{jj}-g_{ii})\\&\quad+\sum_{\substack{k\ne i\\k\ne j}}(v_{ki}g_{ki}g_{kj}-v_{jk}g_{jk}g_{ik})\ ,\end{aligned} \tag{3.18}$$

thus yielding a system of nine (real) coupled equations.

Of course, in the "pure" case discussed here these could have also been written in terms of the two complex quantities x_2 and x_3 (the phase of x_1 being irrelevant). Notice that, when written in terms of the v_{ij}, the number of particles N does not explicitly appear in (3.18).

The TDHF equations of motion are nonintegrable for $n>2$, as opposed to what happens in the SU(2) situation, in which the conservation of $\langle\hat{H}\rangle$ and $\langle\hat{J}^2\rangle$ renders the system one dimensional. Accordingly, the temporal evolution displays a more complex character, so that this model constitutes a more challenging test for the approximations developed than the SU(2) one.

A few words about the time scale would be appropriate here. Our "characteristic time unit" here is of the order of $t=\hbar/(\epsilon_2-\epsilon_1)$. If the denominator is of the order of 500 keV, one would have $t\cong1.31\times10^{-21}$ s, which is large enough compared with the nucleon transversal time ($\sim10^{-22}$ s).

Going back to the system (3.18), this is solved with the help of initial conditions provided via (3.11). The TDHF equations are easily seen to conserve the expectation values C_1,C_2,C_3 of the three Casimir operators entering into this, namely

$$C_1=\sum_i g_{il}\ , \tag{3.19}$$

$$C_2=\sum_{ij}g_{ij}g_{ji}\ , \tag{3.20}$$

$$C_3=\sum_{ijk}g_{ij}g_{jk}g_{kl}\ , \tag{3.21}$$

which have the value 1 in the pure case considered in this work.

It is to be stressed that the solutions of the system (3.17), i.e., the $g_{ij}(t)$, yield the exact (intensive) expectation values $\langle \hat{G}_{ij} \rangle / N$ in the thermodynamic limit ($N \to \infty$).

For finite N, however, we do not obtain accurate results. These in turn, to make the situation even worse, strongly depend on the initial conditions.

Of special interest are the stationary solutions of the system (3.17) (that is, the static HF solutions). Taking, for simplicity,

$$v_{ij} = v(1-\delta_{ij}), \quad \forall\, i,j \tag{3.22}$$

these can be classified into several types, according to the number of s.p. levels that play an active role in the ensuing situation. In this work we shall concern ourselves with solutions of the type

$$x_i = 1, \quad x_j = 0, \quad j \neq i \tag{3.23}$$

where just one of the available s.p. levels is occupied. In this situation there exists just one self-consistent static Hamiltonian $\hat{h}$, which coincides with $\hat{H}_0$. These solutions are the unique ones for

$$|v| < \mathrm{Min}(\epsilon_i - \epsilon_j) = 1, \quad i \neq j \tag{3.24}$$

(in the following we take $\epsilon_1 = 0$, $\epsilon_2 = 1$, $\epsilon_3 = 2$).

C. Higher order approaches

1. *Corrected mean field approach (CMFA)*

We first translate Eq. (2.8) into the present context, employing the useful definition

$$\hat{O}^{(2)}_{kij} = [\hat{G}_{ki},\ \hat{G}_{kj}]_+ = \hat{O}^{(2)}_{kji}\ , \tag{3.25}$$

for the only two-body operators of interest here. We have

$$-i\hbar\, d\langle \hat{G}_{ij} \rangle / dt = (\epsilon_i - \epsilon_j)\langle \hat{G}_{ij} \rangle + \tfrac{1}{2} \sum_k \left(V_{ki} \langle \hat{O}^{(2)}_{kij} \rangle - V_{jk} \langle \hat{O}^{(2)\dagger}_{kij} \rangle \right) \tag{3.26}$$

