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Mean-field approximation to the many-body S matrix

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A nonperturbative method is developed for calculating the excitation of a many-body system by a time-dependent Hamiltonian. The stationary-phase approximation to a functional-integral representation of the interaction-picture many-body evolution operator results in a mean-field approximation to the S matrix which is asymptotically time independent. A one-body temporally nonlocal evolution equation defines the stationary mean-field configurations. The general method and character of the stationary solutions are illustrated by application to the forced harmonic oscillator and forced Lipkin model. Potential applications to realistic nuclear and atomic scattering situations are discussed.

[NUCLEAR REACTIONS Mean-field approximation, many-body S matrix, time-dependent Hartree Fock.]

I. INTRODUCTION

The picture of independent nucleons moving in a self-consistent mean field has proven to be a good first approximation to many aspects of the nuclear many-body problem. Hartree-Fock calculations with phenomenological[1] or realistic[2,3] effective interactions are capable of reproducing ground-state binding energies, charge densities, and single-particle energies for nuclei throughout the periodic table. To describe excited states, the static mean-field picture can be extended to the near equilibrium oscillations of the random-phase approximation (RPA).[4,5] The next logical step in this sequence is to develop a mean-field picture for nuclear collisions. In the past several years, time-dependent Hartree-Fock (TDHF) calculations[6-8] have been shown to be a good description of some inclusive properties of deep inelastic heavy-ion collisions.[9,10] However, it has so far proven impossible to formulate a mean-field method for calculating specific reaction cross sections or, equivalently, elements of the many-body S matrix. This paper presents the first steps toward such a calculation.

To motivate the present investigation, it is useful to recall the well-documented deficiencies of the TDHF approximation as an exclusive description of nuclear *reactions*, rather than as an inclusive description of nuclear *collisions*. The TDHF many-body wave function is assumed at all times to be a single Slater determinant evolving in a nonlinear, self-consistent manner. This evolution differs significantly from that of the exact Schrödinger equation in that, for times long after the collision, the wave function does not decompose into a linear combination of channel eigenstates whose coefficients have a time independent modulus. This so-called "spurious cross-channel correlation"[6,11] therefore defeats any attempt to calculate the S matrix by projection of the TDHF wave function onto channel states.[12] Another difficulty is the fact that the initial TDHF determinant is a wave packet in the space of channel eigenstates, making it difficult to unambiguously isolate a given incident channel.[13] Finally, although the TDHF evolution prescription plausibly represents the mean-field physics expected to dominate at small bombarding energies per nucleon, its precise relation to the exact Schrödinger evolution has only recently come under investigation.[14,15]

Our mean-field methods for calculating the many-body S matrix follow from the Hubbard-Stratonovich representation for the many-body evolution operator.[14,16] For a Hamiltonian consisting of a one-body kinetic energy term and a two-body interaction, the exact Schrödinger propagator can be written as a functional integral over an auxiliary field, the integrand containing only a one-body evolution operator which is functionally dependent on the auxiliary field. The many-body evolution problem is thus reduced to a coherent superposition of a (very infinite) number of one-body evolution problems. For given initial and final states, the saddle point or stationary-phase approximation to the functional integral results in a set of mean-field equations, similar to the TDHF but not identical to it, which define a stationary field configuration, and hence a one-body approximation to the matrix element of the many-body propagator. The remarkable utility and versatility of this general technique for the many-body problem is well illustrated by its recent application to bound-state problems[17] and its potential applications to spontaneous fission lifetimes[18] and the nuclear partition function.[19] An excellent introduction to this approach can be found in Ref. 20.

The definition of the initial and final state in the many-body scattering process is an important aspect of the problem. For simple single-particle potential scattering, these states are plane waves, the eigenstates of the "channel Hamiltonian," which is the free kinetic energy. However, in the many-body case, the solution of the channel Hamiltonian is itself a many-body problem, quite distinct from any approximations to the propagator. The success of any practical calculation therefore depends upon how well an approximate evolution of approximate channel states reproduces the exact results. Because our mean-field approximation uses a one-body evolution problem to determine the stationary auxiliary field, it is most conveniently applied when the channel eigenstates are approximated by Slater determinants, although it is by no means restricted to these cases.

Technical difficulties in achieving a simple but adequate approximation to the channel states prevent us from developing a practical application of the mean-field method to the full nuclear scattering problem, although, as discussed in Sec. IV, we have done so in principle. While this might prove to be possible in the future, our goal here is to answer the quite independent question of how well the mean-field method approximates the exact many-body evolution. For this purpose, we consider the more abstract problem of a many-body system subject to an external perturbation localized in time, and seek to calculate the amplitudes for the various transitions induced by the perturbation between eigenstates (or approximate eigenstates) of the unperturbed Hamiltonian. While this study avoids the problem of finding satisfactory channel eigenstates, it is not devoid of physical interest. Indeed, it is possible to model the scattering problem in a way in which the relative motion of the colliding system is treated semiclassically (as is appropriate for heavy-ion or atomic collisions), and the intrinsic motion is treated quantum mechanically using our mean-field approach. Transitions between intrinsic states are then induced by a potential whose time dependence is due to the relative motion. It is also possible to develop a scheme for including in a self-consistent manner the influence of the intrinsic excitation upon the relative motion.[21]

