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Time-dependent coupled-cluster approximation to nuclear dynamics. I. Application to a solvable model*

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A general hierarchy of approximations to the many-body Schrödinger equation is presented which reduces to the time-dependent mean-field approximation in lowest order and provides systematic corrections in subsequent orders. The theory is applied to two interacting systems described by the Lipkin model Hamiltonian. Comparison of the results of the lowest two orders of approximation with the exact solution demonstrates the practicality of the method and its potential for generalizing nuclear dynamics beyond the mean field theory.

[NUCLEAR STRUCTURE Time-dependent approximation to nuclear dynamics. Corrections to time-dependent mean-field theory. Solution of Lipkin model for two interacting systems.]

I. INTRODUCTION

Given the complexity of the full time-dependent nuclear many-body problem, it is desirable to formulate a general hierarchy of successive approximations for treating nuclear dynamics. Ideally, the lowest order theory should provide an intuitively motivated and physically sound approximation for a wide range of dynamical processes. In addition, there must certainly exist a completely systematic series of corrections so that, at least in principle, the evaluation of an observable to any order is conceptually unambiguous. In view of the appreciable progress in the microscopic theory of the ground states of finite nuclei, it is also desirable that in the special case of stationary states, the theory make contact with existing theories for which convergence properties with nuclear potentials have been explored.

The natural starting point for such a theory of nuclear dynamics is the time-dependent mean-field approximation. The intuitive appeal of the mean-field as the obvious mechanism to govern collective motion and the evolution of the gross behavior of the nuclear wave function is evident, and has been discussed in some detail in the literature.[1] The viability of the mean-field approximation is substantiated by its successful application to light ion collisions,[2] heavy ion collisions,[3] and fission[4] as well as the success of the random phase approximation,[5] which is its infinitesimal amplitude limit.

Since virtually all general methods in fermion many-body theory reduce to the mean-field or Hartree-Fock (HF) approximation in lowest order or some appropriate limit, there is no unique series of systematic corrections to the mean-field theory. Thus, it is useful to motivate the coupled-cluster theory by briefly explaining why it appears preferable to alternative methods that have been considered.

The time-dependent variational principle yields the time-dependent Hartree-Fock (TDHF) approximation when the trial function is restricted to the set of all Slater determinants. The most satisfactory systematic hierarchy of successive variational approximations appears to arise from the extended Jastrow trial functions

$$\Psi^{(M)}(r_1 \cdots r_N) = \prod_i f^{(M)}(r_{i_1} r_{i_2} \cdots r_{i_M}) \prod_j f^{(M-1)}(r_{j_1} r_{j_2} \cdots r_{j_{M-1}}) \cdots \prod_k f^{(2)}(r_{k_1} r_{k_2}) \Phi_{SD}(r_1 r_2 \cdots r_N), \tag{1.1}$$

where $f^{(M)}$ is an M-body correlation function and Φ_{SD} is a Slater determinant. Based on experience with the energy and radial distribution function in liquid helium and nuclear matter,[7] there is every reason to expect rapid convergence in expectation values of few-body operators in this hierarchy. The fundamental problem, however, is the difficulty in obtaining a sufficiently accurate expression for the energy in terms of the correlation functions and single-particle wave functions to use in the variational principle. In the special case of infinite matter and central forces, it is already difficult to solve the time-independent Euler-Lagrange equations in the lowest order Fermi hypernetted

chain (FHNC) approximation.[8] Given the fact the lowest order FHNC is of marginal accuracy, state dependent nuclear potentials have never been treated adequately, and that calculation of finite nuclei requires inclusion of additional terms which vanish in the FHNC infinite-matter limit, the present variational technology is grossly inadequate even for formulation of a time-dependent variational theory containing two-body correlation functions.

An alternative approach is the truncation of a suitable hierarchy of coupled equations for expectation values of products of n pairs of fermion field creation and annihilation operators. Depending upon how one specifies relative time arguments and whether time-ordered products are introduced, the theory may be formulated in terms of n-particle density matrices or n-body Green's functions. In either case, using the Heisenberg equations of motion for the field operators, the time evolution of the expectation value of n pairs of field operators is coupled to the mean value of $(n+1)$ pairs of field operators as well as lower order terms.[9] Truncation of the hierarchy at nth order may then be effected by a physically motivated prescription for approximating the matrix element of $(n+1)$ pairs of field operators in terms of nth and lower order expressions. The TDHF approximation is obtained in this approach by replacing the expectation value of two pairs of creation and annihilation operators by the product of expectation values of single pairs of creation and annihilation operators. In a density-matrix hierarchy, the TDHF equation follows immediately:

$$i\dot{\rho} = [h, \rho] , \tag{1.2a}$$

where

$$\rho_{\alpha\beta} = \langle a_\beta^\dagger a_\alpha \rangle \tag{1.2b}$$

and

$$h_{\alpha\beta} = T_{\alpha\beta} + \sum_{\gamma\delta} v^{\mathrm{AS}}_{\alpha\gamma,\beta\delta}\rho_{\delta\gamma} . \tag{1.2c}$$

In terms of Green's functions, the same result is obtained by combining the equation for $(\partial/\partial t)G(x, t; y, t')\big|_{t'=t^+}$ with its adjoint equation. The Green's function formulation is particularly useful in motivating higher-order truncations, both because of its close connection to diagrammatic perturbation theory and the straightforwardness of ensuring general conservation laws.[10]

The primary disadvantage of the Green's function or density-matrix formulation relative to the coupled-cluster theory described subsequently is the computational cumbersomeness of dealing with n-body density matrices. The integral form of the Green's function hierarchy is clearly inconvenient for time-dependent problems because it involves integrations over relative times. However, even when the differential form of the theory has been reduced to the special case of a single time argument, one is still faced with evolving a function of $2n$ spatial variables, thereby even rendering treatment of two-particle correlations intractable in all but the most oversimplified applications.

The formulation which appears most suited to the present problem is a time-dependent generalization of the $\exp(S)$ or coupled-cluster approximation pioneered by Coester and Kummel[11] and subsequently applied extensively to fermion systems.[12] In this theory, the full many-body wave function is written in the form

$$\Psi = \exp(S)\Phi , \tag{1.3}$$

where

$$S = \sum_{n=1}^{M} S^{(n)} \tag{1.4}$$

and $S^{(n)}$ represents the most general n-particle, n-hole operator defined relative to the Slater determinant of occupied states Φ. The time-independent or time-dependent Schrödinger equation implies a hierarchy of nonlinear, coupled equations for the static or time-dependent n-particle, n-hole amplitude, which may be truncated in the same manner as a density-matrix or Green's-function hierarchy. However, the n-particle amplitude may be expressed in terms of n spatial coordinates and n occupied state labels rather than $2n$ coordinates since $S^{(n)}$ may be written

$$\begin{aligned} S^{(n)} &= \langle x_1 x_2 \cdots x_n | S^{(n)} | \nu_1 \nu_2 \cdots \nu_n \rangle \\ &\quad \times \psi^\dagger(x_1)\psi^\dagger(x_2)\cdots\psi^\dagger(x_n) a_{\nu_n}\cdots a_{\nu_1} \end{aligned} \tag{1.5}$$

where

$$\begin{aligned} &\langle x_1 x_2 \cdots x_n | S^{(n)} | \nu_1 \nu_2 \cdots \nu_n \rangle \\ &\quad \equiv \sum_{\rho_1 \cdots \rho_n} \langle x_1 | \rho_1 \rangle \cdots \langle x_n | \rho_n \rangle \langle \rho_1 \cdots \rho_n | S^{(n)} | \nu_1 \cdots \nu_n \rangle \end{aligned}$$

and $\psi^\dagger(x)$ is the field creation operator at position x. Thus, for finite systems, the coupled-cluster formalism provides a particularly economical description of many-body correlations.

Whereas the basic ideas underlying the coupled-cluster hierarchy are very simple, the technical details involved in applying even the time-independent theory to the most general case are somewhat tedious and notationally cumbersome.[12] Therefore, in this first paper we shall defy the usual custom of expounding general, untested formalism and present only the minimal time-dependent formalism required to solve a specific model. In this way, we hope to emphasize the essential

physics of the approach and establish its viability sufficiently to justify exposition of the general coordinate-space formulation for strong, short-ranged potentials in a subsequent work.

The basic elements of the time-dependent coupled-cluster hierarchy and a particular truncation procedure are briefly described in Sec. II. The model problem, comprised of two interacting systems described by the Lipkin Hamiltonian, is presented in Sec. III and solved exactly.

The first two orders of approximation for the static and time-dependent coupled-cluster theory are derived for the model problem in Secs. IV and V, respectively. These approximations are compared with exact solutions in Sec. VI and the general conclusions arising from this work are presented in Sec. VII.

II. THE TIME-DEPENDENT COUPLED-CLUSTER APPROXIMATION

Since the coupled-cluster approximation for stationary states has recently been described in detail,[12] we shall only review a few basic features of the theory as a foundation for the time-dependent generalization.