and

$$-i\hbar\, d\langle \hat{O}^{(2)}_{kij} \rangle / dt = (2\epsilon_k - \epsilon_i - \epsilon_j)\langle \hat{O}^{(2)}_{kij} \rangle + \tfrac{1}{2} \sum_l \langle \hat{F}_{lkij} \rangle_{\mathrm{HF}}\ , \tag{3.27}$$

where

$$\hat{F}_{lkij} = V_{lk}([\hat{O}^{(2)}_{lik}, \hat{G}_{ki}]_+ + [\hat{O}^{(2)}_{ljk}, \hat{G}_{ki}]_+) - V_{il}([\hat{O}^{(2)\dagger}_{lik}, \hat{G}_{kj}]_+ - V_{jl}[\hat{O}^{(2)\dagger}_{ljk}, \hat{G}_{ki}]_+)\ , \tag{3.28}$$

the sums over k,l being restricted by the condition $V_{ii} = 0$, $\forall i$.

2. *Perturbative treatments*

We next turn our attention to the "perturbative" approaches of Sec. II C. The first one, if we go up to first order ($M = 2$), leads to a set like that posed by (3.26) and (3.27), but with $\hat{F}_{lkij} = 0$. When going up to second order, the following additional equations must be incorporated, in addition to (3.26) and (3.27), (with the exact value of $\langle \hat{F}_{lkij} \rangle$):

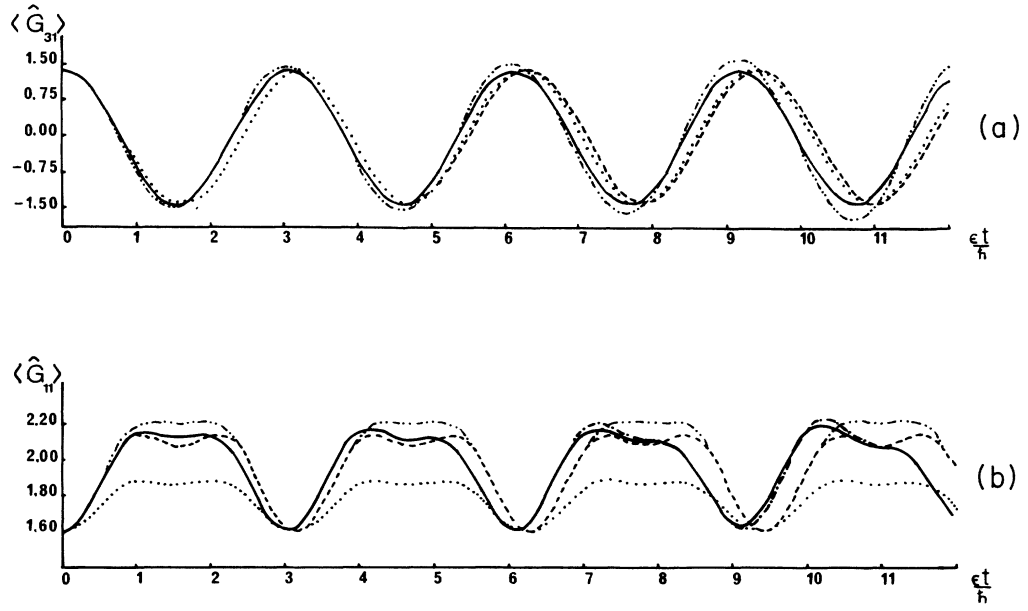

FIG. 1. Temporal evolution of (a) $\mathrm{Re}\langle \hat{G}_{31} \rangle$ and (b) $\langle \hat{G}_{11} \rangle$ for $N = 10$. Initial values are $x^2_1 = 0.4$, $x^2_{2,3} = 0.3$ (all x_i real). The coupling constant is $v = -0.5$. Exact results, ——; TDHF results, · · · ·; CMFA results, —·—·—·; first order perturbative treatment, — — —; second order perturbative treatment, —··—··—. The time in all figures is given in units of $\hbar/\epsilon$, $\epsilon = \epsilon_2 - \epsilon_1$ (see Sec. III B) and expectation values are in units of $N/4$. In (a), the CMFA results cannot be distinguished from exact results on the scale of the figure.

