Time-dependent coupled-cluster approximation to nuclear dynamics. II. General formulation

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A general formulation is presented of the time-dependent coupled-cluster hierarchy of equations introduced previously. Truncations appropriate to potentials with strongly repulsive cores are specified and the properties of the resulting equations of motion are discussed.

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I. INTRODUCTION

In the first paper of this series,[1] hereafter denoted as I, the time-dependent coupled-cluster theory was shown to provide a convenient systematic hierarchy of corrections to the intuitively appealing time-dependent mean-field approximation. This theory, which is formulated in terms of multi-particle-hole amplitudes, offers the significant advantage of representing many-particle correlations much more economically than corresponding density-matrix or Green's function hierarchies. Furthermore, explicit application to the exactly solvable problem of two systems interacting via the Lipkin model Hamiltonian has demonstrated satisfactory convergence of expectation values of few body operators toward the exact values in the first two orders of successive approximations. Hence, the time-dependent coupled-cluster theory demonstrates sufficient promise to warrant application to more realistic nuclear systems with potentials having strongly repulsive cores.

This present work, therefore, addresses the problem of deriving a general coordinate-space formulation suitable for potentials with repulsive cores. For pedagogical purposes, the low order equations are derived two different ways. First, in Sec. II, generalized time-dependent Hartree-Fock (GTDHF) and generalized time-dependent Bethe-Goldstone (GTDBG) equations are derived in terms of subsystem amplitudes. This approach, which follows the time-independent approach of Lührmann,[2] offers the advantage of introducing a minimum of definitions and formalism and renders the physical approximations involved in truncation particularly transparent. Since this method becomes progressively more cumbersome in higher orders, a general derivation is presented in Sec. III using the e^S formulation of Ref. 1. Finally, salient properties of the coupled-cluster equations are discussed in Sec. IV.

II. TIME-DEPENDENT EQUATIONS FOR SUBSYSTEMS

We consider N-particle solutions to the time-dependent Schrödinger equation

$$H|\psi(t)\rangle = i\frac{\partial}{\partial t}|\psi(t)\rangle , \tag{2.1}$$

with Hamiltonian

$$H=\sum_{\alpha\beta} T_{\alpha\beta}a_\alpha^\dagger a_\beta + \tfrac{1}{2}\sum_{\alpha\beta\delta\gamma} V_{\alpha\beta\delta\gamma}a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta . \tag{2.2}$$

The indices α, β, γ, δ labeling creation and annihilation operators represent a complete set of single-particle quantum numbers in an as yet unspecified and possibly time-dependent basis and may range over both normally occupied and unoccupied states. It is useful to define an N-particle determinantal wave function

$$|\Phi\rangle = a_{\nu_1}^\dagger a_{\nu_2}^\dagger \cdots a_{\nu_n}^\dagger |0\rangle , \tag{2.3}$$

with ψ normalized such that $\langle\phi(t)|\psi(t)\rangle = 1$ and to use the convention of Ref. 1 that ν, μ denote normally occupied states and ρ, λ denote normally unoccupied states.

A. Subsystem amplitudes

The set of reduced wave functions introduced by Kümmel,[3] provide a convenient way of decomposing the total wave function of a many body system into parts composed of successively higher correlation functions.

$$\langle x_1\cdots x_n|\psi_n|\nu_1\cdots\nu_n\rangle \equiv \langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle . \tag{2.4}$$

The reduced wave functions ψ_n are antisymmetric under exchange of any two particle labels or any two coordinates by virtue of the anticommutation relations for fermions. These reduced wave func-

tions describe the amplitude for n particles to be at the positions $x_1 \cdots x_n$, while the rest of the particles are required to occupy the states $\nu_{n+1} \cdots \nu_N$. The nth order reduced wave function thus corresponds to an n-body subsystem amplitude, and this physical interpretation will be important in developing approximations. For a non-interacting system, it is obvious from Eq. (2.4) that the n-subsystem amplitude is just $A_\nu[\phi_{\nu_1}(x_1) \cdots \phi_{\nu_n}(x_n)]$, where A_ν antisymmetrizes with respect to the labels $\nu_1 \cdots \nu_n$.

A set of time-dependent correlation amplitudes S_n may then be defined in terms of these subsystem amplitudes:

$$\begin{aligned}
&\langle x_1|\psi_1|\nu_1\rangle = \langle x_1|\nu_1\rangle + \langle x_1|S_1|\nu_1\rangle ,\\
&\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle = A_\nu[\langle x_1|\psi_1|\nu_1\rangle\langle x_2|\psi_1|\nu_2\rangle] + \langle x_1x_2|S_2|\nu_1\nu_2\rangle ,\\
&\langle x_1x_2x_3|\psi_3|\nu_1\nu_2\nu_3\rangle = A_\nu[\langle x_1|\psi_1|\nu_1\rangle\langle x_2|\psi_1|\nu_2\rangle\langle x_3|\psi_1|\nu_3\rangle]\\
&\qquad + A_\nu'[\langle x_1x_2|S_2|\nu_1\nu_2\rangle\langle x_3|\psi_1|\nu_3\rangle + \langle x_1x_3|S_2|\nu_1\nu_3\rangle\langle x_2|\psi_1|\nu_2\rangle\\
&\qquad\quad + \langle x_2x_3|S_2|\nu_2\nu_3\rangle\langle x_1|\psi_1|\nu_1\rangle] + \langle x_1x_2x_3|S_3|\nu_1\nu_2\nu_3\rangle ,
\end{aligned} \tag{2.5}$$

where the prime on the antisymmetrizing operator A_ν' indicates that no labels within any S are to be antisymmetrized.

In each order, S_n is uniquely defined such that it represents that part of ψ_n which cannot be decomposed into an antisymmetrized product of previously defined functions of fewer variables. Since the decomposition of the subsystem amplitudes ψ_n for general n is both unnecessary for the present purpose and somewhat involved, we shall simply summarize the important properties of these correlation amplitudes S_n.

(a) For a vanishing two-body interaction, $S_n = 0$ for $n > 1$.

(b) $\langle x_1 \cdots x_n|S_n|\nu_1 \cdots \nu_n\rangle$ is antisymmetric under exchange of any two coordinate labels or any two hole labels for $n > 1$.

(c) For all $n > 1$, by use of the fermion commutation rules, it is easy to establish the following orthogonality property of the correlation amplitudes S_n with respect to the occupied state wavefunctions ϕ_ν:

$$\int dx_i \phi^*_{\nu_k}(x_i)\langle x_1 \cdots x_i \cdots x_n|S_n|\nu_1 \cdots \nu_i \cdots \nu_n\rangle = 0. \tag{2.6}$$

This relation is a nontrivial nonlocal constraint on admissible forms of S_n.

(d) For finite range forces, as the distance $|x_i - x_j|$ between any pair of coordinates increases, S_n approaches zero.

(e) The interpretation of S_n as an n-body correlation amplitude arises from the fact that it represents that part of ψ_n which cannot be decomposed into products of lower order amplitudes.