Basic elements of time-independent theory

For stationary states, equations for the n-particle, n-hole amplitudes appearing in Eqs. (13) and (14) are obtained by projecting the Schrödinger equation

$$e^{-S}He^{S}\left|\Phi\right\rangle = E\left|\Phi\right\rangle \tag{2.1}$$

onto a complete set of m-particle, m-hole states. Denoting unoccupied states by ρ_i and occupied states by ν_i, the following hierarchy of equations arises:

$$\langle\Phi\left|e^{-S}He^{S}\right|\Phi\rangle = E\,, \tag{2.2a}$$

$$\langle\Phi\left|a_\nu^\dagger a_\rho\, e^{-S}He^{S}\right|\Phi\rangle = 0\,, \tag{2.2b}$$

$$\vdots$$

$$\langle\Phi\left|a_{\nu_1}^\dagger\cdots a_{\nu_m}^\dagger a_{\rho_m}\cdots a_{\rho_1}\, e^{-S}He^{S}\right|\Phi\rangle = 0\,. \tag{2.2c}$$

From the identity

$$e^{-x}\hat{O}e^{x} = \hat{O} + [\hat{O},x] + \frac{1}{2!}[[\hat{O},x],x] + \cdots, \tag{2.3}$$

it is evident that if H contains only one and two-body operators, repeated commutation with H can remove at most two pairs of creation and annihilation operators from the particle-hole operators $S^{(n)}$. Thus, since $e^{-S}He^{S}\left|\Phi\right\rangle$ must connect to $\left|\Phi\right\rangle$ in Eq. (2.2a) and at most two pairs of particle-hole operators have been contracted, the resulting equation can involve only S_1 and S_2. In fact, for the special case of Eq. (2.2a), the exact equation

$$\langle\Phi\left|H(S^{(1)} + \tfrac{1}{2}S^{(1)}S^{(1)} + S^{(2)})\right|\Phi\rangle = E \tag{2.4}$$

is trivially obtained by noting $\langle\Phi\left|S=0\right.$ and expanding e^{S}. Similarly, Eq. (2.2b) involves amplitudes only through $S^{(3)}$ and in general Eq. (2.2c) includes amplitudes through $S^{(m+2)}$. The explicit form of the general equation is somewhat complicated, but follows straightforwardly from substitution of Eq. (2.3), which terminates after 5 terms when $\hat{O}=H$, into Eq. (2.2c).

Since the resulting hierarchy of equations for the $S^{(n)}$'s is equivalent to the original Schrödinger equation, physical approximations are introduced by the method of truncation. The simplest truncation prescription, which we shall use in this present work, is to specify that $S^{(n)}=0$ for all $n>m$. This has the effect of treating particle-hole correlations of up to m particles exactly while retaining only those correlations for more than m particles which arise from products of lower order amplitudes. In terms of familiar perturbation theory, truncation at $m=2$ sums particle-particle and hole-hole ladders as well as RPA ring diagrams, and this approximation has been shown to be accurate for a single Lipkin model and for systems with long-range forces.[12] For potentials which are infinitely repulsive at short distances, it is inconsistent to define the higher $S^{(n)}$'s to be zero and instead one must impose a prescription which makes the wave function vanish when n particles are within a hard core radius. For finite, but strongly repulsive cores, a similar condition is physically reasonable, and this more complicated truncation procedure will be addressed in a subsequent paper.

Retaining only m nonzero amplitudes yields m equations of the form (2.2c) in m unknowns which completely specify the $S^{(n)}$'s. With these amplitudes, Eq. (2.2a) yields an mth order approximation to the energy which is distinct from the expectation value of H with the wave function $\exp(S^{(1)}+S^{(2)}+\cdots+S^{(m)})\left|\Phi\right\rangle$ since $-S\neq S^\dagger$. Truncation at $m=1$ yields the HF approximation, which is most obvious by noting that the most general determinant may be written $\exp(S^{(1)})\left|\Phi\right\rangle$ by Thouless's theorem.[13] In general, one always has the freedom to specify $S^{(1)}\equiv 0$ and to solve an equation for the single-particle wave functions comprising the determinant $\left|\Phi\right\rangle$.

Time-dependent theory

The time-dependent coupled-cluster theory is obtained analogously by projecting the time-dependent Schrödinger equation,

$$e^{-S}He^{S}\left|\Phi\right\rangle = ie^{-S}\frac{\partial}{\partial t}e^{S}\left|\Phi\right\rangle\,, \tag{2.5}$$

onto n-particle, n-hole states,

$$\langle\Phi|e^{-S}He^{S}|\Phi\rangle = i\langle\Phi|e^{-S}(\partial/\partial t)e^{S}|\Phi\rangle\,, \tag{2.6a}$$

$$\langle\Phi|a_\nu^\dagger a_\rho\, e^{-S}He^{S}|\Phi\rangle = i\langle\Phi|a_\nu^\dagger a_\rho\, e^{-S}(\partial/\partial t)e^{S}|\Phi\rangle$$

$$\vdots \tag{2.6b}$$

$$\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_m}^\dagger a_{\rho_m}\cdots a_{\rho_1}e^{-S}He^{S}|\Phi\rangle = i\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_m}^\dagger a_{\rho_m}\cdots a_{\rho_1}e^{-S}(\partial/\partial t)e^{S}|\Phi\rangle\,. \tag{2.6c}$$

The general structure of these equations is observed by noting that

$$e^{-S}\frac{\partial}{\partial t}e^{S} = \frac{\partial}{\partial t} + \dot{S} + \frac{1}{2!}[\dot{S},S] + \frac{1}{3!}[[\dot{S},S],S] + \cdots \tag{2.7}$$

and writing $S^{(n)}$ in an arbitary time-dependent basis,

$$S^n(t) = \sum_{\rho_i\nu_i}\langle\rho_1\cdots\rho_n|S^n(t)|\nu_1\cdots\nu_n\rangle \times a_{\rho_1}^\dagger(t)\cdots a_{\rho_n}^\dagger(t)a_{\nu_1}(t)\cdots a_{\nu_1}(t)\,. \tag{2.8}$$

Since

$$\frac{\partial}{\partial t}a_\alpha^\dagger = \sum_\beta\langle\beta|\dot{\alpha}\rangle a_\beta^\dagger\,, \tag{2.9}$$

each nonvanishing term in $\dot{S}^{(m)}$ either contains an $a_\rho^\dagger$ or a_ν term, for which $[\dot{S}^{(m)},S^{(n)}]=0$ or contains at most one $a_\nu^\dagger$ or a_ρ term, in which case the commutator $[\dot{S}^m,S^n]$ contains only $a_{\rho_i}^\dagger$ and a_{ν_i} operators. Hence, in any case, the multiple commutator $[[\dot{S},S],S]$ must vanish and

$$\langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_m}^\dagger a_{\rho_m}\cdots a_{\rho_1}e^{-S}(\partial/\partial t)e^{S}|\Phi\rangle = \langle\Phi|a_{\nu_1}^\dagger\cdots a_{\nu_m}^\dagger a_{\rho_m}\cdots a_{\rho_1}(\partial/\partial t + \dot{S} + \tfrac{1}{2}[\dot{S},S])|\Phi\rangle\,. \tag{2.10}$$

Although Eq. (2.10) yields many terms, the only nonvanishing term involving the time derivative of an $S^{(n)}$ amplitude, as opposed to the derivative of a basis function $\langle\beta|\dot{\alpha}\rangle$, is $(d/dt)\times\langle\rho_1\cdots\rho_m|S^m(t)|\nu_1\cdots\nu_m\rangle$. Thus, Eq. (2.6b) specifies $(d/dt)\langle\rho|S^{(1)}(t)|\nu\rangle$ in terms of known functions at time t, providing a first-order differential equation in time for the one-particle, one-hole amplitudes. In general, Eq. (2.6c) provides a first-order equation for the m-particle, m-hole amplitude, so that given initial conditions at time $t=0$ the amplitudes may be evolved in time by numerically integrating a system of first-order equations. The first equation, Eq. (2.6a) clearly plays no role in the time evolution since no time derivatives of particle-hole amplitudes survive in the right-hand side. It could be satisfied identically by introducing an appropriate time-dependent phase in the definition of Φ, but since such an overall phase is unobservable, Eq. (2.6a) is devoid of physical content. Formally, it is satisfied identically when the order of truncation, m, equals the number of particles.

Truncation of the time-dependent hierarchy proceeds precisely as in the time-independent theory. In lowest order, setting all $S^{(n)}$'s equal to zero for $n\geq 2$ yields the TDHF approximation, which is again most readily apparent by choosing the basis in which $S^{(1)}$ is identically zero. In this case, Eq. (2.6b) becomes

$$\langle\Phi|a_\nu^\dagger a_\rho(H - i\partial/\partial t)|\Phi\rangle = 0\,, \tag{2.11}$$

which implies the TDHF equation

$$\langle\rho|i\partial/\partial t|\nu\rangle = \langle\rho|h|\nu\rangle\,, \tag{2.12}$$

with h as defined in Eq. (1.2c). Making the usual arbitrary choice for hole-hole matrix elements yield the more familiar form

$$i\frac{\partial}{\partial t}|\nu\rangle = h|\nu\rangle\,. \tag{2.13}$$

Truncation at $n=2$ yields two closed coupled equations for $\dot{S}^{(1)}$ and $\dot{S}^{(2)}$ in terms of $S^{(1)}$ and $S^{(2)}$ which describes the time evolution of two-body correlations and in mth order one obtains m equations for $\dot{S}^{(1)}$ through $\dot{S}^{(m)}$.