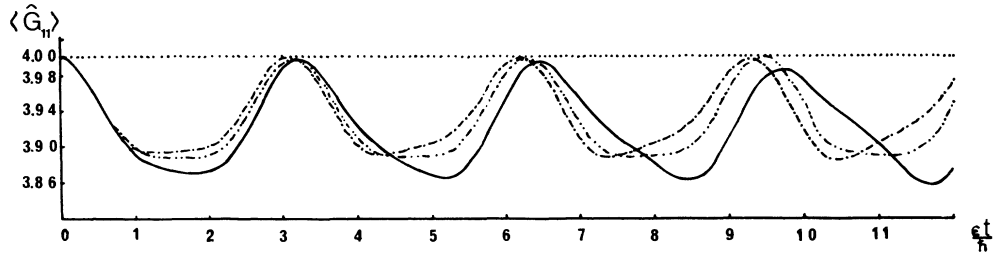

FIG. 2. Temporal evolution of $\langle \hat{G}_{11} \rangle$ for the stationary initial values $x_1=1$, $x_2=x_3=0$, and $v=-0.5$ ($N=10$). The same conventions as Fig. 1 are used. Exact, CMFA, and second order perturbative treatments are shown. Both TDHF and first order perturbations predict a constant evolution. Nondiagonal operators vanish in all treatments.

$$-i\hbar d\langle [\hat{O}^{(2)}_{lik},\hat{G}_{kj}]_+ \rangle /dt = \langle [\hat{H}_0,[\hat{O}^{(2)}_{lik},\hat{G}_{kj}]_+] \rangle = (2\epsilon_l-\epsilon_j-\epsilon_i)\langle [\hat{O}^{(2)}_{lik},\hat{G}_{kj}]_+ \rangle \tag{3.29}$$

and

$$-i\hbar d\langle [\hat{O}^{(2)}_{ljk},\hat{G}_{ki}]_+ \rangle /dt = [2(\epsilon_k-\epsilon_l)+\epsilon_j-\epsilon_i]\langle [\hat{O}^{(2)\dagger}_{ljk},\hat{G}_{ki}]_+ \rangle \ . \tag{3.30}$$

The resulting system is a linear one and can be trivially solved. Three-body expectation values oscillate, as t grows, with the unperturbed frequencies. Of course, for the remaining observables, terms arising from the two-body component of $\hat{H}$ have an effect in their temporal evolution although the corresponding frequencies are independent of the coupling constant.

Finally, if we replace $\hat{H}_0$ with $\hat{h}$ in the system of equations just discussed, we get a nonlinear and much larger system, as the closure of the semialgebra with $\hat{h}$ (3.6) in the last step involves the addition of new operators.

IV. RESULTS

A typical situation that serves to illustrate the various methods discussed up to this point is depicted in Fig. 1. The coupling constant is $v=-0.5$, while the initial constants are of the real kind, with $x_1^2=0.4$ and $x_2^2=x_3^2=0.3$. For the case of nondiagonal operators, the TDHF results soon fall out of phase with the exact ones, their behavior being of a sinusoidal character. In the case of $\langle \hat{G}_{11} \rangle$, which exhibits a highly nonlinear behavior, the TDHF approach fails to provide correct amplitudes even in the course of the first temporal oscillation. On the contrary, the results obtained with the method introduced in Sec. II B (CMFA) are quite accurate, even for $M=2$ (first order). Neither of the two perturbative techniques described in Sec. II C match these CMFA results, although the corresponding values constitute an improvement upon the TDHF ones. Notice that second order perturbative figures are inferior to the first-order ones provided by the set of equations (3.26) and (3.27). Of course, for sufficiently long periods, all approximations will deviate from the exact evolution. See, however, the remark concerning time units in Sec. III B.