(f) Although we have not stressed the relation, the S_n's are precisely the n-particle–n-hole amplitudes in Eq. (1.1) of Ref. 1 occurring in the equation

$$|\psi\rangle = \exp\sum_m S_m \ |\phi\rangle .$$

This relation may be straightforwardly derived[4] by evaluating

$$\langle x_1 \cdots x_n|\psi_n|\nu_1 \cdots \nu_n\rangle = \left\langle \phi \left| a^\dagger_{\nu_1} \cdots a^\dagger_{\nu_n} a(x_n) \cdots a(x_1) \exp\left(\sum_{m=1}^{n} S_m\right) \right| \phi \right\rangle \tag{2.7}$$

for each n with

$$S_m = \frac{1}{(m!)^2}\langle x_1 \cdots x_m|S_m|\nu_1 \cdots \nu_m\rangle a^\dagger(x_1) \cdots a^\dagger(x_m) a_{\nu_m} \cdots a_{\nu_1} , \tag{2.8a}$$

where

$$\langle x_1 \cdots x_m|S_m|\nu_1 \cdots \nu_m\rangle \equiv \sum_{\rho_1 \cdots \rho_m} \langle x_1|\rho_1\rangle \cdots \langle x_m|\rho_m\rangle\langle\rho_1 \cdots \rho_m|S_m|\nu_1 \cdots \nu_m\rangle . \tag{2.8b}$$

B. Projection

By projecting the Schrödinger equation (2.1) onto a complete set of states, we can generate the following set of exact relations:

$$\langle\Phi|\left(H-i\frac{\partial}{\partial t}\right)|\Psi\rangle=0, \tag{2.9a}$$

$$\langle\Phi|a_\nu^\dagger a(x)\left(H-i\frac{\partial}{\partial t}\right)|\Psi\rangle=0, \tag{2.9b}$$

$$\langle\Phi|a_{\nu_1}^\dagger a_{\nu_2}^\dagger a(x_2)a(x_1)\left(H-i\frac{\partial}{\partial t}\right)|\Psi\rangle=0, \tag{2.9c}$$

$$\cdots$$

$$\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)\left(H-i\frac{\partial}{\partial t}\right)|\Psi\rangle=0. \tag{2.9d}$$

The terms involving the time derivative in Eqs. (2.6) are evaluated making use of Eq. (2.9) of Ref. 1:

$$\frac{\partial}{\partial t}a_\alpha^\dagger=\sum_\beta\langle\beta|\dot\alpha\rangle a_\beta^\dagger. \tag{2.10}$$

Thus

$$\begin{aligned}
&\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)\frac{\partial}{\partial t}|\Psi\rangle\\
&=\frac{\partial}{\partial t}\langle x_1\cdots x_n|\psi_n|\nu_1\cdots\nu_n\rangle-\sum_{i=1}^n\langle\Phi|a_{\nu_1}^\dagger\cdots\dot a_{\nu_i}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\\
&\quad-\left(\frac{\partial}{\partial t}\langle\Phi|\right)a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\\
&=\frac{\partial}{\partial t}\langle x_1\cdots x_n|\psi_n|\nu_1\cdots\nu_n\rangle-\sum_{i=1}^n\sum_\nu\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_{i-1}}^\dagger a_\nu^\dagger a_{\nu_{i+1}}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\langle\nu|\dot\nu_i\rangle\\
&\quad-\sum_{\alpha\nu}\langle\Phi|a_\nu^\dagger a_\alpha a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\langle\dot\nu|\alpha\rangle.
\end{aligned} \tag{2.11}$$

By use of the anticommutation rules, the last term in Eq. (2.11) above is

$$\begin{aligned}
&\sum_{\alpha\nu}\langle\Phi|a_\nu^\dagger a_\alpha a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\langle\dot\nu|\alpha\rangle\\
&=\sum_\nu\langle x_1\cdots x_n\dot\nu|\psi_{n+1}|\nu_1\cdots\nu_n\nu\rangle+\sum_{i=1}^n\sum_\nu\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_{i-1}}^\dagger a_\nu^\dagger a_{\nu_{i+1}}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)|\Psi\rangle\langle\dot\nu|\nu_i\rangle,
\end{aligned} \tag{2.12}$$

where we have used the notation

$$\begin{aligned}
\langle x_1\cdots x_n\dot\nu|\psi_{n+1}|\nu_1\cdots\nu_n\nu\rangle&\equiv\sum_\alpha\langle\dot\nu|\alpha\rangle\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a_\nu^\dagger a_\alpha a(x_n)\cdots a(x_1)|\Psi\rangle\\
&=\int dx\dot\phi_\nu^*(x)\langle x_1\cdots x_n x|\psi_{n+1}|\nu_1\cdots\nu_n\nu\rangle.
\end{aligned} \tag{2.13}$$

Combining Eqs. (2.11) and (2.12), and recognizing that for an orthonormal basis

$$\langle\nu|\dot\nu_i\rangle+\langle\dot\nu|\nu_i\rangle=\frac{d}{dt}\langle\nu|\nu_i\rangle=0, \tag{2.14}$$

the time derivative terms of Eqs. (2.9) become

$$\left\langle\Phi\left|a_{\nu_1}^\dagger\cdots a_{\nu_n}^\dagger a(x_n)\cdots a(x_1)i\frac{\partial}{\partial t}\right|\Psi\right\rangle=i\frac{\partial}{\partial t}\langle x_1\cdots x_n|\psi_n|\nu_1\cdots\nu_n\rangle-i\sum_\nu\langle x_1\cdots x_n\dot\nu|\psi_{n+1}|\nu_1\cdots\nu_n\nu\rangle. \tag{2.15}$$

The Hamiltonian (2.2) can now be inserted into Eqs. (2.9) and, after some algebra, we obtain the following equations, corresponding to Eqs. (2.9a), (2.9b), and (2.9c), respectively:

$$\sum_{\nu}\langle\nu|T\psi_1|\nu\rangle+\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V\psi_2|\nu\nu'\rangle=-i\sum_{\nu}\langle\dot{\nu}|\psi_1|\nu\rangle\,, \tag{2.16a}$$

$$T(x)\langle x|\psi_1|\nu\rangle+\sum_{\nu'}\langle\nu' x|T\psi_2|\nu'\nu\rangle+\sum_{\nu'}\langle\nu' x|V\psi_2|\nu'\nu\rangle+\tfrac{1}{2}\sum_{\nu'\nu''}\langle\nu'\nu'' x|V\psi_3|\nu'\nu''\nu\rangle=i\frac{\partial}{\partial t}\langle x|\psi_1|\nu\rangle-i\sum_{\nu'}\langle x\dot{\nu}'|\psi_2|\nu\nu'\rangle\,, \tag{2.16b}$$

$$\begin{aligned}[T(x_1)+T(x_2)+V(x_1x_2)]\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle&+\sum_{\nu}\langle\nu x_1x_2|T\psi_3|\nu\nu_1\nu_2\rangle\\&+\sum_{\nu}\langle\nu x_1x_2|[V(xx_1)+V(xx_2)]\psi_3|\nu\nu_1\nu_2\rangle+\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu' x_1x_2|V\psi_4|\nu\nu'\nu_1\nu_2\rangle\\&=i\frac{\partial}{\partial t}\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle-i\sum_{\nu}\langle\dot{\nu}x_1x_2|\psi_3|\nu\nu_1\nu_2\rangle\,,\end{aligned} \tag{2.16c}$$

where, following Ref. 2, we have introduced the abbreviations

$$\langle\nu x_1\cdots x_{n-1}|T\psi_n|\mu_1\cdots\mu_n\rangle\equiv\int dx\langle\nu|x\rangle T(x)\langle xx_1\cdots x_{n-1}|\psi_n|\mu_1\cdots\mu_n\rangle\,, \tag{2.17a}$$

$$\langle\nu\nu' x_1\cdots x_{n-2}|V\psi_n|\mu_1\cdots\mu_n\rangle\equiv\int dxdx'\langle\nu|x\rangle\langle\nu'|x'\rangle V(xx')\langle xx' x_1\cdots x_{n-2}|\psi_n|\mu_1\cdots\mu_n\rangle\,, \tag{2.17b}$$

$$\langle\nu x_1\cdots x_{n-1}|V(xx_i)\psi_n|\mu_1\cdots\mu_n\rangle\equiv\int dx\langle\nu|x\rangle V(xx_i)\langle xx_1\cdots x_{n-1}|\psi_n|\mu_1\cdots\mu_n\rangle\,, \tag{2.17c}$$

and

$$\langle\nu x_1|V\psi_2|\mu_1\mu_2\rangle\equiv\langle\nu x_1|V(xx_1)\psi_2|\mu_1\mu_2\rangle\,. \tag{2.17d}$$

From Eqs. (2.16) it is evident that each additional equation generated by higher order projection introduces one new unknown amplitude, so some physically motivated approximation is required to truncate the hierarchy of exact equations.