The balance of this paper is organized as follows. In Sec. II, we set up the formalism for our method. We show that intrinsic defects of the mean-field approximation to the Schrödinger picture evolution require a reformulation of the problem in the interaction picture to achieve an S matrix which is asymptotically time independent. The equations defining the stationary auxiliary field configurations are presented and their properties discussed. In Sec. III we illustrate our method by applying it to the forced harmonic oscillator, for which it gives the exact results, and to the forced Lipkin model, where we investigate the limits of its validity. Section IV contains a discussion of several open questions and of the potential application of the mean-field approximation to various realistic reaction situations in nuclear and atomic physics.

II. FORMALISM

A. Statement of the problem

As discussed in the Introduction, the type of problem we shall consider is the excitation of a many-body system with pairwise interactions by an external, time-dependent one-body field. The Hamiltonian for such a problem can be written as

$$H(t)=H_0+V(t). \tag{2.1}$$

Here, H_0 is the unperturbed Hamiltonian composed of the one-body kinetic energies t_i and the two-body interparticle interaction v_{ij}, which we take to be local in coordinate space

$$H_0=\sum_i t_i+\tfrac{1}{2}\sum_{i\neq j} v(x_i-x_j). \tag{2.2}$$

The external, time-dependent perturbing field is taken to be of the one-body form

$$V(t)=\sum_i V(x_i,t) \tag{2.3}$$

with $|V(x,t)|\to 0$ sufficiently rapidly as $|t|\to\infty$, although our treatment below can be simply generalized to a two-body perturbation.

In a second-quantized notation, H_0 can be written in terms of the anticommuting field operators $\psi(x), \psi^\dagger(x)$ as

$$H_0=T+\tfrac{1}{2}\iint dx\,dx'\,\psi^\dagger(x)\psi^\dagger(x')v(x-x')\psi(x')\psi(x), \tag{2.4}$$

where

$$T=\frac{1}{2m}\int dx\,\nabla\psi^\dagger(x)\cdot\nabla\psi(x) \tag{2.5}$$

is the total kinetic energy operator (we henceforth put $\hbar=1$). Similarly

$$V(t)=\int dx\, V(x,t)\psi^\dagger(x)\psi(x)\,. \tag{2.6}$$

For simplicity we omit the explicit specification of spin and isospin coordinates.

Our goal is to calculate the S matrix for the above problem. Specifically, if the system is in a state β as $t\to-\infty$, the amplitude to observe it in the state β' as $t\to+\infty$ is defined as

$$S_{\beta'\beta}=\langle\beta'|S|\beta\rangle\,. \tag{2.7}$$

It then follows that $|S_{\beta'\beta}|^2$ is the probability to excite the state β', that $S_{\beta\beta}$ describes "elastic" propagation of the state β, and that S is unitary in the sense that $\sum_{\beta''} S^*_{\beta''\beta'}S_{\beta''\beta}=\delta_{\beta'\beta}$.

The operator S in (2.7) is defined as the long-time limit of the interaction-picture evolution operator[22]

$$S=\lim_{t\to\infty} U_0(0,t)U(t,-t)U_0(-t,0)\,. \tag{2.8}$$

Here $U(t_2,t_1)$ is the Schrödinger-picture evolution operator for H from time t_1 to t_2, and satisfies

$$i\frac{\partial}{\partial t_2}U(t_2,t_1)=H(t_2)U(t_2,t_1) \tag{2.9}$$

with the boundary condition

$$U(t_1,t_1)=1\,. \tag{2.10}$$

The free evolution operator U_0 is defined similarly, but with $H(t)$ replaced by H_0.

In the ordinary state of affairs, $|\beta\rangle$ and $|\beta'\rangle$ are eigenstates of H_0, with eigenvalues E_β and $E_{\beta'}$, respectively. In this case, $S_{\beta'\beta}$ may also be written as

$$S_{\beta'\beta}=\lim_{t\to\infty} e^{i(E_\beta+E_{\beta'})t}\langle\beta'|U(t,-t)|\beta\rangle\,. \tag{2.11}$$

In view of the general intractability of the many-body problem, any approximation to S involves two separate and independent approximations. First, the generally unknown eigenstates of H_0 must be approximated, often by a single determinant or by a linear combination of a small number of determinants. The best that one may then assume is that such wave functions are "narrow" wave packets in the space of exact eigenstates, and that the matrix elements of S between such wave packets therefore approximate the exact S matrix. The validity of this assumption will, of course, vary from problem to problem. It should also be remarked that this necessarily approximate nature of the initial and final states makes Eq. (2.11) time dependent, even as $t\to\infty$, so that Eq. (2.8) is then more appropriate.