A particularly attractive feature of the theory is the fact that solutions to the truncated time-independent equations at any order m are stationary solutions to the truncated time-dependent equations truncated at the same order by virtue of the fact that the left-hand terms of Eqs. (2.2) are identical to those of Eqs. (2.6). Thus, appropriate initial conditions for time-dependent problems can be obtained by turning on interactions or arranging collisions between systems which are in initial eigenstates calculated with precisely the same approximation. A further advantage is the fact that the static equations may actually be solved by evolving an initial guess for a wave function in complex time or by beginning with a solution to a one-body Hamiltonian, $H_0 = T+U$, and adiabatically switching on the interaction $H' = V-U$ in the time-dependent theory.

Approximation of mean values and wave functions

Finally, it is important to emphasize at the outset the essential difference between calculating expectation values of few-body operators and overlaps between N-body wave functions. Just as in perturbation theory, to which the coupled-cluster theory is intimately related,[12] low order truncations can yield excellent approximations to expectation values of few-body operators while pro-

ducing arbitrarily poor approximations to the full N-particle wave function. Physically the mean value of a finite-range two-body operator, for example, depends on the local two-body correlations of the system. Errors in describing the behavior of other particles far away from a correctly correlated pair are irrelevant and just contribute an arbitrary normalization factor which cancels out of the numerator and denominator of $\langle \hat{O} \rangle = \langle \Psi_T | \hat{O} | \Psi_T \rangle / \langle \Psi_T | \Psi_T \rangle$, where Ψ_T is a truncated approximation to Ψ. The overlap with some other many-body wave function $\langle \Phi | \Psi_T \rangle$, however, may be arbitrarily inaccurate. An extreme example is the lowest order of truncation, in which the mean-field approximation represents the full wave function as a single determinant. In the familiar hypothetical case in which the probability of exciting any particle out of its normally occupied state is some small value ϵ, the probability that all N-particles are simultaneously in their normally occupied states is evidently $(1-\epsilon)^N \sim e^{-N\epsilon}$. Thus, the determinental wave function will represent expectation values of one-body operators very well, with errors only of order ϵ, whereas the overlap with the true wave function is exponentially small.

The distinction between mean values and overlaps of N-body wave function is particularly crucial in addressing time-dependent problems. Sloppiness in making the corresponding distinction for stationary states is seldom disastrous because virtually all experimental measurements deal with expectation values of one- or two-body operators. Thus, binding energies, removal energies and charge densities don't really probe the full wave function, but rather just the expectation value of the Hamiltonian and one-body density operator. Similarly, despite loose talk about testing RPA wave functions, in practice only transition densities induced by one-body operators can be compared with experiment. Time-dependent applications, however, are far more dangerous since experimentalists insist on confronting theorists with S-matrix elements, which are overlaps of N-body wave functions evolved through some interaction with other appropriate N-particle wave functions describing final asymptotic states. From the previous discussion, it is clear that neither perturbation theory nor a low order coupled-cluster approximation has any hope of accurately describing S-matrix elements. Thus, the present theory must be applied only to the calculation of mean values of appropriate few-body operators. In heavy ion collisions, such operators might include the fragment mean proton number, neutron number, and c.m. momentum. Because of the crucial importance of distinguishing between mean values of few-body operators and S-matrix elements and our view that serious errors exist in the recent literature in this connection, we shall explicitly demonstrate this distinction in the case of the solvable model presented below.

III. INTERACTING LIPKIN SYSTEMS

The Lipkin model[14] consists of a system of N identical but distinguishable fermions, each fermion having only two possible states, which are separated by an energy ϵ. The second quantized Hamiltonian for the system is

$$H^N = \frac{\epsilon}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} + \frac{V}{2} \sum_{pp'\sigma} a^\dagger_{p\sigma} a^\dagger_{p'-\sigma} a_{p'-\sigma} a_{p-\sigma} , \quad (3.1)$$

where p labels the N particles and $\sigma = +1$ denotes the upper state and $\sigma = -1$ denotes the lower state. Operators with different particle labels commute with each other. The interaction term scatters a pair of particles from the same level to the other level. A single-particle state may be represented as a Pauli spinor, and the noninteracting ground state with $V = 0$ is a direct product of spinors. Introducing the quasispin operators J_z, J_+, and J_-

$$J_z = \tfrac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} ,$$

$$J_+ = \sum_p a^\dagger_{p+} a_{p-} , \quad (3.2)$$

$$J_- = J_+^\dagger ,$$

the Hamiltonian can be rewritten as

$$H^N = \epsilon J_z + \tfrac{1}{2} V (J_+^2 + J_-^2) . \quad (3.3)$$

The operators J_z, J_+, and J_- satisfy the usual angular momentum algebra, and the operator $J^2 \equiv J_z^2 + \frac{1}{2}(J_+ J_- + J_- J_+)$ commutes with each angular momentum component and therefore with the Hamiltonian. The Hamiltonian also commutes with the parity operator $\hat{\pi}$ and the number operator for the p'th fermion $\hat{n}_{p'}$, where

$$\hat{\pi} = e^{-i\pi J_z} , \quad \hat{n}_{p'} = a^\dagger_{p'+} a_{p'+} + a^\dagger_{p'-} a_{p'-} . \quad (3.4)$$

The eigenstates of H may thus be labeled by the eigenvalues of $\hat{\pi}$ and J. Since the interaction does not connect states of different J, the ground state may be calculated in the $J = N/2$ subspace, which contains the noninteracting ground state. Excitations of single particle-hole pairs are forbidden, and hence the Hartree Fock equations are trivially satisfied in the noninteracting ground state basis.

The interacting eigenstates of the Hamiltonian in the $J = N/2$ subspace may be expanded in the natural basis,

$$|J\alpha\rangle = \sum \omega_{J\alpha}(m_J) |Jm_J\rangle . \quad (3.5)$$

The expansion coefficients $\omega_{J\alpha}(m_J)$ and the eigenvalues corresponding to the states $|J\alpha\rangle$ are determined from the solution of

$$\det|\langle J\alpha'|H|J\alpha\rangle - \epsilon_\alpha \delta_{\alpha\alpha'}| = 0 . \tag{3.6}$$

To obtain a solvable model problem which bears some analogy to a nuclear collision, we consider the extreme caricature of two interacting Lipkin systems. Initially, like two distantly approaching nuclei, particles in each isolated system interact only among themselves, with each system evolving in its respective ground state. At time $t=0$ each particle is allowed to interact with any particle in either system, like nucleons within two nuclei which are passing through each other. Finally, after some interaction time τ, the fragments are assumed to have separated by more than the range of interaction and again particles are restricted to interact only with other particles in the same system. Although questions of c.m. motion and particle transfer are completely eliminated from the model, one does address the essential problem of mutual excitation of two interacting systems which have an exceeding large number of accessible states.

Distinguishing operators for particles in the two systems by subscripts and assuming the systems contain N_1 and N_2 particles, respectively, the Hamiltonian for the two interacting systems is

$$H(t) = H^{N_1} + H^{N_2} + [\Theta(t) - \Theta(t-\tau)]H_{\rm INT} , \tag{3.7}$$

where

$$H_{\rm INT} = V(J_{1_+}J_{2_+} + J_{1_-}J_{2_-}) . \tag{3.8}$$

For times prior to $t=0$, the two systems are in their respective interacting ground states,

$$|\Psi\rangle = |J_1\alpha_0\rangle\,|J_2\beta_0\rangle = \sum_{J\gamma} C_{J\gamma}(0)\,|J\gamma\rangle . \tag{3.9}$$

By orthogonality, we find

$$C_{J\gamma}(0) = \langle J_1\alpha_0 J_2\beta_0|J\gamma\rangle . \tag{3.10}$$

The quantities $\langle J_1\alpha_0 J_2\beta_0|J\gamma\rangle$ may be expressed in terms of the eigenvectors and the Clebsch-Gordan coefficients.

$$\langle J_1\alpha_0 J_2\beta_0|J\gamma\rangle = \sum_{m_{J_1}m_{J_2}} \omega_{J_1\alpha_0}(m_{J_1})\omega_{J_2\beta_0}(m_{J_2}) \times \omega_{J\gamma}(m_{J_1}+m_{J_2}) \times \langle J_1J_2m_{J_1}m_{J_2}|Jm_{J_1}+m_{J_2}\rangle . \tag{3.11}$$

During the interaction interval $0<t<\tau$, the Hamiltonian describes a "compound nucleus" with known eigenstates. Hence, application of the time evolution operator to the initial state yields

$$|\Psi(t)\rangle = \sum_{J\gamma} C_{J\gamma}(0)e^{-i\epsilon_{J\gamma}t}\,|J\gamma\rangle . \tag{3.12}$$

It should be noted that the simple form above would have been impossible to achieve if ϵ or V had been chosen to be different for the two systems.