C. Truncation of the subsystem hierarchy

For systems without strong short range forces, a reasonable and unambiguous approximation is to set all $S_m=0$ for $m>n$ as in Ref. 1, thereby obtaining a closed set of equations for S_1 through S_n. However, such a truncation is not appropriate to the nuclear many-body problem where the hard core requires that the wave function vanish inside the core.

To truncate the set of Eqs. (2.16) to depend only on ψ_1 and ψ_2, or equivalently S_1 and S_2, it is necessary to approximate the ψ_3 term in (2.16b) and the ψ_3 and ψ_4 terms in (2.16c). As in Refs. 2–4, physical insight suggests distinct approximations for the potential energy terms and the kinetic and time derivative terms. For the potential terms in (2.16b) and (2.16c), it is absolutely crucial that the subsystem amplitudes ψ_3 and ψ_4 at least become small when the relative coordinate occurring in the potential becomes small. Thus, for the potential terms in (2.16b) and (2.16c), the quantity $V\psi_3$ is approximated as follows:

$$\begin{aligned}&V(xx')\langle xx' y|\psi_3|\nu_1\nu_2\nu_3\rangle\\&\quad\approx A'_{\nu}[V(xx')\langle xx'|\psi_2|\nu_1\nu_2\rangle\langle y|\psi_1|\nu_3\rangle]\,.\end{aligned} \tag{2.18}$$

Comparison with Eq. (2.15) indicates that this is different from specifying $S_3=0$. Whereas antisymmetry is thereby relinquished, just those terms involving products of $S_2\psi_1$ are dropped so as to allow $\langle xx' y|\psi_3|\nu_1\nu_2\nu_3\rangle$ to vanish like the two-body correlation function for small values of $|x-x'|$. Thus, Eq. (2.18) singles out a distinct pair of particles, namely those which will interact via the two-body interaction, and specifies that they propagate as an independent pair uncorrelated with the third particle. In the same spirit, a corresponding approximation is introduced for $V\psi_4$ in Eq. (2.16c)

$$\begin{aligned}&V(xx')\langle xx' x_1x_2|\psi_4|\nu\nu'\nu_1\nu_2\rangle\\&\quad\approx A'_{\nu}[V(xx')\langle xx'|\psi_2|\nu\nu'\rangle\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle]\,.\end{aligned} \tag{2.19}$$

Here again, the pair of interacting particles is singled out to propagate as a correlated pair independent of the other pair of spectator particles, relinquishing antisymmetry in order to force ψ_4 to vanish for small values of the relative coordinates of the two interacting particles.

For the terms involving $T(x)$ or $\dot{\phi}^{\dagger}_{\nu}(x)$ acting on $\langle xx_1x_2|\psi_3|\nu\nu_1\nu_2\rangle$ in Eq. (2.16c), there is no reason for these operators to single out any specific subsystem or for the behavior of small values of any particular relative coordinate to be important. Thus, a totally antisymmetric truncation is introduced by setting $S_3=0$ in Eq. (2.5). Denoting either $\dot{\phi}^{\dagger}_{\nu}(x)$ or $T(x)$ by $\mathcal{O}(x)$, the following approx-

imation is made:

$$\begin{aligned}\Theta(x)&\langle xx_1x_2|\psi_3|\nu\nu_1\nu_2\rangle\\ &\approx\Theta(x)A'_\nu[\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle\langle x|\psi_1|\nu\rangle\\ &\quad+\langle x_1|\psi_1|\nu_1\rangle\langle xx_2|S_2|\nu\nu_2\rangle\\ &\quad+\langle x_2|\psi_1|\nu_2\rangle\langle xx_1|S_2|\nu\nu_1\rangle].\end{aligned}\tag{2.20}$$

By the definition of S_2 in Eq. (2.5), this expression is manifestly antisymmetric.

Two crucial questions have not been addressed in this very elementary and intuitive discussion of truncation. The first is whether Eqs. (2.18)–(2.20) represent a systematic procedure which may be unambiguously extended to all orders. The procedure is, in fact, completely general. Terms of the form $\Theta(x)\langle xx_1\cdots x_m|\psi_{m+1}|\nu\nu_1\cdots\nu_m\rangle$ may be systematically truncated at order m by imposing the condition $S_{m+1}=0$, and Eq. (2.7) provides a general relation between S_{m+1} and the ψ's. Consistent with our philosophy of avoiding unnecessary formalism, we have not introduced the reduced subsystem amplitudes $\chi_m^{(ij)}$ of Appendix B of Ref. 4. For strongly repulsive potentials, the general truncation of potential terms at order m may be effected in terms of these amplitudes by imposing the condition $\chi_{m+1}^{(ij)}=\chi_{m+2}^{(ij)}=0$ in the terms $V(x_ix_j)\psi_{m+1}$ and $V(x_ix_j)\psi_{m+2}$. Equations (2.18) and (2.19) correspond to the special case of $m=2$.

The second question concerns the convergence of this truncation procedure for realistic potentials. In the case of stationary states, the application of this procedure to light nuclei summarized in Ref. 4 yields very satisfactory apparent numerical convergence with the Reid potential. Given that the time-independent hierarchy truncated in this way appears to be the most satisfactory microscopic formalism yet to be implemented, we believe that the present truncation provides the most promising candidate for the time-dependent hierarchy. The only terms containing time derivatives requiring truncation have the same structure in the kinetic terms and consistency thus requires that they be truncated analogously. The need for consistency is particularly evident for stationary states in an arbitrary potential, in which case $i\dot\phi_\nu=\epsilon_\nu\phi_\nu$ and thus

$$\begin{aligned}\int dx&[\phi_\nu^*(x)T(x)+i\dot\phi_\nu^*(x)]\langle xx_1x_2|\psi_3|\nu\nu_1\nu_2\rangle\\ &=\int dx\phi_\nu^*(x)[T(x)-\epsilon_\nu]\langle xx_1x_2|\psi_3|\nu\nu_1\nu_2\rangle.\end{aligned}\tag{2.21}$$

D. Truncated one- and two-particle equations

Truncated equations of motion for S_1 and S_2 may be obtained by applying approximations (2.18) through (2.20) to Eqs. (2.16a)–(2.16c).

We first note that Eq. (2.16a) requires no approximation and specifies nothing about the dynamics of any S_n. Each of the terms is proportional to the number of particles in the system, N, and in the case of stationary states, this equation specifies the exact energy.