The second major approximation concerns the propagators U and U_0, which are difficult many-body operators. We propose to evaluate them in the mean-field limit as described below, turning the many-body evolutions into a set of coupled, one-body evolutions. This is, of course, most convenient for determinantal approximations for β and β', but, in view of the independence of the propagation and initial-final state approximations, it may, in principle, be investigated for any β,β'.

B. The mean-field approximation to the propagator

To evaluate Eq. (2.8) we must develop tractable expressions for U and U_0. We focus here on U, the transcription to U_0 being simply accomplished by putting $V=0$.

In terms of the density operator,

$$\rho(x)=\psi^\dagger(x)\psi(x)\,, \tag{2.12}$$

the Hamiltonian can be written as

$$H(t)=K+\tfrac{1}{2}\iint dx\,dx'\rho(x)v(x-x')\rho(x')+\int dx\, V(x,t)\rho(x)\,. \tag{2.13}$$

Here, K is the kinetic energy operator, corrected for the self-interaction term

$$K=T-\tfrac{1}{2}v(0)\int dx\,\rho(x)=\sum_i k_i\,. \tag{2.14}$$

To simplify the notation we define a scalar product (A,B) as

$$(A,B)=\int dx\, A(x)B(x)\,. \tag{2.15}$$

Note that A and B can be either c numbers or operators. Equation (2.13) then becomes

$$H(t)=K+\tfrac{1}{2}(\rho,v\rho)+(V(t),\rho)\,, \tag{2.16}$$

where v is viewed as a matrix in x space

$$(v\rho)(x)=\int dx'\, v(x-x')\rho(x')\,. \tag{2.17}$$

The evolution operator U defined by Eqs. (2.9) and (2.10) is given by

$$U(t,-t)=T\exp\left[-i\int_{-t}^{t}d\tau\, H(\tau)\right]=T\exp\left\{-i\int_{-t}^{t}d\tau\,[K+\tfrac{1}{2}(\rho,v\rho)+(V(\tau),\rho)]\right\}, \tag{2.18}$$

where T denotes the time-ordered product. To evaluate this expression we adopt a technique first introduced by Hubbard and Stratonovich[16] in statistical mechanics, and applied recently to nuclear physics by Kleinert[23] and Levit.[14] The details can be found in these references. In broad terms, we linearize the quadratic form $(\rho, v\rho)$ in Eq. (2.18) by introducing a functional integration over an auxiliary field, $\sigma(x,\tau)$. The many-body propagator is thus expressed as a superposition of an infinite number of one-body propagators. Although superficially complicated, this exact representation of U is a useful starting point for the approximations discussed below. In the following, we assume for simplicity that the fermions are distinguishable, thus neglecting exchange terms. These may be included in a relatively straightforward, but cumbersome manner.[17]

The Hubbard-Stratonovich representation of U is

$$U(t,-t)=\int D[\sigma]\exp\left[\frac{i}{2}\int_{-t}^{t}d\tau\,(\sigma(\tau),v\sigma(\tau))\right]U_\sigma(t,-t)\,, \tag{2.19}$$

where

$$U_\sigma(t,-t)=T\exp\left[-i\int_{-t}^{t}d\tau\,H_\sigma(\tau)\right], \tag{2.20}$$

and

$$H_\sigma(\tau)=K+(\sigma(\tau),v\rho)+(V(\tau),\rho)\,. \tag{2.21}$$

The auxiliary field $\sigma(\tau)$ is a time-dependent *scalar c* number in x space, $\sigma(\tau)\equiv\sigma(x,\tau)$, while the functional integral in Eq. (2.19) is over all possible σ fields. This integral and its measure $D[\sigma]$ are best understood by choosing a discrete mesh of uniformly spaced points (x_i, t_j) in space time, with spacing $\Delta x, \Delta t$. Then[14]

$$D[\sigma]\equiv\frac{(\det v)^{1/2}}{(2\pi i)^{N/2}}\prod_{i=1}^{N}\left[\Delta x\Delta t\left(\prod_j d\sigma(x_i,t_j)\right)\right], \tag{2.22}$$

where $N(\to\infty)$ is the number of spatial points.

The Hamiltonian H_σ as defined by Eq. (2.21) is the second-quantized representation of a one-body operator

$$H_\sigma=\sum_i h_\sigma^{(i)}\,, \tag{2.23}$$

where h_σ is the single particle Hamiltonian

$$h_\sigma(\tau)=k+(\sigma,v)+V(\tau)\,. \tag{2.24}$$

Thus, the potential experienced by a particle includes the external potential and a potential obtained by convoluting the two-body interaction over the σ field. It follows from Eq. (2.23) that U_σ is a one-body propagator and can be decomposed into a product of single-particle propagators

$$U_\sigma(t,-t)=\prod u_\sigma^{(i)}(t,-t)\,,$$

where

$$u_\sigma(t_2,t_1)=\exp\left[-i\int_{t_1}^{t_2}d\tau\,h_\sigma(\tau)\right]. \tag{2.25}$$

Of course, u_σ satisfies

$$i\frac{\partial}{\partial t_2}u_\sigma(t_2,t_1)=h_\sigma(t_2)u_\sigma(t_2,t_1) \tag{2.26}$$

with $u_\sigma(t_1,t_1)=1$.