The static s.p. mean field Hamiltonian $\hat{H}_0$ [Eq. (3.3)] has been used in all cases as the unperturbed Hamiltonian. The use of the dynamic s.p. Hamiltonian (3.6) in place of $\hat{H}_0$ does not improve appreciably the accuracy of the results in all treatments, and in some circumstances the results are even worse, in spite of the approaches becoming much more involved.

The situation in which the initial conditions correspond to a static HF solution (Fig. 2) deserves special attention. In this case the TDHF approach predicts no evolution at all, contrary to what happens in the exact instance (these HF solutions do not provide us, of course, with exact eigenstates of $\hat{H}$). Our approach yields, instead, a nonstationary temporal evolution (even for $M=2$). On the other hand, the perturbative approaches will not take us out of the stationary situation if we stop at first order, forcing one to go at least up to second order. The CMFA results of Fig. 2 are rather satisfactory ones.

Still a different type of circumstance is illustrated in Fig. 3. Although the TDHF approach gives the right initial tendency of the system when the number of parti-

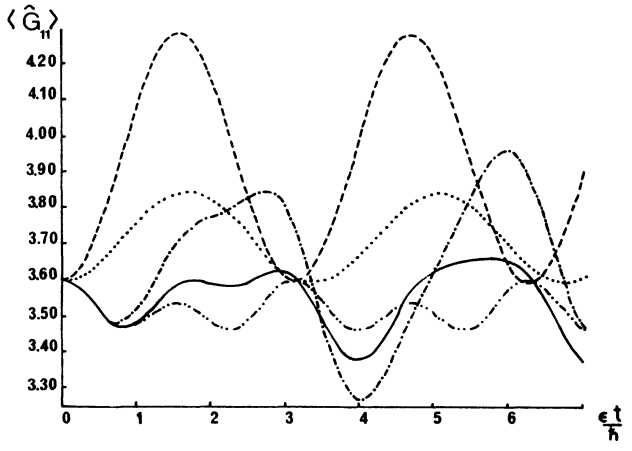

FIG. 3. Mean value of $\langle \hat{G}_{11} \rangle$ vs time for $x_1^2=0.9$, $x_2^2=0.1$, $N=10$, and $v=-0.95$. Details are similar to those of Fig. 1. The initial trend of TDHF differs from that of the exact behavior.

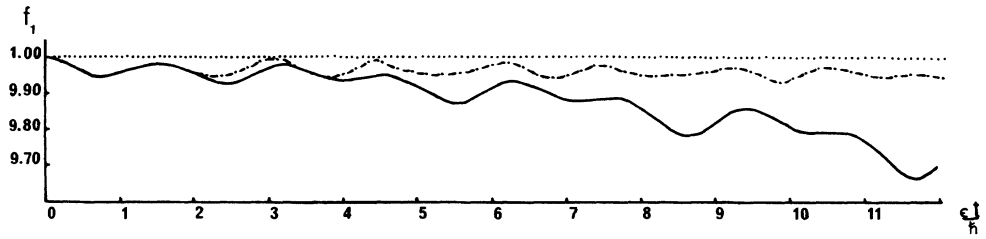

FIG. 4. The greatest eigenvalue of the s.p. density matrix (f_1) vs time for the same conditions of Fig. 1. Exact results (——) and CMFA results (—·—·—·). f_1 remains equal to 1 in TDHF (· · · ·), reflecting the idempotent character of this approach.

cles N is large, it may not be so if N is sufficiently small (but not necessarily too small). In the example considered, the initial values of $\langle \hat{G}_{ij} \rangle$ are all real and, consequently, all the first time derivatives of real parts of $\langle \hat{G}_{ij} \rangle$ vanish initially for Hamiltonian (3.3). Since the second time derivative is not guaranteed by the TDHF approach, we cannot assure in this case the correct initial behavior.