The equation of motion for ψ_1, and thus S_1, is obtained from Eq. (2.16b). Substituting approximation (2.18) and writing the full expressions for the abbreviations (2.13) and (2.17) yields the equation

$$\begin{aligned}&T(x)\langle x|\psi_1|\nu\rangle+\sum_{\nu'}\int dx'\langle\nu'|x'\rangle T(x')\langle x'x|\psi_2|\nu'\nu\rangle+\sum_{\nu'}\int dx'\langle\nu'|x'\rangle V(x,x')\langle x'x|\psi_2|\nu'\nu\rangle\\ &+\tfrac12\sum_{\nu'\nu''}\int dx'dx''\langle\nu'|x'\rangle\langle\nu''|x''\rangle V(x'x'')\{\langle x'x''|\psi_2|\nu'\nu''\rangle\langle x|\psi_1|\nu\rangle+\langle x''x|\psi_2|\nu''\nu\rangle\langle x'|\psi_1|\nu'\rangle\\ &+\langle xx'|\psi_2|\nu\nu'|\rangle\langle x''|\psi_1|\nu''\rangle\}-i\frac{\partial}{\partial t}\langle x|\psi_1|\nu\rangle+i\sum_{\nu'}\int dx'\langle\nu'|x'\rangle\langle xx'|\psi_2|\nu\nu'\rangle=0.\end{aligned}\tag{2.22}$$

This equation contains terms like $[T(x)-i\partial/\partial t]\langle x|\psi_1|\nu\rangle$ which are independent of the number of particles in the system and specify the evolution of the one-particle amplitude $\langle x|\psi_1|\nu\rangle$. However, substituting the equation for ψ_2, Eq. (2.5), in Eq. (2.22) yields the following three terms proportional to N:

$$\sum_{\nu'}\int dx'\langle\nu'|x'\rangle T(x')\langle x'|\psi_1|\nu'\rangle\langle x|\psi_1|\nu\rangle,\tag{2.23a}$$

$$\tfrac12\sum_{\nu'\nu''}\int dx'dx''\langle\nu'|x'\rangle\langle\nu''|x''\rangle V(x'x'')\langle x'x''|\psi_2|\nu'\nu''\rangle\langle x|\psi_1|\nu\rangle,\tag{2.23b}$$

and

$$i\sum_{\nu'}\int dx''\langle\dot\nu'|x'\rangle\langle x'|\psi_1|\nu'\rangle\langle x|\psi_1|\nu\rangle.\tag{2.23c}$$

Just as in the case of stationary-state linked cluster expansions, a viable theory for large N requires the systematic removal of all such unlinked terms that factorize into independent products and thus introduce improper N-dependence. In the case of Eq. (2.22), this cancellation is trivially accomplished by multiplying Eq. (2.16a) by $\langle x|\psi_1|\nu\rangle$ and subtracting. Collecting terms and utilizing our abbreviations for compactness yields the generalized time dependent Hartree-Fock (GTDHF) equation

$$T(x)\langle x|\psi_1|\nu\rangle+\sum_{\nu'}\langle x\nu'|TS_2|\nu\nu'\rangle+\sum_{\nu'}\langle x\nu'|V\psi_2|\nu\nu'\rangle-\sum_{\nu'}\langle x|\psi_1|\nu'\rangle h_{\nu'\nu}$$
$$=i\frac{\partial}{\partial t}\langle x|\psi_1|\nu\rangle-i\sum_{\nu'}[\langle x\dot{\nu}'|S_2|\nu\nu'\rangle-\langle\dot{\nu}'|\psi_1|\nu\rangle\langle x|\psi_1|\nu'\rangle], \tag{2.24}$$

where the matrix $h_{\nu_1\nu_2}$ is defined by

$$h_{\nu_1\nu_2}=\langle\nu_1|T\psi_1|\nu_2\rangle+\sum_{\nu}\langle\nu_1\nu|V\psi_2|\nu_2\nu\rangle. \tag{2.25}$$

To derive the equation of motion for S_2, we substitute the approximations (2.18)–(2.20) into the exact second order equation (2.16c). The resulting equation again contains unlinked terms which may be cancelled by use of the two lower order equations (2.16a) and (2.16b). Straightforward algebra yields the generalized time-dependent Bethe-Goldstone (GTDBG) equation:

$$[T(x_1)+T(x_2)]\langle x_1x_2|S_2|\nu_1\nu_2\rangle-\sum_{\nu}[\langle\nu x_2|TS_2|\nu_1\nu_2\rangle\langle x_1|\psi_1|\nu\rangle+\langle x_1\nu|TS_2|\nu_1\nu_2\rangle\langle x_2|\psi_1|\nu\rangle]$$
$$+V(x_1x_2)\langle x_1x_2|\psi_2|\nu_1\nu_2\rangle-\sum_{\nu}[\langle\nu x_2|V\psi_2|\nu_1\nu_2\rangle\langle x_1|\psi_1|\nu\rangle+\langle x_1\nu|V\psi_2|\nu_1\nu_2\rangle\langle x_2|\psi_1|\nu\rangle]$$
$$+\tfrac{1}{2}\sum_{\nu'\nu''}\langle\nu'\nu''|V\psi_2|\nu_1\nu_2\rangle\langle x_1x_2|\psi_2|\nu'\nu''\rangle-\sum_{\nu}[h_{\nu\nu_1}\langle x_1x_2|S_2|\nu\nu_2\rangle+h_{\nu\nu_2}\langle x_1x_2|S_2|\nu_1\nu\rangle]$$
$$=i\frac{\partial}{\partial t}\langle x_1x_2|S_2|\nu_1\nu_2\rangle+i\sum_{\nu}[\langle\dot{\nu}x_2|S_2|\nu_1\nu_2\rangle\langle x_1|\psi_1|\nu\rangle+\langle x_1\dot{\nu}|S_2|\nu_1\nu_2\rangle\langle x_2|\psi_1|\nu\rangle$$
$$+\langle\dot{\nu}|\psi_1|\nu_1\rangle\langle x_1x_2|S_2|\nu\nu_2\rangle+\langle\dot{\nu}|\psi_1|\nu_2\rangle\langle x_1x_2|S_2|\nu_1\nu\rangle]. \tag{2.26}$$

Although this procedure could be straightforwardly extended to any order, it is clearly desirable to establish a general linked expansion, which is the subject of the next section.

III. LINKED CLUSTER EXPANSION

Having utilized equations for subsystem amplitudes to emphasize the physical approximations introduced in truncation and to display the cancellation of unlinked terms in low orders, we now establish the general linked cluster expansion. It is convenient to write the wave function in the exp(s) form:

$$|\Phi\rangle=e^{\hat{s}}|\Phi\rangle, \tag{3.1}$$

where

$$\hat{S}=\sum_{n=1}^{N}\hat{S}_n, \tag{3.2a}$$

and $\hat{S}_n$ is specified by Eq. (2.8) or in particle-hole representation by

$$\hat{S}_n=\frac{1}{(n!)^2}\sum\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle a^\dagger_{\rho_1}\cdots a^\dagger_{\rho_n}a_{\nu_n}\cdots a_{\nu_1}. \tag{3.2b}$$

As remarked earlier, with these definitions Eqs. (2.5) follow immediately from the definition of the subsystem amplitudes.

Instead of projecting as in Eqs. (2.9), a completely linked expansion is obtained by projecting the Schrödinger equation as follows:

$$\langle\Phi|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-\hat{s}}He^{\hat{s}}|\Phi\rangle=\left\langle\Phi\left|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-\hat{s}}i\frac{\partial}{\partial t}e^{\hat{s}}\right|\Phi\right\rangle. \tag{3.3}$$

Since the left-hand side of Eq. (3.3) occurs in the time-independent coupled-cluster theory, it has been evaluated in general and shown to be completely linked.[4] Thus, we need only evaluate the right-hand side of Eq. (3.3) and demonstrate that it is also linked.