Let us now consider how these expressions can be used to approximate the matrix elements of the propagator. We defer to the following section consideration of the product U_0UU_0 required by Eq. (2.8), and as an illustrative example consider instead the quantity $\langle\beta'|U(t,-t)|\beta\rangle$. According to Eq. (2.19), this is given as

$$\langle\beta'|U(t,-t)|\beta\rangle=\int D[\sigma]\exp\left[\frac{i}{2}\int d\tau(\sigma,v\sigma)\right]\langle\beta'|U_\sigma|\beta\rangle$$

$$=\int D[\sigma]\,|\langle\beta'|U_\sigma|\beta\rangle|\,\exp(i\varphi[\sigma])\,, \tag{2.27}$$

where we have omitted for convenience the arguments $(t,-t)$ and τ from U_σ and σ, respectively. The effective "action"

$$\varphi[\sigma]=\tfrac{1}{2}\int d\tau(\sigma,v\sigma)+\arg(\langle\beta'|U_\sigma|\beta\rangle)$$

$$=\tfrac{1}{2}\int d\tau(\sigma,v\sigma)+\mathrm{Im}\ln\langle\beta'|U_\sigma|\beta\rangle \tag{2.28}$$

is a complicated functional of σ.

The exact evaluation of Eq. (2.27) is, of course, out of the question. However, one may expect that in certain situations (e.g., the "classical" limit), φ will vary sufficiently rapidly with σ so that the stationary phase method will furnish an adequate approximation. Following Ref. 14, we therefore consider a stationary field $\sigma^0(x,\tau)$ which satisfies

$$\left.\frac{\delta\varphi[\sigma]}{\delta\sigma(x,\tau)}\right|_{\sigma=\sigma^0}=0\,, \tag{2.29}$$

and expand φ through second order about this field:

$$\varphi[\sigma]\approx\varphi[\sigma_0]+\tfrac{1}{2}\iint d\tau\,d\tau'\left(\delta\sigma(\tau),\left.\frac{\delta^2\varphi}{\delta\sigma(\tau)\delta\sigma(\tau')}\right|_{\sigma^0}\delta\sigma(\tau')\right). \tag{2.30}$$

With this approximation the functional integral (2.27) is of the multi-Gaussian type [in the variables $\delta\sigma(x,\tau)$], and can be evaluated exactly to give

$$\langle\beta'|U(t,-t)|\beta\rangle \simeq \left(\frac{\det[v(x-x')\delta(\tau-\tau')]}{\det[\delta^2\varphi/\delta\sigma(x,\tau)\delta\sigma(x',\tau')]}\right)^{1/2} |\langle\beta'|U_{\sigma^0}(t,-t)|\beta\rangle| \exp(i\varphi[\sigma_0]) \tag{2.31a}$$

$$\equiv S_2[\sigma^0] \exp\left[\frac{i}{2}\int_{-t}^{t} d\tau(\sigma^0, v\sigma^0)\right]\langle\beta'|U_{\sigma^0}(t,-t)|\beta\rangle . \tag{2.31b}$$

The quantity $S_2[\sigma^0]$, which we shall refer to as the quadratic correction to the zeroth-order amplitude [the balance of Eq. (2.31b)] is given by

$$S_2[\sigma^0] = \left(\frac{\det[v(x-x')\delta(\tau-\tau')]}{\det[\delta^2\varphi/\delta\sigma(x,\tau)\delta\sigma(x',\tau')]}\right)^{1/2}\Bigg|_{\sigma^0} . \tag{2.32}$$

This is generally very difficult to evaluate, since it involves calculating the determinant of a continuous matrix in space-time, although this matrix depends only on the local properties of $\varphi[\sigma^0]$. However, we show below that because of certain properties of Eq. (2.8), the zeroth order evaluation is often sufficient, and S_2 may be set to unity. We therefore concentrate on the determination of σ^0 and $\varphi[\sigma^0]$. We have, of course, assumed in Eq. (2.31) that only one stationary field exists. If there are several such fields, then $\langle\beta'|U|\beta\rangle$ is the coherent sum of contributions of the form (2.31) corresponding to each stationary path.