We now consider transition amplitudes to excited states of the single systems at the end of the interaction period τ. The amplitude $\tilde{C}_{\alpha\beta}(\tau)$ for finding the final state with system 1 in state α and system 2 in state β is clearly the analog of an S-matrix element for this simple model and is given by

$$|\Psi(\tau)\rangle = \sum_{\alpha\beta} \tilde{C}_{\alpha\beta}(\tau)\,|J_1\alpha\rangle\,|J_2\beta\rangle . \tag{3.13}$$

Matching Eq. (3.13) at $t=\tau$ to Eq. (3.12) and projecting, we obtain

$$\tilde{C}_{\alpha\beta}(\tau) = \sum_{J\gamma} C_{J\gamma}(0)e^{-i\epsilon_{J\gamma}t}\langle J_1\alpha J_2\beta|J\gamma\rangle . \tag{3.14}$$

This expression for the transition amplitudes yields all the results to be compared subsequently with appropriate solutions. Since evaluation of $\tilde{C}_{\alpha\beta}(\tau)$ requires knowledge of only the single system eigenvectors and the relevant Clebsch-Gordan coefficients, it is feasible to calculate solutions for large numbers of particles.

IV. SOLUTION IN THE TDHF APPROXIMATION

The lowest order truncation of the coupled-cluster equations, in the representation in which $S^{(1)} \equiv 0$, yields the static HF equation

$$\langle\phi|a_\nu^\dagger a_\rho H|\phi\rangle = 0 \tag{4.1}$$

and the TDHF equation

$$\langle\phi|a_\nu^\dagger a_\rho(H(t) - i\partial/\partial t)|\phi\rangle = 0 . \tag{4.2}$$

A convenient parametrization for ϕ is obtained by introducing the general unitary transformation[5,6]

$$\begin{bmatrix}\gamma_{p_+}^\dagger\\ \gamma_{p_-}^\dagger\end{bmatrix} \equiv \begin{bmatrix}\cos(\tfrac{1}{2}\alpha) & -i\sin(\tfrac{1}{2}\alpha)e^{i\psi}\\ -i\sin(\tfrac{1}{2}\alpha)e^{-i\psi} & \cos(\tfrac{1}{2}\alpha)\end{bmatrix}\begin{bmatrix}a_{p_+}^\dagger\\ a_{p_-}^\dagger\end{bmatrix} \tag{4.3}$$

and defining

$$|\phi\rangle = \prod_p \gamma_{p_-}^\dagger\,|0\rangle . \tag{4.4}$$

The noninteracting ground state, obtained by choosing $\alpha=\psi=0$ is a trivial solution to Eqs. (4.1) and (4.2), as may be noted by observing that H and $i\partial/\partial t$ do not connect the noninteracting ground state to any one-particle, one-hole states.

A general solution is obtained by defining the operators I_z, I_+, and I_- in analogy to the J operators,

$$I_z = \tfrac{1}{2}\sum_{p\sigma}\sigma\gamma^\dagger_{p\sigma}\gamma_{p\sigma}\,,$$
$$I_+ = \sum_p \gamma^\dagger_{p_+}\gamma_{p_-}\,, \tag{4.5}$$
$$I_- = I^\dagger_+\,.$$

The I operators preserve the commutation relations for angular momentum operators. As before, operators defined for the two separate systems are distinguished by an integer subscript and operators not belonging to the same system commute. The transformation between the two sets of operators is

$$\begin{bmatrix} J_z \\ J_+ \\ J_- \end{bmatrix} = \begin{bmatrix} \cos\alpha & -\tfrac{1}{2}i\sin\alpha\, e^{-i\psi} & \tfrac{1}{2}i\sin\alpha\, e^{i\psi} \\ -i\sin\alpha\, e^{i\psi} & \tfrac{1}{2}(1+\cos\alpha) & \tfrac{1}{2}(1-\cos\alpha)e^{2i\psi} \\ i\sin\alpha\, e^{-i\psi} & \tfrac{1}{2}(1-\cos\alpha)e^{-2i\psi} & \tfrac{1}{2}(1+\cos\alpha) \end{bmatrix} \begin{bmatrix} I_z \\ I_+ \\ I_- \end{bmatrix} \tag{4.6}$$

and for $\psi = 0$ each quasispin is simply rotated through the same angle α about the x axis. The Hamiltonian $H(t)$ can now be expressed in terms of the I operators. The simplicity of the original representation is lost, however, and there are now 9 nonzero coefficients for the 9 independent linear and bilinear combinations of I_z, I_+, and I_-. We note that the Hamiltonian will contain nondiagonal one-body terms in this representation so that Eq. (4.4) will not in general satisfy the TDHF equation.

The wave function for the two systems is given by

$$|\Phi\rangle = |\phi_1\rangle|\phi_2\rangle\,, \tag{4.7}$$

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are defined by Eq. (4.4) for each system. Although the model may consist of arbitrarily many particles, by symmetry in the particle labels, each system is completely specified by the two parameters α_i and ψ_i.

The static HF solution for a single system is obtained by noting that with $|\phi\rangle$ defined in Eq. (4.4), the only projections onto particle-hole states which are not trivially zero in Eq. (4.1) are

$$\langle\phi|\gamma^\dagger_{p_-}\gamma_{p_+}H|\phi\rangle = 0\,. \tag{4.8}$$

By symmetry in the particle labels, these N equations may be replaced by the single equation obtained by summing over p

$$\langle\phi|I_-H|\phi\rangle = 0\,. \tag{4.9}$$

Substitution of J_z, J_+, and J_- from Eq. (4.6) and the definition of H from Eq. (3.3) in Eq. (4.9) yields the result

$$i\tfrac{1}{2}N\sin\alpha\, e^{-i\psi}[\epsilon - (N-1)V(i\sin 2\psi + \cos 2\psi\cos\alpha)] = 0\,. \tag{4.10}$$

The root $\alpha = 0$ reproduces the noninteracting ground state as the HF solution. This weak-coupling solution exists for arbitrarily small values of V and has energy

$$\langle\phi|H|\phi\rangle = -\tfrac{1}{2}N\epsilon\,. \tag{4.11}$$

The second root

$$\psi = 0, \quad \cos\alpha = \frac{\epsilon}{V(N-1)}\,, \tag{4.12}$$

exists only for $V > \epsilon/(N-1)$ and corresponds to the strong coupling solution. The HF energy for this root is

$$\langle\phi|H|\phi\rangle = -\frac{\epsilon N}{4}\left(\frac{1}{(N-1)V/\epsilon} + (N-1)\frac{V}{\epsilon}\right). \tag{4.13}$$

The transition between the weak and strong coupling solutions occurs at $V_T = \epsilon/(N-1)$ with both $E(V)$ and (dE/dV) continuous at V_T.

The time evolution of the parameters α_1, α_2, and ψ_1, ψ_2 is obtained from the TDHF equation, Eq. (4.2), with $H(t)$ given in Eq. (3.7). As in Eqs. (4.8) and (4.9), it is useful to write the nonzero $a^\dagger_\nu a_\rho$ terms as $\gamma^\dagger_{\rho_-}\gamma_{\rho_+}$ and sum over the particles in the ith system, yielding the two equations

$$\langle\Phi|I_{i_-}(H(t) - i\partial/\partial t)|\Phi\rangle = 0\,. \tag{4.14}$$

The transformation Eq. (4.3) may be differentiated with respect to time and combined with the corresponding inverse transformation and yields the following equation of motion for $\gamma^\dagger_{p\sigma}$:

$$\begin{bmatrix} \dot\gamma^\dagger_{p_{i+}} \\ \dot\gamma^\dagger_{p_{i-}} \end{bmatrix} = \begin{bmatrix} i\dot\psi_i\sin^2(\tfrac{1}{2}\alpha_i) & -\tfrac{1}{2}(i\dot\alpha_i - \dot\psi_i\sin\alpha_i)e^{i\psi_i} \\ -\tfrac{1}{2}(i\dot\alpha_i + \dot\psi_i\sin\alpha_i)e^{-i\psi_i} & -i\dot\psi_i\sin^2(\tfrac{1}{2}\alpha_i) \end{bmatrix} \begin{bmatrix} \gamma^\dagger_{p_{i+}} \\ \gamma^\dagger_{p_{i-}} \end{bmatrix}. \tag{4.15}$$

The time derivative of $|\phi_i\rangle$ is then given by

$$i\frac{\partial}{\partial t}|\phi_i\rangle = i\sum_j \gamma^\dagger_{1-}\cdots\dot{\gamma}^\dagger_{j-}\cdots\gamma^\dagger_{N_i-}|0\rangle$$
$$= \tfrac{1}{2}(\dot{\alpha}_i - i\dot{\psi}_i\sin\alpha_i)e^{-i\psi_i}I_{i+}|\phi_i\rangle + \dot{\psi}_i\sin^2(\tfrac{1}{2}\alpha_i)|\phi_i\rangle \quad (4.16)$$

and contains one component proportional to $|\phi_i\rangle$ and a second component of one-particle, one-hole excitations. Hence

$$\langle\Phi|I_{i-}i\partial/\partial t|\Phi\rangle = \tfrac{1}{2}N_i(\dot{\alpha}_i - i\dot{\psi}_i\sin\alpha_i)e^{-i\psi_i}. \quad (4.17)$$