Using the identity

$$e^{-\hat{S}}\frac{\partial}{\partial t}e^{\hat{S}}=\frac{\partial}{\partial t}+\dot{\hat{S}}+\frac{1}{2!}[\dot{\hat{S}},\hat{S}]+\frac{1}{3!}[[\dot{\hat{S}},\hat{S}],\hat{S}]+\cdots, \tag{3.4}$$

and Eqs. (2.8) and (2.10), it was shown in Eq. (2.10) of I that the multiple commutators all vanish yielding the result

$$\langle\Phi|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-\hat{S}}i\frac{\partial}{\partial t}e^{\hat{S}}|\Phi\rangle=\left\langle\Phi\left|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}\left(i\frac{\partial}{\partial t}+i\dot{\hat{S}}+\frac{1}{2}[i\dot{\hat{S}},\hat{S}]\right)\right|\Phi\right\rangle. \tag{3.5}$$

Furthermore, each nonvanishing term in $[\dot{\hat{S}},\hat{S}]$ arises from a term in $\dot{\hat{S}}$ containing $a^{\dagger}_{\nu_i}$ or a_{ρ_i} which yields a nonzero commutator with a_{ν_i} or $a^{\dagger}_{\rho_i}$ in S. Hence, the nonvanishing terms in $[\dot{\hat{S}},\hat{S}]$ are necessarily linked by a common index ν_i or ρ_i and Eq. (3.5) is thus completely linked.

We now evaluate Eq. (3.5) for general $n>1$. By Eq. (2.10) the first term on the right-hand side contributes only for $n=1$ since $(\partial/\partial t)|\Phi\rangle$ generates at most one-particle, one-hole excitations. The second term yields

$$\begin{aligned}
&\langle\Phi|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}i\frac{\partial}{\partial t}\sum_{m=1}^{N}\frac{1}{(m!)^2}\sum_{\nu,\mu}\langle\lambda_1\cdots\lambda_m|S_m|\mu_1\cdots\mu_m\rangle a^{\dagger}_{\lambda_1}\cdots a^{\dagger}_{\lambda_m}a_{\mu_m}\cdots a_{\mu_1}|\Phi\rangle\\
&=i\frac{\partial}{\partial t}\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle+\sum_{i=1}^{n}\sum_{\lambda}\langle\rho_i|\dot{\lambda}\rangle\langle\rho_i\cdots\rho_{i-1}\lambda\rho_{i+1}\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle\\
&+i\sum_{i=1}^{n}\sum_{\mu}\langle\dot{\mu}|\nu_i\rangle\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\nu_{i-1}\mu\nu_{i+1}\cdots\nu_n\rangle+i\sum_{\lambda\mu}\langle\mu|\dot{\lambda}\rangle\langle\lambda\rho_1\cdots\rho_n|S_{n+1}|\mu\nu_1\cdots\nu_n\rangle.
\end{aligned} \tag{3.6}$$

Extending the abbreviation (2.13) to the particle-hole amplitude S_n in the obvious way

$$\begin{aligned}
\langle\dot{\alpha}\rho_2\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle&\equiv\sum_{\rho}\langle\dot{\alpha}|\rho\rangle\langle\rho\rho_2\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle,\\
\langle\rho_1\cdots\rho_n|S_n|\dot{\alpha}\nu_2\cdots\nu_n\rangle&\equiv\sum_{\nu}\langle\nu|\dot{\alpha}\rangle\langle\rho_1\cdots\rho_n|S_n|\nu\nu_2\cdots\nu_n\rangle,
\end{aligned} \tag{3.7}$$

and using Eq. (2.14),

$$\begin{aligned}
\langle\Phi|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}i\dot{\hat{S}}|\Phi\rangle&=i\frac{\partial}{\partial t}\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle-i\sum_{i}\langle\rho_1\cdots\dot{\rho}_i\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle\\
&-i\sum_{i}\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\dot{\nu}_i\cdots\nu_n\rangle-i\sum_{\nu}\langle\dot{\nu}\rho_1\cdots\rho_n|S_{n+1}|\nu\nu_1\cdots\nu_n\rangle.
\end{aligned} \tag{3.8}$$

The third term may be rewritten

$$\begin{aligned}
&\frac{1}{2}\left\langle\Phi\left|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}\left[i\frac{\partial\hat{S}}{\partial t},\hat{S}\right]\right|\phi\right\rangle\\
&=\frac{i}{2}\langle\Phi|a^{\dagger}_{\nu_1}\cdots a^{\dagger}_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}\sum_{k+l=n+1}\frac{1}{(k!)^2(l!)^2}\sum_{\lambda\mu\lambda'\mu'}\Bigg[\sum_{i\beta}\{\langle\beta|\dot{\lambda}_i\rangle a^{\dagger}_{\lambda_1}\cdots a^{\dagger}_{\lambda_{i-1}}a^{\dagger}_{\beta}a^{\dagger}_{\lambda_{i+1}}\cdots a^{\dagger}_{\lambda_k}\cdots a_{\mu_k}\cdots a_{\mu_1}\\
&\qquad+\langle\dot{\mu}_i|\beta\rangle a^{\dagger}_{\lambda_1}\cdots a^{\dagger}_{\lambda_k}a_{\mu_k}\cdots a_{\mu_{i+1}}a_{\beta}a_{\mu_{i-1}}\cdots a_{\mu_1}\},\ a^{\dagger}_{\lambda'_1}\cdots a^{\dagger}_{\lambda'_l}a_{\mu'_l}\cdots a_{\mu_1}\Bigg]\\
&\qquad\times\langle\lambda_1\cdots\lambda_k|S_k|\mu_1\cdots\mu_k\rangle\langle\lambda'_1\cdots\lambda'_l|S_l|\mu'_1\cdots\mu'_l\rangle|\Phi\rangle\\
&=\sum_{k+l=n+1}\frac{ikl}{2(k!)^2(l!)^2}(-1)^{kl}A_{\mu}A_{\rho}\sum_{\nu,\lambda}\{\langle\mu|\dot{\lambda}\rangle\langle\rho_{l+1}\cdots\rho_{n-1}\lambda|S_k|\nu_1\cdots\nu_k\rangle\langle\rho_1\cdots\rho_l|S_l|\nu_{k+1}\cdots\nu_{n-1}\mu\rangle\\
&\qquad-\langle\dot{\mu}|\lambda\rangle\langle\rho_1\cdots\rho_k|S_k|\nu_{l+1}\cdots\nu_{n-1}\mu\rangle\langle\rho_{k+1}\cdots\rho_{n-1}\lambda|S_l|\nu_1\cdots\nu_l\rangle\}\\
&=i\sum_{k+l=n+1}(-1)^{kl+1}A'_{\nu}A'_{\rho}\sum_{\mu}\langle\rho_{l+1}\cdots\rho_{n-1}\dot{\mu}|S_k|\nu_1\cdots\nu_k\rangle\langle\rho_1\cdots\rho_l|S_l|\nu_{k+1}\cdots\nu_{n-1}\mu\rangle,
\end{aligned} \tag{3.9}$$

where, by Eq. (2.14), the two series involving $\langle\mu|\dot{\lambda}\rangle$ and $\langle\dot{\mu}|\lambda\rangle$ are equal and cancel the factor $\frac{1}{2}$ and the $k!(k-1)!(l-1)!l!$ permutations of ρ's and ν's within S_k and S_l cancel the remaining combinational factor.