Stationary solutions σ^0 are found by applying Eq. (2.29). Since

$$\delta U_\sigma = -i\int d\tau\, U_\sigma(t,\tau)\delta H_\sigma(\tau)U_\sigma(\tau,-t) , \tag{2.33}$$

and

$$\delta H_\sigma(\tau) = (\delta\sigma(\tau), v\rho) , \tag{2.34}$$

$$\delta\varphi = \int d\tau\left((\delta\sigma(\tau), v\sigma(\tau)) - \left\{\delta\sigma(\tau), v\,\mathrm{Re}\left[\frac{\langle\beta'|U_\sigma(t,\tau)\rho U_\sigma(\tau,-t)|\beta\rangle}{\langle\beta'|U_\sigma(t,-t)|\beta\rangle}\right]\right\}\right) . \tag{2.35}$$

It then follows that σ^0 satisfies the equation

$$\sigma^0(x,\tau) = \mathrm{Re}\left[\frac{\langle\beta'|U_{\sigma^0}(t,\tau)\rho(x)U_{\sigma^0}(\tau,-t)|\beta\rangle}{\langle\beta'|U_{\sigma^0}(t,-t)|\beta\rangle}\right] . \tag{2.36}$$

It is now convenient to introduce a more transparent notation. We define $|\beta(\tau)\rangle$ to be the wave function which develops forward in time under the one-body propagator U_{σ^0} from $|\beta\rangle$ at time $-t$:

$$|\beta(\tau)\rangle \equiv U_{\sigma^0}(\tau,-t)|\beta\rangle . \tag{2.37}$$

Similarly, $\langle\beta'(\tau)|$ is the wave function which develops backwards from β' at time t:

$$\langle\beta'(\tau)| \equiv \langle\beta'|U_{\sigma^0}(t,\tau) . \tag{2.38}$$

By Eq. (2.20) and its adjoint, these states evolve according to

$$i\frac{d}{d\tau}|\beta(\tau)\rangle = H_{\sigma^0}(\tau)|\beta(\tau)\rangle , \tag{2.39a}$$

$$i\frac{d}{d\tau}\langle\beta'(\tau)| = -\langle\beta(\tau)|H_{\sigma^0}(\tau) . \tag{2.39b}$$

In terms of these states, Eq. (2.36) reads

$$\sigma^0(\tau) = \mathrm{Re}\left[\frac{\langle\beta'(\tau)|\rho|\beta(\tau)\rangle}{\langle\beta'(\tau)|\beta(\tau)\rangle}\right] . \tag{2.40}$$

Note that the denominator in this expression is actually independent of τ, since $U_\sigma(t,\tau)U_\sigma(\tau,-t) = U_\sigma(t,-t)$. Equation (2.40) is a self-consistent equation for σ^0, in the sense that both $|\beta(\tau)\rangle$ and $\langle\beta'(\tau)|$ have a complicated functional dependence upon the values of σ^0 at all times. Note also that the solution σ^0 depends upon which matrix element of U is being calculated, i.e., upon $|\beta\rangle$ and $\langle\beta'|$.

As has been emphasized in Ref. 17, the mean-field approximation to the evolution operator reduces the many-body problem to a set of nonlinear one-body problems. In this regard, it is very similar to the well-known and much exploited time-dependent Hartree-Fock (TDHF) method. Indeed, Eq. (2.39a) is identical with the TDHF if Eq. (2.40) is replaced by

$$\sigma^0_{\mathrm{TDHF}}(x,\tau) = \mathrm{Re}\left[\frac{\langle\beta(\tau)|\rho(x)|\beta(\tau)\rangle}{\langle\beta(\tau)|\beta(\tau)\rangle}\right] , \tag{2.41}$$

where here $\langle\beta(\tau)| = (|\beta(\tau)\rangle)^\dagger$ [*not* the state implied by Eq. (2.38) with $\beta'=\beta$]. The denominator here is, of course, unity. Although Eq. (2.41) has the advantage of reducing the self-consistency problem to a time-local one, (and the mean field is independent of β'), it should be noted that there is no *a priori* justification for it, and that the mean field defined by Eq. (2.40) is that which follows rigorously from the stationary phase approximation.

The difficulty mentioned above concerning Eq. (2.11) rather than Eq. (2.8) should now be even more apparent, i.e., $\langle\beta'|U(t,-t)|\beta\rangle$ in either the mean field or TDHF approximations, continues to oscillate nontrivially with t, so that the limit $t\to\infty$ is not defined and the S matrix cannot be computed. This has earlier been termed spurious cross-channel correlation,[11] and is due to the complex, nonlinear evolution of $\sigma(\tau)$, even after $V(t)$ has vanished. The phase $\exp[i(E_{\beta'}+E_\beta)t]$ in Eq. (2.11) cannot compensate for this evolution, whether β' is an exact eigenstate of H_0 (in which case time dependence is due to the mean-field approximation made in evaluating U) or whether β' is a HF approximation to the exact state (in which case σ^0 would have to approach σ_{HF} as $t\to\infty$, which is not guaranteed). It should also be noted that in the mean-field approximation, these spurious oscillations are even more severe than in the TDHF, since they exist in the former case for both $t\to\infty$ and $t\to-\infty$, whereas in the TDHF they are present only as $t\to\infty$ when β is a static HF state. Efforts to define an S matrix by averaging out such oscillations in TDHF calculations[11,12] appear to us to be *ad hoc*.