The matrix element $\langle\Phi|I_{i-}H(t)|\Phi\rangle$ is evaluated by substituting the Hamiltonian $H(t)$ of Eq. (3.7) after using the transformation Eq. (4.6) to express it in terms of the I operators. For the interval $0<t<\tau$, straightforward algebra yields

$$\langle\Phi|I_{1-}H(t)|\Phi\rangle = -\tfrac{1}{2}iN_1[\epsilon\sin\alpha_1 e^{-i\psi_1} + VN_2\sin\alpha_2(\sin^2(\tfrac{1}{2}\alpha_1)e^{-i2\psi_1-i\psi_2} - \cos^2\tfrac{1}{2}\alpha_1)e^{i\psi_2}) + V(N_1-1)\sin\alpha_1(\cos^2\tfrac{1}{2}\alpha_1)e^{i\psi_1} - \sin^2(\tfrac{1}{2}\alpha_1)e^{-i3\psi_1})]. \quad (4.18)$$

Equating the real and imaginary parts of Eq. (4.14) to zero yields the equations of motion for the parameters α_i, ψ_i,

$$\begin{bmatrix} N_1\cos\psi_1 & -N_1\sin\alpha_1\sin\psi_1 & 0 & 0 \\ -N_1\cos\psi_1 & -N_1\sin\alpha_1\cos\psi_1 & 0 & 0 \\ 0 & 0 & N_2\cos\psi_2 & -N_2\sin\alpha_2\sin\psi_2 \\ 0 & 0 & -N_2\cos\psi_2 & -N_2\sin\alpha_2\cos\psi_2 \end{bmatrix}\begin{bmatrix}\dot{\alpha}_1\\ \dot{\psi}_1\\ \dot{\alpha}_2\\ \dot{\psi}_2\end{bmatrix} = \begin{bmatrix}\mathrm{Re}\langle\Phi|I_{1-}H|\Phi\rangle\\ \mathrm{Im}\langle\Phi|I_{1-}H|\Phi\rangle\\ \mathrm{Re}\langle\Phi|I_{2-}H|\Phi\rangle\\ \mathrm{Im}\langle\Phi|I_{2-}H|\Phi\rangle\end{bmatrix} \quad (4.19)$$

The off-diagonal blocks are zero in the above equation, a feature which does not survive in approximations in higher order than the mean-field theory. The two systems are coupled only through the appearance of both α's and ψ's in $\langle\Phi|I_{i-}H(t)|\Phi\rangle$.

Inversion of the above matrix yields the final form of the TDHF equations,

$$\begin{bmatrix}\dot{\alpha}_i\\ \dot{\psi}_i\end{bmatrix} = \frac{2}{N_i}\begin{bmatrix}\cos\psi_i & -\sin\psi_i\\ -\dfrac{\sin\psi_i}{\sin\alpha_i} & -\dfrac{\cos\psi_i}{\sin\alpha_i}\end{bmatrix}\begin{bmatrix}\mathrm{Re}\langle\Phi|I_{i-}H(t)|\Phi\rangle\\ \mathrm{Im}\langle\Phi|I_{i-}H(t)|\Phi\rangle\end{bmatrix}. \quad (4.20)$$

Since the noninteracting ground state trivially satisfies the TDHF equations at all times, the only interesting TDHF solution arises from the strong coupling initial condition given in Eq. (4.12). Starting with the values

$$\psi_i(0) = 0, \quad \alpha_i(0) = \cos^{-1}\left[\frac{\epsilon}{V(N_i-1)}\right] \quad (4.21)$$

and discretizing the time variable, the set of equations (4.20) may be solved numerically, thus determining the TDHF approximation to the combined state vector as a function of time. Although our TDHF equations are equivalent to those investigated by Krieger,[15] the initial conditions (4.21) and thus the physical interpretation of our results differ significantly.

V. SOLUTION IN THE TWO-BODY CLUSTER APPROXIMATION

The form of the most general wave function having $S^{(n)}\equiv 0$ for all $n>2$ is especially simple for the Lipkin systems considered in this work. One-particle, one-hole amplitudes may be omitted by using $|\phi\rangle$ and $|\Phi\rangle$ of the form of Eqs. (4.4) and (4.7) and all the physical content of $S^{(1)}$ resides in the parameters α_i and ψ_i. For a single system, by symmetry in the particle labels, $S^{(2)}$ is characterized by a single parameter $\mathcal{S}^{(2)}$,

$$S^{(2)} = \tfrac{1}{2}\sum\langle pp'|S^{(2)}|pp'\rangle\gamma^\dagger_{p+}\gamma^\dagger_{p'+}\gamma_{p'-}\gamma_{p-} \equiv \tfrac{1}{2}\mathcal{S}^{(2)}I_+^{\,2}, \quad (5.1)$$

and for two interacting systems, the general form of $S^{(2)}$ is

$$S^{(2)}(t) = \tfrac{1}{2}\mathcal{S}_1^{(2)}(t)I_{1+}^{\,2} + \tfrac{1}{2}\mathcal{S}_2^{(2)}(t)I_{2+}^{\,2} + \mathcal{S}_{12}^{(2)}(t)I_{1+}I_{2+}. \quad (5.2)$$

Summing over particle labels as in Eqs. (4.8) and (4.4) reduces the general static and time dependent equations (2.2) and (2.6) to the following simple form:

$$\langle\phi|He^{S^{(2)}}|\phi\rangle = E\,, \tag{5.3a}$$

$$\langle\phi|I_-e^{-S^{(2)}}He^{S^{(2)}}|\phi\rangle = 0\,, \tag{5.3b}$$

$$\langle\phi|I_-^2e^{-S^{(2)}}He^{S^{(2)}}|\phi\rangle = 0\,, \tag{5.3c}$$

and

$$\langle\Phi|I_{i_-}e^{-S^{(2)}(t)}(H-i\partial/\partial t)e^{S^{(2)}(t)}|\Phi\rangle = 0\,, \tag{5.4a}$$

$$\langle\Phi|I_{i_-}^2e^{-S^{(2)}(t)}(H-i\partial/\partial t)e^{S^{(2)}(t)}|\Phi\rangle = 0\,, \tag{5.4b}$$

$$\langle\Phi|I_{1-}I_{2-}e^{-S^{(2)}(t)}(H-i\partial/\partial t)e^{S^{(2)}(t)}|\Phi\rangle = 0\,. \tag{5.4c}$$

The static equations (5.3) are solved by angular momentum algebra after expressing H in terms of the I operators, with the results

$$E = -\tfrac{1}{4}\epsilon N\cos\alpha\left[\frac{\chi}{\cos\alpha}(1-\mathcal{S}_2) - \chi\cos\alpha(1+\mathcal{S}_2)+2\right], \tag{5.5a}$$

$$\cos\alpha = \frac{1-(N-1)\mathcal{S}_2}{[1-(N-3)\mathcal{S}_2]\chi}\,, \tag{5.5b}$$

$$(N^2-7N+9)(1+\cos^2\alpha)\chi(\mathcal{S}_2)^2 + [6\chi(N-2)(1-\cos^2\alpha)+4(N-1)\cos\alpha]\mathcal{S}_2 + (1+\cos^2\alpha)\chi = 0\,, \tag{5.5c}$$

where χ is a dimensionless parameter

$$\chi = \frac{V(N-1)}{\epsilon}\,. \tag{5.6}$$

The last two equations above combine to give a single quartic equation in $\mathcal{S}^{(2)}$. The appropriate root is real, yields a real value for α, and corresponds to an energy which is continuously connected to the HF energy. In the approximation $\mathcal{S}^{(2)}=0$, Eq. (5.5a) reduces to the corresponding weak and strong coupling HF results. Note that when including $\mathcal{S}^{(2)}$, the transition between weak and strong coupling solutions no longer occurs at $\chi = 1$.[16]

The time-dependent equations, Eq. (5.4), involve a total of ten independent real functions of time: the four parameters $\alpha_1\alpha_2\psi_1\psi_2$ and the real and imaginary parts of the complex amplitudes $\mathcal{S}_1^{(2)}$, $\mathcal{S}_2^{(2)}$, and $\mathcal{S}_{12}^{(2)}$. The initial values of these quantities are fixed by requiring $\alpha_i(0)$ and $\mathcal{S}_i^{(2)}(0)$ to satisfy the static equations, and requiring the other quantities to be zero.

Evaluation of the time derivatives in Eqs. (5.4) proceeds as in Sec. II using Eq. (2.7). The time derivative of I_{i_+} is

$$\frac{\partial}{\partial t}I_{i_+} = i\dot\psi_i(1-\cos\alpha_i)I_{i_+} + (i\dot\alpha_i - \dot\psi_i\sin\alpha_i)e^{i\psi_i}I_{iz}\,, \tag{5.7}$$

which is established by differentiating I_{i_+} and using the operator equations of motion Eq. (4.15).