The general result is thus:

$$\langle\Phi|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-S}i(\partial/\partial t)e^{S}|\Phi\rangle = i\frac{\partial}{\partial t}\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle - i\sum_i\langle\rho_1\cdots\dot\rho_i\cdots\rho_n|S_n|\nu_1\cdots\nu_n\rangle$$
$$- i\sum_i\langle\rho_1\cdots\rho_n|S_n|\nu_1\cdots\dot\nu_i\cdots\nu_n\rangle - i\sum_\nu\langle\dot\nu\rho_1\cdots\rho_n|S_{n+1}|\nu\nu_1\cdots\nu_n\rangle$$
$$+ i\sum_{k+l=n+1}(-)^{kl+1}A'_\nu A'_\rho\langle\rho_{l+1}\cdots\rho_{n-1}\dot\mu\,|S_k|\nu_1\cdots\nu_k\rangle$$
$$\times\langle\rho_1\cdots\rho_l|S_l|\nu_{k+1}\cdots\nu_{n-1}\mu\rangle\,. \tag{3.10}$$

It is instructive to explicitly evaluate Eq. (3.10) for the case $n=2$ and transform to coordinate space. Multiplication of Eq. (3.10) for the case $n=2$ by $\langle x_1|\rho_1\rangle\langle x_2|\rho_2\rangle$ and summation over ρ_1 and ρ_2 yields

$$\langle\Phi|a^\dagger_{\nu_1}a^\dagger_{\nu_2}a(x_2)a(x_1)e^{-S}i(\partial/\partial t)e^{S}|\Phi\rangle$$
$$= i\sum_{\rho_1\rho_2}\langle x_1|\rho_1\rangle\langle x_2|\rho_2\rangle\Big\{\frac{\partial}{\partial t}\langle\rho_1\rho_2|S_2|\nu_1\nu_2\rangle - \sum_\nu\langle\dot\nu\rho_1\rho_2|S_3|\nu\nu_1\nu_2\rangle$$
$$+\Big[-\langle\rho_1\rho_2|S_2|\nu_1\dot\nu_2\rangle - \langle\rho_1\dot\rho_2|S_2|\nu_1\nu_2\rangle + \sum_\nu\left(\langle\dot\nu|S_1|\nu_2\rangle\langle\rho_1\rho_2|S_2|\nu_1\nu\rangle + \langle\rho_1\dot\nu|S_2|\nu_1\nu_2\rangle\langle\rho_2|S_1|\nu\rangle\right)\Big]$$
$$+\Big[-\langle\rho_1\rho_2|S_2|\dot\nu_1\nu_2\rangle - \langle\dot\rho_1\rho_2|S_2|\nu_1\nu_2\rangle + \sum_\nu\left(\langle\dot\nu|S_1|\nu_1\rangle\langle\rho_1\rho_2|S_2|\nu\nu_2\rangle + \langle\dot\nu\rho_2|S_2|\nu_1\nu_2\rangle\langle\rho_1|S_1|\nu\rangle\right)\Big]\Big\}. \tag{3.11}$$

Evaluation of the first term in square brackets using Eqs. (2.5), (2.14), and (3.8) yields

$$i\sum_\nu\left(\langle\dot\nu|\nu_2\rangle + \langle\dot\nu|S_1|\nu_2\rangle\right)\langle x_1x_2|S_2|\nu_1\nu\rangle + i\sum_\rho\left[\langle x_2|\left(1-\sum_\nu|\nu\rangle\langle\nu|\right)|\dot\rho\rangle + \sum_\nu\langle\dot\nu|\rho\rangle\langle x_2|S_1|\nu\rangle\right]\langle x_1\rho|S_2|\nu_1\nu_2\rangle$$
$$= i\int dx\sum_\nu\langle\dot\nu|x\rangle\left(\langle x|\psi_1|\nu_2\rangle\langle x_1x_2|S_2|\nu_1\nu\rangle + \langle x_2|\psi_1|\nu\rangle\langle x_1x|S_2|\nu_1\nu_2\rangle\right) + i\sum_\rho\langle x_2|\dot\rho\rangle\langle x_1\rho|S_2|\nu_1\nu_2\rangle\,, \tag{3.12}$$

and the second term in brackets yields the corresponding result with 1 and 2 interchanged. Finally, noting that

$$\frac{\partial}{\partial t}\langle x_1x_2|S_2|\nu_1\nu_2\rangle = \sum_{\rho_1\rho_2}\left[\left(\langle x_1|\dot\rho_1\rangle\langle x_2|\rho_2\rangle + \langle x_1|\rho_1\rangle\langle x_2|\dot\rho_2\rangle\right)\langle\rho_1\rho_2|S_2|\nu_1\nu_2\rangle + \langle x_1|\rho_1\rangle\langle x_2|\rho_2\rangle\frac{\partial}{\partial t}\langle\rho_1\rho_2|S_2|\nu_1\nu_2\rangle\right], \tag{3.13}$$

we obtain

$$\langle\Phi|a^\dagger_{\nu_1}a^\dagger_{\nu_2}a(x_2)a(x_1)e^{-S}i\frac{\partial}{\partial t}e^{S}|\Phi\rangle$$
$$= i\frac{\partial}{\partial t}\langle x_1x_2|S_2|\nu_1\nu_2\rangle + i\int dx\sum_\nu\langle\dot\nu|x\rangle\left(\langle x|\psi_1|\nu_2\rangle\langle x_1x_2|S_2|\nu_1\nu\rangle + \langle x_2|\psi_1|\nu\rangle\langle x_1x|S_2|\nu_1\nu_2\rangle\right.$$
$$\left. + \langle x|\psi_1|\nu_1\rangle\langle x_1x_2|S_2|\nu\nu_2\rangle + \langle x_1|\psi_1|\nu\rangle\langle xx_2|S_2|\nu_1\nu_2\rangle - \langle xx_1x_2|S_3|\nu\nu_1\nu_2\rangle\right). \tag{3.14}$$

Truncation by requiring $S_3=0$ as before reproduces the right-hand side of the GTDBG equation, Eq. (2.26).

IV. PROPERTIES OF THE TRUNCATED COUPLED-CLUSTER EQUATIONS

A. Equations in the maximum overlap basis

Truncation at the $n=2$ level yields the set of three coupled nonlinear integrodifferential equations (2.16a), (2.24), and (2.26). Although the equations are written in a general time-dependent basis, the truncation, which involves approximating multi-particle-hole amplitudes beyond $n=2$, is certainly basis dependent. Thus, the final basis choice necessitates a compromise between structural simplicity and physical considerations.

For small oscillations about the ground state solution, a static basis well suited tc the ground state problem would appear sensible. The structure of Eqs. (2.24) and (2.26) is then especially simple with only $i(\partial/\partial t)\langle x|S_1|\nu\rangle$ and $i(\partial/\partial t)\times\langle x_1x_2|S_2|\nu_1\nu_2\rangle$ appearing on the right-hand sides, respectively. This basis would be ideal, for example, to generalize the random phase approximation to include two-body correlations. For large amplitude motion, as well as fission and collisions, it is desirable to select a basis which follows the shape of the system as closely as possible. Consider, for example, a determinant $|\Phi\rangle$ with a shape quite different from $|\psi\rangle$. It is true that by Thouless's theorem,[5] any determinant $|\phi\rangle$, including one of the desired shape, may be written $|\Phi'\rangle = e^{S_1}|\Phi\rangle$. Nevertheless, the wave function

$e^{S_1+S_2}|\Phi\rangle = e^{S_2}|\Phi'\rangle$ only permits two-particle, two-hole excitations defined relative to the original, nonoptimal determinant $|\Phi\rangle$. Intuitively one would expect to obtain a better approximation with the wave function $e^{S_1'+S_2'}|\Phi'\rangle$, where $|\Phi'\rangle$ is required to have the proper size, shape, and other one-body properties.