C. Mean-field approximation for the interaction picture

The interaction-picture representation of S, Eq. (2.8), has none of the difficulties discussed above. To approximate Eq. (2.8) we apply the Hubbard-Stratonovich transformation for each of the three U's appearing there. Thus,

$$S=\lim_{t\to\infty}\iiint D[\sigma_i]D[\sigma]D[\sigma_f]\exp\left[\frac{i}{2}\oint(\sigma,v\sigma)d\tau\right]\times U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)\,, \quad (2.42)$$

where

$$\oint d\tau(\sigma,v\sigma)\equiv\int_0^{-t}d\tau(\sigma_i,v\sigma_i)+\int_{-t}^{t}d\tau(\sigma,v\sigma)+\int_t^0 d\tau(\sigma_f,v\sigma_f)\,. \quad (2.43)$$

The propagator S is now expressed as a functional integral over a set of three fields: σ_i, σ, and σ_f. For each such set, there is an "interaction picture" evolution $U_{\sigma_f}U_\sigma U_{\sigma_i}$, weighted by $\exp[(i/2)\oint d\tau\times(\sigma,v\sigma)]$.

The integrand of Eq. (2.42) can be visualized in the simple diagram shown in Fig. 1. Evolution is represented by motion along a loop, which consists of three sections:

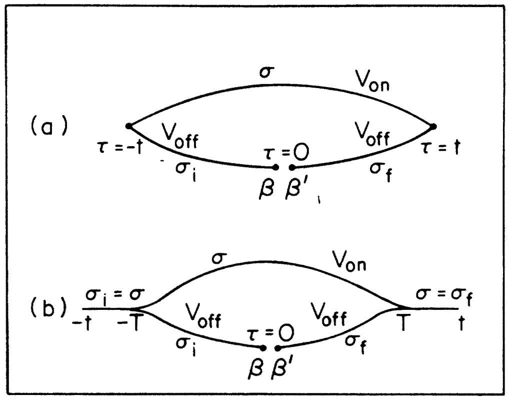

FIG. 1. (a) The "loop" illustrating the time-evolution used in computing the S matrix. (b) The collapse of the loop ends when $V(\tau)=0$ for $|\tau|>T$.

(i) The system starts at $\tau=0$ in the lower middle and moves backward in time along the lower left-hand side of the loop (to time $-t$) with the mean-field σ_i and with the interaction V turned off. This "prepares" the interaction process and is governed by

$$U_{\sigma_i}(-t,0)=T\exp\left[-i\int_0^{-t}d\tau\,H_{\sigma_i}(\tau)\right] \quad (2.44a)$$

with

$$H_{\sigma_i}=K+(\sigma_i,v\rho)\,. \quad (2.44b)$$

(ii) The system evolves forward in time from $-t$ to t along the upper section of the loop with the field σ and the interaction V turned on. This is the interaction process itself and is given formally by

$$U_\sigma(t,-t)=T\exp\left[-i\int_{-t}^{t}d\tau H_\sigma(\tau)\right]\,, \quad (2.45a)$$

where

$$H_\sigma=K+(\sigma,v\rho)+(V,\rho)\,. \quad (2.45b)$$

(iii) In the final analysis process, the system moves backward in time from t to 0 along the lower right-hand portion of the loop with a mean field σ_f and the interaction V turned off. This stage is necessary, as is the preparation, to compensate for undesirable transitions caused by the mean-field approximation long after the interaction ceases. This final stage corresponds to the evolution

$$U_{\sigma_f}(0,t)=T\exp\left[-i\int_t^0 d\tau\,H_{\sigma_f}(\tau)\right], \quad (2.46a)$$

where

$$H_{\sigma_f}=K+(\sigma_f,v\rho)\,. \quad (2.46b)$$

The integral (2.43) can now be interpreted as going around the loop ($\oint d\tau$), with $(\sigma, \nu\sigma)$ taken to be the appropriate quantity $[(\sigma_i, \nu\sigma_i)$, $(\sigma_f, \nu\sigma_f)$, or $(\sigma, \nu\sigma)]$ in each section.

Using the expansion (2.42), a specific S-matrix element can be written as

$$\langle\beta'|S|\beta\rangle = \lim_{t\to\infty}\iiint D[\sigma_f]D[\sigma]D[\sigma_i]\,|\langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle| \times \exp(i\varphi[\sigma_f,\sigma,\sigma_i]), \tag{2.47}$$

where

$$\varphi[\sigma_f,\sigma,\sigma_i] = \tfrac{1}{2}\oint(\sigma,\nu\sigma)d\tau + \mathrm{Im}\,[\ln\langle\beta'|U_{\sigma_f}U_\sigma U_{\sigma_i}|\beta\rangle]. \tag{2.48}$$

The stationary phase evaluation of each of the three functional integrals proceeds analogously to that of the single integral for $\langle\beta'|U(t,-t)|\beta\rangle$ following Eq. (2.29). For notational convenience, we drop the superscript "0" denoting the stationary fields and introduce the following wave functions along different sections of the loop.