For instance, the second initial time derivative of $\langle \hat{G}_{ii} \rangle$ in the mean field approach is given in this case by

$$d^2\langle \hat{G}_{ii} \rangle_{\mathrm{HF}}/dt^2 \mid_{t=0} = -4v/(N\hbar^2) \sum_{k\neq i} (\langle \hat{G}_{ki} \rangle_0 \langle [\hat{h}, \hat{G}_{ki}] \rangle_0)$$
$$= -4v/(N\hbar^2) \sum_{k\neq i} \langle \hat{G}_{ki} \rangle_0^2 [(\epsilon_k - \epsilon_i) + v/N \langle (-\hat{G}_{kk} + \hat{G}_{ii}) \rangle_0] \tag{4.1a}$$

(0 denotes initial value), whereas the exact value is

$$d^2\langle \hat{G}_{ii} \rangle_{\mathrm{exact}}/dt^2 \mid_{t=0} = -2V/\hbar^2 \sum_{k\neq i} (\langle [\hat{H}, \hat{G}_{ki}^2] \rangle_0)$$
$$= -2V/\hbar^2 \sum_{k\neq i} \left[2(\epsilon_k - \epsilon_i) \langle \hat{G}_{ki}^2 \rangle_0 + \sum_{l\neq m} V/2 \langle [\hat{G}_{lm}^2, \hat{G}_{ki}^2] \rangle_0 \right] . \tag{4.1b}$$

Thus, for $N = 10$ and $x_1^2 = 0.9$ and $x_2^2 = 0.1$, $\langle \hat{G}_{11} \rangle$ increases initially if $0 > v > -1.250$ according to (4.1a), and $0 > v > -0.568$ according to (4.1b), and, consequently, there is a range in which the TDHF approach fails to give the correct initial tendency.

The power of the CMFA, which allows for the right Mth time derivative, is in this instance amply demonstrated (already in first order). The perturbative treatments give also the correct answer here, but one needs to go up to second order.

Moreover, the CMFA is able to detect effects appearing at (considerable) later times, which indicates the fact that this technique is not a mere "parabolic" estimate of the time evolution (the first two time derivatives are correct).

Figure 4 depicts the behavior of the largest eigenvalue of the s.p. density matrix (the largest occupation number), which is constant in the TDHF treatment. The CMFA s.p. density matrix will cease to be an idempotent one for $t > 0$. Indeed, its eigenvalues (i.e., the occupation numbers) will not be constant as t grows, contrary to what happens in the TDHF instance. This reflects the influence of the correlations we are including in this treatment. Once more, this fact provides us with fresh additional evidence in favor of the CMFA.

Of course, the accuracy of both the CMFA and the TDHF approach decreases as the coupling constant increases, but does so in a slower fashion for the former than for the latter.

V. CONCLUSIONS

We have introduced and illustrated a new method for the description of the temporal evolution that allows for a systematic way of improving the renowned TDHF approach.

This method is not more difficult to handle than the TDHF one, and can be applied, consequently, to a wide class of physical problems. It is quite accurate [at least within the U(3) framework here discussed] in those instances in which TDHF works fairly well, and is still reliable in circumstances not tractable within the TDHF scope.

The central idea governing our extended treatment is that of closing (albeit in nonlinear fashion) a partial Lie algebra under commutation with the Hamiltonian. Alternative ways of effecting this closure have also been discussed and illustrated. A novel feature of these methods is that the approach yields the desired order of

accuracy just for those operators we are interested in, whereas ordinary methods deal with the corresponding wave function or density operator, making them much more difficult to apply (and to extract the desired expectation values). The present technique is based directly and explicitly on expectation values.

We do not assume any relaxation time approximation. Our methods are based on a suitable truncation of the corresponding semialgebra formed by the Hamiltonian on one hand, and the observables we are interested in on the other.

An essential feature of the CMFA is the self-consistent evaluation of those terms that are discarded in a perturbative treatment. This evaluation is seen to provide a degree of accuracy similar to that obtained in going up one step in the perturbative series. Accordingly, the correct Mth-order initial time derivative of s.p. mean values is attained. Of course, we do not pretend to offer an approach that may replace the TDHF one, but a technique that may complement it in some special circumstances that ask for increased accuracy.

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