A quantitative procedure to implement these intuitive notions is to select the maximum overlap basis by requiring $S_1 = 0$. As shown by Coester and Kümmel,[6] this may be done for the exact ψ so that the exact hierarchy of Eqs. (2.16) may be written with $\langle x|\psi_1|\nu\rangle = \langle x|\nu\rangle$. Truncation at $n=2$ thus yields coupled equations for $i(d/dt)\langle x|\nu\rangle$ and $i(d/dt)\langle x_1x_2|S_2|\nu_1\nu_2\rangle$.

In the maximum overlap basis, the GTDHF equation becomes

$$T(x)\langle x|\nu\rangle + \sum_{\nu'}\langle x\nu'|TS_2|\nu\nu'\rangle + \sum_{\nu'}\langle x\nu'|\psi_2|\nu\nu'\rangle - \sum_{\nu'}\langle x|\nu'\rangle h_{\nu'\nu} = i\frac{\partial}{\partial t}\langle x|\nu\rangle - i\sum_{\nu'}[\langle x\dot{\nu}'|S_2|\nu\nu'\rangle - \langle\dot{\nu}'|\nu\rangle\langle x|\nu'\rangle], \tag{4.1}$$

where

$$h_{\nu_1\nu_2} = \langle\nu_1|T|\nu_2\rangle + \sum_{\nu}\langle\nu_1\nu|V\psi_2|\nu_2\nu\rangle. \tag{4.2}$$

In this basis, the connection to the TDHF equation is directly obtained by setting $S_2 = 0$. Defining

$$\langle x|h_{HF}|x'\rangle \equiv \delta(x'-x)T(x') + \sum_{\nu'}\delta(x-x')\int dx''V(x,x'')\langle\nu'|x''\rangle\langle x''|\nu'\rangle - \sum_{\nu'}V(x,x')\langle\nu'|x\rangle\langle x'|\nu'\rangle, \tag{4.3}$$

Eq. (4.1) becomes

$$\left\langle x\left|h_{HF} - i\frac{\partial}{\partial t}\right|\nu\right\rangle = \sum_{\nu'}\left(\left\langle\nu'\left|h_{HF} - i\frac{\partial}{\partial t}\right|\nu\right\rangle\right)\langle x|\nu'\rangle, \tag{4.4}$$

with the usual TDHF solution

$$i\frac{\partial}{\partial t}\langle x|\nu\rangle = \int dx'\langle x|h_{HF}|x'\rangle\langle x'|\nu\rangle. \tag{4.5}$$

Just as in the case of the GTDHF equation, the GTDBG equation is greatly simplified in the maximum overlap basis and the connection with the ordinary Bethe-Goldstone equation is clarified. Introducing the definitions

$$\langle x_1|\Lambda|x_1'\rangle \equiv \sum_{\nu}\langle x_1|\psi_1|\nu\rangle\langle\nu|x_1'\rangle, \tag{4.6}$$

$$\langle x_1x_2|Q|x_1'x\rangle \equiv \langle x_1|1-\Lambda|x_1'\rangle\langle x_1|1-\Lambda|x_2'\rangle, \tag{4.7}$$

and

$$\eta^{\nu_1\nu_2}(x_1x_2) \equiv \sum_{\nu}[\langle\mathring{\nu}x_2|S_2|\nu_1\nu_2\rangle\langle x_1|\psi_1|\nu\rangle + \langle x_1\mathring{\nu}|S_2|\nu_1\nu_2\rangle\langle x_2|\psi_1|\nu\rangle + \langle\mathring{\nu}|\psi_1|\nu_1\rangle\langle x_1x_2|S_2|\nu\nu_2\rangle + \langle\mathring{\nu}|\psi_1|\nu_2\rangle\langle x_1x_2|S_2|\nu_1\nu\rangle] \tag{4.8}$$

in Eq. (2.26), the TDBG equation becomes

$$\langle x_1x_2|Q(T_1+T_2)S_2|\nu_1\nu_2\rangle + \langle x_1x_2|QV\psi_2|\nu_1\nu_2\rangle + \tfrac{1}{2}\sum_{\nu'\nu''}\langle x_1x_2|S_2|\nu'\nu''\rangle\langle\nu'\nu''|V\psi_2|\nu_1\nu_2\rangle$$
$$- \sum_{\nu}[h_{\nu\nu_1}\langle x_1x_2|S_2|\nu\nu_2\rangle + h_{\nu\nu_2}\langle x_1x_2|S_2|\nu_1\nu\rangle]$$
$$= i\frac{\partial}{\partial t}\langle x_1x_2|S_2|\nu_1\nu_2\rangle + i\eta^{\nu_1\nu_2}(x_1x_2). \tag{4.9}$$

In the case $S_1 = 0$, Q becomes the familiar Pauli operator. Specializing to the case of a stationary state, which makes the right-hand side vanish; considering a translationally invariant system, which makes $h_{\nu\nu'}$ diagonal; and omitting the third term on the left-hand side, which generates hole-hole ladders; Eq. (4.9) reduces to the familiar Bethe-Goldstone equation

$$(QT-h)S_2=-QV\psi_2 \tag{4.10a}$$

or

$$\psi_2=\phi-\frac{1}{QT-h}QV\psi_2, \tag{4.10b}$$

where we denote the antisymmetrized product of two plane waves $A_\nu\langle x|\nu\rangle\langle x'|\nu'\rangle$ by ϕ.

B. Consistency

Thus far, we have not discussed the zeroth order equation, Eq. (2.16a), which in the maximum overlap basis becomes

$$\sum_\nu\langle\nu|T|\nu\rangle+\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V\psi_2|\nu\nu'\rangle=-i\sum_\nu\langle\dot\nu|\nu\rangle. \tag{4.11}$$

In general, truncation of Eqs. (2.16) at level n yields $n+1$ equations. The second equation specifies the evolution of S_1 (or $\langle x|\nu\rangle$), the third specifies $\dot S_2$ and the $(n+1)$th specifies $\dot S_n$. Thus, the truncated system becomes overdetermined and there is no guarantee that the first equation is ever satisfied for a truncated hierarchy.

When Eq. (2.16a) is not fulfilled exactly in any finite order, one might worry about the essential consistency of the theory, since it has been used repeatedly either explicitly or implicitly to eliminate unlinked terms in all higher order equations. One argument supporting the consistency of the present set of equations instead of those resulting from truncating some arbitrary linear combination of them arises from their linked structure. Since all terms in our untruncated equations have the same N dependence in the large N limit, the truncated equations are guaranteed to have the proper N dependence, as well. We do not see how this feature could be ensured in any other alternative formulation.