(i) At any point τ along the lower left-hand side of the loop $(-t<\tau<0)$ we define

$$|\beta_i(\tau)\rangle = U_{\sigma_i}(\tau,0)|\beta\rangle, \tag{2.49a}$$

$$\langle\beta_i'(\tau)| = \langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,\tau). \tag{2.49b}$$

(ii) At any point τ along the upper portion of the loop $(-t<\tau<t)$, we define

$$|\beta(\tau)\rangle = U_\sigma(\tau,-t)U_{\sigma_i}(-t,0)|\beta\rangle, \tag{2.50a}$$

$$\langle\beta'(\tau)| = \langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,\tau). \tag{2.50b}$$

(iii) Along the lower right-hand side of the loop $(0<\tau<t)$ we define

$$|\beta_f(\tau)\rangle = U_{\sigma_f}(\tau,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle, \tag{2.51a}$$

$$\langle\beta_f'(\tau)| = \langle\beta'|U_{\sigma_f}(0,\tau). \tag{2.51b}$$

When convenient, we shall also use the subscript l as a generic label instead of i, "no subscript," or f. The definitions (2.49)–(2.51) may be summarized by two very simple rules: to find $|\beta_l\rangle$ at any point on the loop, evolve $|\beta\rangle$ from $\tau=0$ (in the lower portion) clockwise along the loop to the given point. Similarly, for $\langle\beta_l'|$, evolve $\langle\beta'|$ counterclockwise from $\tau=0$. The evolution equations for all of these states follow simply from Eqs. (2.44)–(2.46).

With these definitions, the stationary conditions for Eq. (2.47) can be written as

$$\frac{\delta\varphi}{\delta\sigma_l} = 0 \quad\text{or}\quad \sigma_l(\tau) = \mathrm{Re}\frac{\langle\beta_l'(\tau)|\rho|\beta_l(\tau)\rangle}{\langle\beta_l'(\tau)|\beta_l(\tau)\rangle}. \tag{2.52}$$

The denominator in this expression is l independent

$$\begin{aligned}\langle\beta_i'(\tau)|\beta_i(\tau)\rangle = \langle\beta'(\tau)|\beta(\tau)\rangle = \langle\beta_f'(\tau)|\beta_f(\tau)\rangle\\ = \langle\beta'|U_{\sigma_f}(0,t)U(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle\end{aligned} \tag{2.53}$$

and is also independent of τ. In addition, the σ fields are continuous at the two endpoints of the loop, $\tau=\pm t$:

$$\sigma_i(-t) = \sigma(-t), \tag{2.54a}$$

$$\sigma(t) = \sigma_f(t). \tag{2.54b}$$

Our stationary phase approximation is completed by the zeroth order expression for the S matrix:

$$\langle\beta'|S|\beta\rangle \simeq \lim_{t\to\infty}\exp\left[\frac{i}{2}\oint d\tau(\sigma,\nu\sigma)\right]\langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle, \tag{2.55}$$

evaluated at the stationary field configuration. It is, of course, possible to simply write down the "quadratic correction" for this expression, analogous to the $S_2[\sigma]$ appearing in Eq. (2.31b). However, it is generally not practical to evaluate this correction. Fortunately, as we show below, it is often unimportant.

Equations (2.52) are three implicit coupled equations which must be solved self-consistently and simultaneously for the three stationary fields σ_i, σ, and σ_f. Nevertheless, the many-body evolution has been simplified substantially, since the wave functions defining the σ's propagate under a one-body evolution where the effects of the two-body interaction are approximated by the mean field.

D. Asymptotic behavior

The S matrix defined by Eqs. (2.52) and (2.55) becomes time independent for t greater than the time during which V is nonvanishing, and so has a well-defined limit as $t\to\infty$. Although we shall now prove this statement only for the zeroth order approximation to $S_{\beta'\beta}$, Eq. (2.55), it can also be shown to hold for the quadratic corrections to this expression.

The time independence of Eq. (2.55) is a consequence of the asymptotic behavior of the σ fields. Suppose that there is a time T for which we may safely take $V(\tau)=0$ when $|\tau|>T$. Then, if $t>T$, we will demonstrate that

$$\sigma_i(\tau)=\sigma(\tau) \text{ for } -t<\tau<-T\,, \tag{2.56a}$$

$$\sigma(\tau)=\sigma_f(\tau) \text{ for } T<\tau<t\,, \tag{2.56b}$$

i.e., at any point in space σ coincides with σ_i before the interaction starts, and with σ_f after the interaction ceases. Thus, the evolution caused by U_σ for $T<|\tau|<t$ is canceled by U_{σ_i} when $\tau<0$ and by U_{σ_f} when $\tau>0$. This may be represented by modifying Fig. 1(a) to Fig. 1(b), since no net evolution takes place along the "collapsed" ends of the loop.