To illustrate the procedure for calculating the matrix elements of the time derivative operator, we shall evaluate Eq. (5.4a) and simply quote the other results,

$$\left\langle\Phi\left|I_{1-}e^{-S^{(2)}}i\frac{\partial}{\partial t}e^{S^{(2)}}\right|\Phi\right\rangle = \left\langle\Phi\left|I_{1-}\,i\frac{\partial}{\partial t}\right|\Phi\right\rangle + \tfrac{1}{2}\mathcal{S}_1^{(2)}\left\langle\Phi\left|I_{1-}\left(I_{1+}\frac{\partial}{\partial t}I_{1+} + \frac{\partial}{\partial t}I_{1+}I_{1+}\right)\right|\Phi\right\rangle + \tfrac{1}{2}\mathcal{S}_{12}^{(2)}\left\langle\Phi\left|I_{1-}\left(I_{1+}\frac{\partial}{\partial t}I_{2+} + \frac{\partial}{\partial t}I_{1+}I_{2+}\right)\right|\Phi\right\rangle. \tag{5.8}$$

Using Eq. (5.7), this simplifies to

$$\left\langle\Phi\left|I_{1-}e^{-S^{(2)}}i\frac{\partial}{\partial t}e^{S^{(2)}}\right|\Phi\right\rangle = \tfrac{1}{2}N_1(\dot\alpha_1 - i\dot\psi_1\sin\alpha_1)e^{-i\psi_1} + \tfrac{1}{2}N_1(N_1-1)\mathcal{S}_1^{(2)}(\dot\alpha_1 + i\dot\psi_1\sin\alpha_1)e^{i\psi_1} + \tfrac{1}{2}N_1N_2\mathcal{S}_{12}^{(2)}(\dot\alpha_2 + i\dot\psi_2\sin\alpha_2)e^{i\psi_2}. \tag{5.9}$$

By equating the real and imaginary parts of Eq. (5.9) to the real and imaginary parts of $\langle\Phi|I_{1-}e^{-S^{(2)}}He^{S^{(2)}}|\Phi\rangle$ and repeating with the labels 1 and 2 interchanged, we arrive at a 4×4 matrix equation similar in form to (4.19) but with nonzero off-diagonal blocks. The elements of the matrix may be easily worked out, and will not be displayed here.

By similar manipulations, the time derivative parts of Eqs. (5.4b) and (5.4c) are, respectively,

$$\langle\Phi|I_{1-}^2e^{-S^{(2)}}i\frac{\partial}{\partial t}e^{S^{(2)}}|\Phi\rangle = N_1(N_1-1)\left(i\frac{\partial}{\partial t}\mathcal{S}_1^{(2)} - 2\mathcal{S}_1^{(2)}(1-\cos\alpha_1)\dot\psi_1\right), \tag{5.10a}$$

$$\langle\Phi|I_{1-}I_{2-}e^{-S^{(2)}}i\frac{\partial}{\partial t}e^{S^{(2)}}|\Phi\rangle = N_1N_2\left\{i\frac{\partial}{\partial t}\mathcal{S}_{12}^{(2)} - \mathcal{S}_{12}^{(2)}[(1-\cos\alpha_1)\dot\psi_1 + (1-\cos\alpha_2)\dot\psi_2]\right\}. \tag{5.10b}$$

On equating these results to $\langle\Phi|I_{1-}^2e^{-S^{(2)}}He^{S^{(2)}}|\Phi\rangle$ and $\langle\Phi|I_{1-}I_{2-}e^{-S^{(2)}}He^{S^{(2)}}|\Phi\rangle$, respectively, we arrive at the equations of motion for $\mathcal{S}_1^{(2)}(t)$, $\mathcal{S}_2^{(2)}(t)$, and $\mathcal{S}_{12}^{(2)}(t)$. As shown in general in Sec. II, these differential equations are first order in time for $\mathcal{S}_i^{(2)}$ and $\mathcal{S}_{12}^{(2)}$ and are thus in a form directly suitable for numerical evolution.

Finally, we turn to the problem of evaluating the matrix elements of the collision Hamiltonian in Eqs. (5.4). Although one can use the straightforward means employed previously in the TDHF case, the amount of algebra is prohibitive, given the relatively complicated form of the Hamiltonian when expressed in I operators. Hence all operators have been represented by matrices of finite dimension, and the desired matrix elements obtained numerically by matrix multiplication. As an example, consider a typical matrix element which we wish to evaluate,

$$\langle\Phi|I_{1-}{}^{2}e^{-S^{(2)}}H(t)e^{S^{(2)}}|\Phi\rangle = \langle\Phi|I_{1-}{}^{2}\{H(t)+[H(t),S^{(2)}] + \frac{1}{2!}[[H(t),S^{(2)}],S^{(2)}]+\cdots\}|\Phi\rangle . \tag{5.11}$$

Since $H(t)$ is bilinear in the operators I_{iz}, I_{i+}, I_{i-} and $S^{(2)}$ is bilinear in I_{i+}, and since the number of raising and lowering operators must occur in equal numbers for each i in order for the matrix element to be nonzero, the infinite series in Eq. (5.11) terminates in finite order. In this example, the highest power of I_{i+} or I_{i-} which can occur is 4.

To represent the operators I_{iz}, I_{i+}, I_{i-} by finite dimensional matrices, it is sufficient to impose the following conditions:

(a) All matrices with $i=1$ commute with all matrices with $i=2$.

(b) For $n \leq 4$ and $i=1,2$,

$$I_{iz}^{n}|\phi_i\rangle = (-\tfrac{1}{2}N)^{n}|\phi_i\rangle , \tag{5.12a}$$

$$I_{i+}^{n}|\phi_i\rangle = [n!(N_i-n+1)(N_i-n+2)\cdots N_i]^{1/2} \times |I_i=\tfrac{1}{2}N_i, m_{I_i}=-\tfrac{1}{2}N_i+n\rangle . \tag{5.12b}$$

A set of matrices which fulfill these conditions is explicitly given in Appendix A.

VI. NUMERICAL RESULTS FOR INTERACTING LIPKIN SYSTEMS

In order to quantitatively assess the validity of the lowest two orders of approximation in the coupled-cluster hierarchy, we have compared the approximations of Secs. IV and V with the exact solution of Sec. III. Both of the interacting systems were chosen to contain 14 particles, since more than 28 particles in the combined system renders exact solution cumbersome and costly. The level spacing ϵ was chosen to be 1 MeV and thus crudely representative of nuclear energy scales. Interaction times up to 1.2×10^{-21} sec were considered, representing the time required for projectiles with energies of 10–40 MeV per particle to interpenetrate 5–10 fm, respectively. Wide variations in N, V, and ϵ make little difference in the qualitative features of the solutions, so the limited results reported here are in fact representative of the general applicability of the coupled-cluster theory for this model.

Static solutions

Figure 1 shows the exact energy, E, for a single 14-particle system and the deviation between

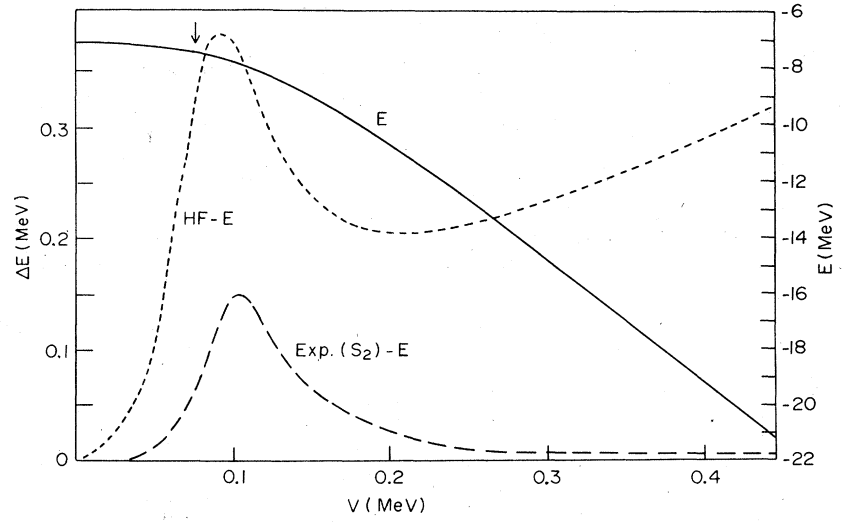

FIG. 1. The exact ground state energy E (solid line), deviation from E of the HF energy (short dashes), and deviation from E of the coupled-cluster energy including $S^{(2)}$ (long dashes). Note that E is referred to the scale at the right and the energy deviations use the scale at the left.