A second argument concerns the fact that Eqs. (2.16a) and (4.11) are essentially associated only with an overall multiplicative constant in the wave function. Imagine adding a time-dependent c number to the Hamiltonian:

$$\tilde H\equiv H+C(t) \tag{4.12}$$

in which case

$$\tilde\Psi(t)=\exp\left(-i\int^t C(t)\right)\Psi(t). \tag{4.13}$$

This transformation does not affect the equations of motion for any of the S_n since

$$\langle\Phi|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-\hat S}\left(H-i\frac{\partial}{\partial t}\right)e^{\hat S}|\Phi\rangle$$

$$=\left\langle\Phi\left|a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}a_{\rho_n}\cdots a_{\rho_1}e^{-\hat S}\ \tilde H-i\frac{\partial}{\partial t}\ e^{\hat S}\right|\Phi\right\rangle. \tag{4.14}$$

The zeroth order equation, Eq. (4.4), becomes

$$\sum_\nu\langle\nu|T|\nu\rangle+\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V\psi_2|\nu\nu'\rangle+C(t)=-i\sum_\nu\langle\dot\nu|\nu\rangle. \tag{4.15}$$

Thus, any discrepancy in fulfilling Eq. (4.11) is physically equivalent to an overall multiplicative factor in this wave function. In the event C is real, one is dealing only with a physically unobservable phase. A simple example of such a phase is provided by the TDHF truncation obtained by setting $S_2=0$. Then by Eq. (4.5)

$$-i\langle\dot\nu|\nu\rangle=i\langle\nu|\dot\nu\rangle$$

$$=\langle\nu|T|\nu\rangle+\sum_{\nu'}\langle\nu\nu'|V|\nu\nu'-\nu'\nu\rangle, \tag{4.16}$$

so that from Eq. (4.15),

$$C(t)=\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V|\nu\nu'-\nu'\nu\rangle, \tag{4.17}$$

which is manifestly real. In the stationary state case, this is just the proper phase factor to convert the sum of the single particle energies into the total HF energy:

$$\psi(t)=e^{iCt}\tilde\psi(t)$$

$$=\exp\left[i\left(\tfrac{1}{2}\sum_{\nu\nu'}\langle\nu\nu'|V|\nu\nu'-\nu'\nu\rangle-\sum_\nu\langle\nu|T|\nu\rangle\right.\right.$$

$$\left.\left.-\sum_{\nu\nu'}\langle\nu\nu'|V|\nu\nu'-\nu'\nu\rangle\right)t\right]$$

$$=\exp(-iE_{\mathrm{HF}}t).$$

Any complex component of C would indicate that the truncated hierarchy is not exactly preserving the norm of the wave function, and we can make no general statements regarding the reality of C. Indeed, in the case of the Lipkin model in Ref. 1, the norm was not conserved. A complex C would be neither a surprise, since it is obvious that all particle-hole components are required to obtain the proper norm, nor necessarily of physical consequence since in any event we will be more concerned with the expectation values of few body operators than the entire wave function.

Although we cannot prove that the norm of $|\psi\rangle$ is conserved for a general truncation, it is trivial to prove that the particle number is conserved. Noting that

$$\left[\sum_\alpha a_\alpha^\dagger a_\alpha, \hat{S}_n\right]=0 \tag{4.19}$$

since every particle contribution exactly cancels a hole contribution, it follows that

$$\frac{d}{dt}\langle\hat{N}\rangle=\frac{d}{dt}\frac{\langle\Phi|e^{\hat{s}^\dagger}\sum_\alpha a_\alpha^\dagger a_\alpha e^{\hat{s}}|\Phi\rangle}{\langle\Phi|e^{\hat{s}^\dagger}e^{\hat{s}}|\Phi\rangle}$$

$$=\frac{d}{dt}N=0 \tag{4.20}$$

for any $\hat{S}$.

A second question of consistency concerns the orthonormality of the basis ϕ_ν and orthogonality conditions (2.6) which were assumed to hold at each instant of time. It remains to be shown that the truncated equations of motion preserve these conditions if they are satisfied at the initial time. Consider first the GTDHF equation (2.24) and project it with the operator $\int dx\langle\nu'|x\rangle$. Invoking the orthogonality conditions (2.6) at the time t and using Eq. (2.25), the sum of all the terms on the left-hand side yields zero. Using (2.6) on the right-hand side and rearranging yields the result

$$\frac{d}{dt}\int dx\langle\nu'|x\rangle\langle x|S_1|\nu\rangle=0. \tag{4.21}$$

Similarly, projecting the TDBG equation, Eq. (2.26), with $\int dx_1\langle\nu'|x_1\rangle$ or $\int dx_2\langle\nu'|x_2\rangle$ yields the result

$$\frac{d}{dt}\int dx_1\langle\nu'|x_1\rangle\langle x_1x_2|S_2|\nu_1\nu_2\rangle$$

$$=\frac{d}{dt}\int dx_2\langle\nu'|x_2\rangle\langle x_1x_2|S_2|\nu_1\nu_2\rangle=0. \tag{4.22}$$

Hence the orthogonality conditions are indeed preserved in time.

For the formulation in an arbitrary basis, we assumed orthonormality of the single-particle wave functions, so it is also necessary to show that the optimal overlap wave functions defined by Eq. (4.1) remain orthonormal. Simply projecting Eq. (4.1) with $\int dx\langle\nu'|x\rangle$ and using (2.6) as above yields the desired result.

$$\frac{d}{dt}\langle\nu'|\nu\rangle=0. \tag{4.23}$$

C. Concluding comments

Although we have presented a formal framework which we believe to provide the most promising systematic generalization of the time-dependent mean-field theory for potentials with strongly repulsive cores, substantial practical problems remain to be resolved before it can be implemented in a realistic calculation. Initial attempts at numerical solution of a simple model in coordinate space have indicated some of the major issues.

Based on experience with the TDHF theory, it is clearly desirable to deal with wave functions defined on a discrete coordinate space grid.[7] One immediate problem arises from the fact that our hierarchy does not correspond to a variational wave function.[8] Hence, in contrast to the familiar TDHF case, we must forgo the convenience of first discretizing a variational functional and then obtaining automatically consistent equations of motion by varying this discretized functional. Secondly, since $\langle x_1x_2|S_2|\nu_1\nu_2\rangle$ is defined on an exceedingly large number of grid points, it is highly desirable to implement the physical condition that it should become small at large values of $|x_1-x_2|$. The simplest prescriptions are precluded by the need to strictly enforce the orthogonality conditions (2.6).

Little is known about the stability of discrete approximations to the sets of inhomogeneous nonlinear equations (2.24) and (2.26) or (4.1) and (4.9). Although there exist obvious candidates,[7] no algorithm completely analogous to the simple unitarized approximations to the evolution operator used in TDHF has been found which both insures against exponential error propagation and exactly enforces the orthogonality relations.

As discussed in I and in Refs. 7 and 8, evolution in complex time offers an efficient means of solving the corresponding static equations. A new feature relative to the analogous TDHF complex time technique is the necessity of choosing initial S_n's which satisfy all the orthogonality relations. The simplest method we have devised to obtain such amplitudes is to begin with a pure determinant comprised of eigenfunctions of some convenient one-body potential U. Then the true Hamiltonian is adiabatically switched on by evolution with the Hamiltonian

$$H(t)=T+\lambda(t)V+[1-\lambda(t)]U, \tag{4.24}$$

where $\lambda(t)$ gradually increases from zero to one. Introduction of an imaginary time component during switching on inhibits the build-up of excited state components. Whereas we can make no general statements about convergence of evolution in complex time, it is clear from Eq. (3.3) that if one ever reaches a solution in which the S_n's become time independent, these amplitudes necessarily satisfy the static equations. In simple explatory cases we have investigated, this procedure appears to converge satisfactorily.

Since only expectation values of few-body operators are physically reliable in this theory, even when numerically stable solutions to the equations of motion have been obtained it is still necessary to determine the one- and two-body density ma-

trices from the S_n's. Presumably, techniques analogous to those of Ref. 9 can be developed to obtain suitable approximations for the density matrices commensurate with the approximations introduced into the equations of motion.

In summary, then, we have derived the formal foundations of a general theory which still requires resolution of important technical details for successful implementation.

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