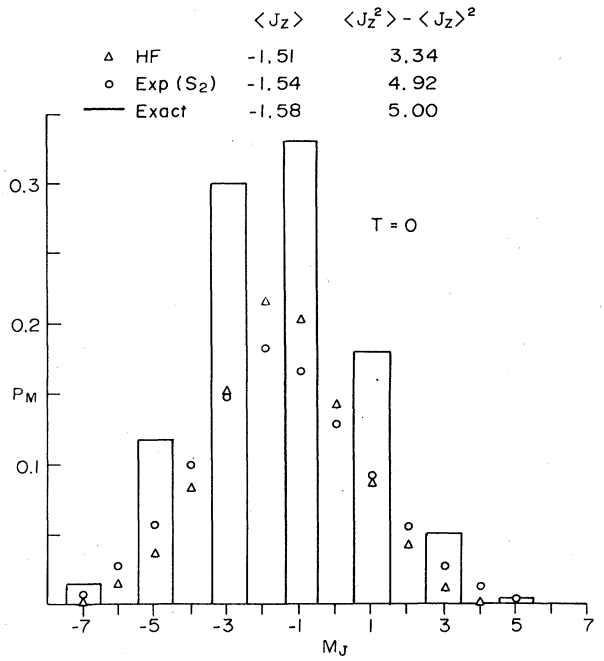

FIG. 2. Probability $P=|\langle\frac{1}{2}N, M_J|\psi\rangle|^2$ of projecting a component with M_J from the exact, HF, and second-order coupled cluster stationary-state wave functions.

truncated approximations to $\langle H\rangle$ and E as a function of interaction strength V. Since we use $\langle H\rangle$ instead of the approximate energy in Eq. (5.5a), it is clear by the variational principle that the deviation is positive definite. The error in the HF approximation near the transition point, $V_T=\epsilon/(N-1)\sim 0.077$ denoted by the arrow in Fig. 1, is at most 5%, and in the strong coupling limit the deviation increases with V. Including S_2 significantly decreases the deviation, not only in the weak coupling limit explored by Lührmann,[17] but also even more dramatically in the strong coupling limit. For the time-dependent calculations, we have selected $NV=5$ MeV, so that the potential strength $V\approx 0.36$ is well into the strong coupling region and yields a nontrivial TDHF solution. Other observables besides the energy for the static solutions with $N=14$ and $NV=5$ are presented in Fig. 2 and as the $T=0$ results in the time-dependent solutions.

Figure 2 displays the probability of observing the ground state in each state of the natural basis of Eq. (3.5)

$$P_{M_J}=|\langle JM_J|\psi\rangle|^2. \tag{6.1}$$

Since H commutes with J^2, the only nonzero amplitudes correspond to $J=\frac{1}{2}N$ and this label is suppressed for notational convenience. Because V only excites pairs of particles between levels, adiabatically evolving Ψ from the noninteracting ground state $|\frac{14}{2},-\frac{14}{2}\rangle$ can only yield amplitudes with odd values of M_J. Thus, the exact solution yields the histogram of Fig. 2 with all even probabilities exactly zero and a broad, Gaussian-type distribution for the odd probabilities. The most essential features of the distribution are characterized by the mean, $\langle J_z\rangle$ and width $\langle J_z^2\rangle-\langle J_z\rangle^2$ tabulated in the figure.

The probabilities $\langle JM_J|\exp(\sum_{n=1}^{k}S_n|\Phi\rangle$ for truncated wave functions of any order $k<N$ differ fundamentally from the exact probabilities. Since only an N-particle correlation can enforce the condition that even numbers of particles occupy each level, there is no way of attaining the dramatic even-odd alternation characterizing the exact solution. One observes this complete lack of even-odd alternation explicitly in the numerical results for the lowest two orders denoted by triangles and circles in Fig. 2.

Figure 2 thus succinctly emphasizes the fundamental distinction between approximating the wave function and expectation values of few-body operators. In no sense do successive truncated approximations converge to the exact probabilities. In contrast, however, the mean values of $\langle J_z\rangle$ and $\langle J_z^2\rangle-\langle J_z\rangle^2$ shown in the top of the figure are approximated extremely well even in very low orders.

Time-dependent solutions

The projection of the wave function of one 14 particle fragment onto the natural basis after an interaction time of 4×10^{-23} sec is shown in Fig. 3. As in Fig. 2, the exact solution has pronounced odd-even staggering although nonvanishing even M_J states are now possible through excitation of pairs comprised of one particle from each system. As in Fig. 2, although there is no convergence for the individual probabilities, good approximations are obtained for mean values of J_z and $(J_z-\langle J_z\rangle)^2$. To the degree to which $\langle JM_J|\psi(t)\rangle$ is a meaningful analog of an S-matrix element in a realistic scattering problem, this example reinforces our emphasis on approximating mean values rather than S-matrix elements.

A quantitative comparison between exact and approximate mean values of particularly relevant operators as a function of interaction time is presented in Fig. 4. The excitation energy, ΔE, is defined as the mean value $\frac{1}{2}\langle H^{N_1}+H^{N_2}\rangle$ for the combined system at time T minus the same quantity evaluated at time $T=0$ (which is just the stationary state energy for a single system in the same approximation.) Roughly half of the true excitation energy is described in the mean-field approximation and for the time scales under consideration the

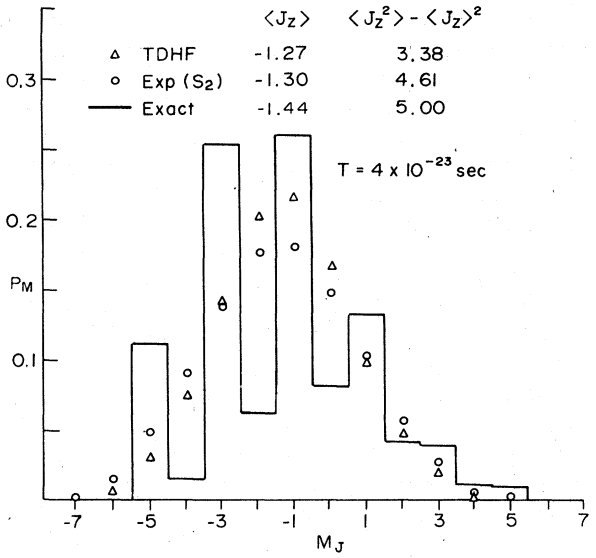

FIG. 3. Same as Fig. 2 for time dependent wave functions at time $T = 4\times10^{-23}$ s.

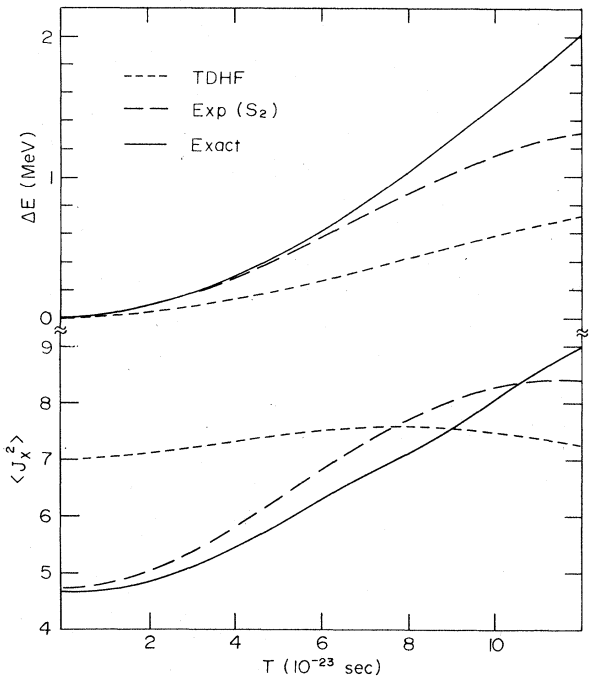

FIG. 4. Excitation energy ΔE and mean value of J_x^2 as a function of interaction time for exact, TDHF, and second-order coupled-cluster wave functions.

$S^{(2)}$ truncation yields a reasonably accurate approximation to the full excitation energy. Similarly for $\langle J_x^2\rangle$, defined as $\frac{1}{2}\langle J_{x1}^2 + J_{x2}^2\rangle$ for the combined system, when the suppressed zero of the graph is considered, the mean-field approximation yields a result of the correct order of magnitude and the inclusion of two-body clusters produces quantitative agreement with the exact solution. In both cases, the operators under consideration involved two-body components so significant contributions from $S^{(2)}$ should be expected and, in fact, do arise. Whereas $S^{(2)}$ contributes linearly to both $\langle H\rangle$ and $\langle J_x^2\rangle$, since J_z is diagonal in $a_p^\dagger a_p$, $\langle J_z^2\rangle$ only depends quadratically on $S^{(2)}$, which explains why $\langle J_z^2\rangle$ in Fig. 3 is not as accurate as $\langle J_x^2\rangle$ in Fig. 4 in the $e^{S^{(2)}}$ approximation.

One-body operators should be much more accurately reproduced in the mean-field approximation than the operators discussed above containing two-body components. Indeed, the tabulated values for $\langle J_z\rangle$ in Figs. 2 and 3 bear out this expectation. Unfortunately, since $\langle J_x\rangle = 0$, J_x does not provide an additional test.

One important question arising in the coupled-cluster hierarchy is whether inaccuracy in computing mean values occurs primarily from errors in the $S^{(n)}$ amplitudes arising from the fact that they are obtained from solving a truncated Schrödinger equation, or whether the inaccuracy in mean values should be attributed to the explicit contribution of higher-order amplitudes to the expectation value. Although we cannot provide a general answer, the results in Tables I and II indicate that in the present model, the dominant error arises from explicit omission of higher correlation amplitudes in mean values. In the basis $|\Phi\rangle$ defined in Eq. (4.7) with the parameters $\alpha(t)$ and $\psi(t)$ in $\gamma_p^\dagger$ satisfying Eq. (5.4a), the $n=2$ coupled cluster wave function for a symmetric system has the form

$$|\Psi^{(2)}\rangle = \exp[\tfrac{1}{2}\mathcal{S}^{(2)}(I_{1_+}^2 + I_{2_+}^2) + \mathcal{S}_{12}^{(2)} I_{1_+} I_{2_+}]|\Phi\rangle. \quad (6.2)$$

In the same basis, the exact wave function, Eq. (3.12), may be written

TABLE I. Wave function amplitudes defined in Eqs. (6.2) and (6.3).

T (10^{-22} s)	C	$\hat{\mathcal{S}}^{(1)}$	$\hat{\mathcal{S}}^{(2)}$	$\mathcal{S}^{(2)}$	$\hat{\mathcal{S}}_{12}^{(2)}$	$\mathcal{S}_{12}^{(2)}$
0	0.489	0.0015	0.0156	0.0151	0	0
0.66	0.489	0.0013	0.0101	0.0097	0.0107	0.0109
1.18	0.491	0.0016	0.0024	0.0050	0.0134	0.0129

TABLE II. Comparison of expectation values with various wave functions at times $T=0$ and $T=1.18\times10^{-22}$ s.

	$\langle J_z(0)\rangle$	$\langle J_z^2(0)\rangle$	$\langle J_z(1.18)\rangle$	$\langle J_z^2(1.18)\rangle$
ψ	−1.58	7.49	−0.74	6.44
$\psi^{(2)}$	−1.54	7.28	−0.11	3.55
$\hat{\psi}^{(2)}$	−1.56	7.40	−0.12	3.52

$$|\Psi\rangle = C\exp\Big(\hat{S}^{(1)}(I_{1_+}+I_{2_+}) + \tfrac{1}{2}\hat{S}^{(2)}(I_{1_+}^2+I_{2_+}^2) + \hat{S}_{12}^{(2)}I_{1_+}I_{2_+} + \sum_{n=3}^{N} S^{(n)}\Big)|\Phi\rangle. \tag{6.3}$$

By projecting the exact solution onto $|\Phi\rangle$, $I_{1_+}|\Phi\rangle$, $I_{1_+}^2|\Phi\rangle$ and $I_{1_+}I_{2_+}|\Phi\rangle$, the values C, $\hat{S}^{(1)}$, $\hat{S}^{(2)}$, and $\hat{S}_{12}^{(2)}$ were obtained and are tabulated in Table I for comparison with the corresponding coupled-cluster amplitudes $S^{(n)}$. Since the discrepancies $(S^{(2)}-\hat{S}^{(2)})$ and $(S^{(1)}-0)$ are small relative to the dominant amplitude at each time, we conclude that the S's evolved with the truncated Schrödinger equation are quite adequate. The normalization constant, C, indicates that only one fourth of the total wave function is comprised of one-particle, one-hole, and two-particle, two-hole components.

Table II shows values of J_z and J_z^2 calculated with the exact wave function ψ, the coupled-cluster wave function $\psi^{(2)}$ defined in Eq. (6.2), and a truncated wave function $\hat{\psi}^{(2)}$ obtained by using the exact $\hat{S}^{(1)}$, $\hat{S}^{(2)}$, and $\hat{S}_{12}^{(2)}$ amplitudes in Eq. (6.3) and omitting $\sum_{n=3}^{N}S^{(n)}$. Since $\psi^{(2)}$ agrees much more closely with $\hat{\psi}^{(2)}$ than with ψ, clearly the dominant error arises from omission of the sum $\sum_{n=3}^{N}S^{(n)}$ rather than the small discrepancies between the S and $\hat{S}$ amplitudes.

VII. SUMMARY AND CONCLUSIONS

The time-dependent coupled-cluster theory introduced in this work provides a convenient framework for a systematic hierarchy of corrections to the intuitively appealing time-dependent mean-field approximation. Formulated in terms of particle-hole amplitudes, the theory represents many-particle correlations far more economically than the corresponding density-matrix or Green's function hierarchies. The consistency between the static and time-dependent theories renders the considerable progress in applying the static theory to nuclear systems directly relevant, provides natural initial conditions utilizing strictly analogous approximations, and provides the alternative technique of evolution in complex time and adiabatic switching on for solving the stationary state equations. Although the simplest truncation prescription of setting $S^{(m)}=0$ for all $m>n$ has been used exclusively in this work, the general theory also admits alternative truncations more suitable for the nuclear interaction.

Application to the specific solvable model of two Lipkin systems explicitly demonstrates the theory's viability and provides valuable insight into how it actually works in practice. The lowest order mean-field approximation yields good results for one-body operators and qualitatively correct behavior for two-body operators for the interaction times investigated in this work, which were an order of magnitude longer than the "lifetime" of a determinant[18] in this model, $T_D=1.3\times10^{-23}$ s. Inclusion of two-particle, two-hole amplitudes yields quantitative agreement for observables containing two-body operators.

The crucial distinction between expectation values of few-body operators and overlap of N-body wave functions was emphasized theoretically and explicitly demonstrated for the projection of the Lipkin model wave function onto the natural basis. Although it is conceivable that certain approximate S-matrix elements defined in terms of projection onto consistently approximated stationary states for the final channel are more meaningful than the projections onto the natural basis examined in this work, there certainly exist formidable obstacles in substantiating such a conjecture, and in view of our pessimistic theoretical arguments and results, the burden of proof lies upon the proponent.

The interacting Lipkin systems considered in this work clearly provide a highly unrealistic caricature of colliding nuclei, and thus strong inferences concerning realistic nuclei are unwarranted. In particular, since there are only two single-particle states for each particle, each particle interacts equally with every other particle, and there are only three distinct two-particle, two-hole amplitudes, the solution in this model is drastically more coherent than for a nucleus. The major emphasis of our subsequent work will therefore be generalization of the method to treat strongly repulsive potentials and application to more realistic model systems.

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APPENDIX A

A representation of the algebra of Eq. (5.12) is provided by 25 dimensional matrices acting on the column vector $|\Phi\rangle$

$$|\Phi\rangle = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \tag{A1}$$

Using the convention that omitted matrix elements are zero, we first define the following 5×5 matrices:

$$A = \begin{bmatrix} -\frac{1}{2}N_1+4 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2}N_1+3 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2}N_1+2 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2}N_1+1 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}N_1 \end{bmatrix}, \tag{A2}$$

$$B = \begin{bmatrix} 0 & [4(N_1-3)]^{1/2} & 0 & 0 & 0 \\ 0 & 0 & [3(N_1-2)]^{1/2} & 0 & 0 \\ 0 & 0 & 0 & [2(N_1-1)]^{1/2} & 0 \\ 0 & 0 & 0 & 0 & (N_1)^{1/2} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{A3}$$

and the 5×5 unit matrix denoted as ϵ_I.

In terms of these matrices, I_{iz} and I_{i+} have the following block form:

$$I_{1z} = \begin{bmatrix} A & 0 & 0 & 0 & 0 \\ 0 & A & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 \\ 0 & 0 & 0 & A & 0 \\ 0 & 0 & 0 & 0 & A \end{bmatrix}, \tag{A4}$$

$$I_{2z} = \begin{bmatrix} (-\frac{1}{2}N_2+4)\epsilon_I & 0 & 0 & 0 & 0 \\ 0 & (-\frac{1}{2}N_2+3)\epsilon_I & 0 & 0 & 0 \\ 0 & 0 & (-\frac{1}{2}N_2+2)\epsilon_I & 0 & 0 \\ 0 & 0 & 0 & (-\frac{1}{2}N_2+1)\epsilon_I & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}N_2\epsilon_I \end{bmatrix}, \tag{A5}$$

$$I_{1+} = \begin{bmatrix} 0 & B & 0 & 0 & 0 \\ 0 & 0 & B & 0 & 0 \\ 0 & 0 & 0 & B & 0 \\ 0 & 0 & 0 & 0 & B \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{A6}$$

$$I_{2+}=\begin{bmatrix} 0 & [4(N_2-3)]^{1/2}\epsilon_I & 0 & 0 & 0 \\ 0 & 0 & [3(N_2-2)]^{1/2}\epsilon_I & 0 & 0 \\ 0 & 0 & 0 & [2(N_2-1)]^{1/2}\epsilon_I & 0 \\ 0 & 0 & 0 & 0 & (N_2)^{1/2}\epsilon_I \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{A7}$$

All other operators, such as H or S, are constructed as appropriate linear or bilinear combinations of the above matrices. This scheme of dealing with the $S^{(2)}$ level truncation can be easily extended to investigate any higher level of truncation, whereas algebraic evaluation would be almost impossible beyond the two-body approximation.

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