To prove Eqs. (2.56), we assume them to be true and then demonstrate that this assumption is consistent with the equations (2.52) defining the σ's. Suppose $-t<\tau<-T$. Then using the composition property of the U's, Eq. (2.52) for $l=i$ can be written as

$$\sigma_i(\tau)=\mathrm{Re}\,\frac{\langle\beta'(\tau)|\,U_\sigma(\tau,-t)U_{\sigma_i}(-t,\tau)\rho\,|\,\beta_i(\tau)\rangle}{\langle\beta'(\tau)\,|\,\beta(\tau)\rangle}\,, \tag{2.57a}$$

and Eq. (2.52) for $l=$"no subscript" can be cast as

$$\sigma(\tau)=\mathrm{Re}\,\frac{\langle\beta'(\tau)\,|\,\rho U_\sigma(\tau,-t)U_{\sigma_i}(-t,\tau)\,|\,\beta_i(\tau)\rangle}{\langle\beta'(\tau)\,|\,\beta(\tau)\rangle}\,. \tag{2.57b}$$

But, if we invoke Eq. (2.56a) and realize that for this interval of time $V=0$, we have $U_\sigma(\tau,-t)=U_{\sigma_i}(\tau,-t)$ and thus $U_\sigma(\tau,-t)U_{\sigma_i}(-t,\tau)=1$. The right-hand sides of Eqs. (2.57a) and (2.57b) are therefore equal, verifying Eq. (2.56a). A similar proof holds for Eq. (2.56b).

Having established Eqs. (2.56), we may also conclude that the σ fields for $|\tau|<T$ are independent of t as long as $t>T$. This property, together with Eqs. (2.56), established the t independence of Eq. (2.55) for $t>T$. Note that although σ_i continues to cause nontrivial evolution during the preparation stage for $-t<\tau<-T$, this evolution is precisely canceled by that due to σ during the same interval of the interaction process. A similar cancellation of the effects of σ_f occurs for $T<\tau<t$. Such cancellation is a very positive aspect of our approximation for $S_{\beta'\beta}$. Even though the mean-field evolution induced by U_σ may be a very poor approximation to the effects of the exact U, its deficiencies are, to a large extent, compensated for by the effects of U_{σ_i} and U_{σ_f}. We demonstrate this explicitly below in our study of the forced harmonic oscillator.

E. Time reversal symmetry

Several properties of the exact S matrix follow from the underlying symmetries of the exact Hamiltonian. It is not *a priori* obvious that these properties are preserved by our zeroth order mean-field approximation (2.55). While the conservation of energy, linear momentum, and angular momentum are not relevant for the more abstract, time-dependent problem we have presented here, it can be shown that these properties hold when our methods are properly applied to realistic scattering problems.[21] The unitarity and time-reversal symmetries of S are separate issues, however. With regard to the former, since the stationary field solutions σ_i, σ, and σ_f are generally different for each pair of states β, β', there is no guarantee that $S_{\beta'\beta}$ as defined by Eq. (2.55) is unitary. Indeed, we show in our model calculations below that for many cases $\sum_{\beta'}|S_{\beta\beta'}|^2\leq 1$, although individual S-matrix elements are often quite well reproduced. Time reversal is a symmetry of S only when $V(t)$ has such a symmetry, of course. Our approximation for S preserves this symmetry, as we now demonstrate.

We begin by extending the usual treatment of time-reversal symmetry to the evolution of nonconservative systems (i.e., those with a time-dependent Hamiltonian). Following the notation and methods of Ref. 24, we let K be the antiunitary operator effecting time reversal (complex conjugation in the case of spinless particles), so that $KK^\dagger = K^\dagger K = 1$. There will be a time reversal symmetry in the exact evolution problem when $KH(t)K^\dagger = H(-t)$, or, if H_0 is time reversal invariant ($KH_0K^\dagger = H_0$), when $KV(t)K^\dagger = V(-t)$. In this case, it may be shown that

$$K^\dagger U^\dagger(t_1, t_2)K \simeq U(-t_2, -t_1)\,, \qquad (2.58)$$

where $\simeq$ denotes equality within an arbitrary phase. This reduces to the familiar result for conservative systems, $K^\dagger U^\dagger(t_1, t_2)K \simeq U(t_1, t_2)$ upon exploiting the time-translation invariance of U for such cases, i.e., $U(t_1, t_2)$ depends only upon $t_1 - t_2$.

Since U_0 also satisfies Eq. (2.58), we may perform the following sequence of manipulations on the exact S-matrix elements defined by Eq. (2.8):

$$S_{\beta'\beta} = \lim_{t\to\infty} \langle \beta' | U_0(0,t)U(t,-t)U_0(-t,0) | \beta\rangle \qquad (2.59a)$$

$$= \lim_{t\to\infty} \langle \beta | U_0^\dagger(-t,0)U^\dagger(t,-t)U_0^\dagger(0,t) | \beta'\rangle^* \qquad (2.59b)$$

$$\simeq \lim_{t\to\infty} \langle \beta | K[K^\dagger U_0^\dagger(-t,0)K][K^\dagger U^\dagger(t,-t)K] \times [K^\dagger U_0^\dagger(0,t)K]K^\dagger | \beta'\rangle^* \qquad (2.59c)$$

$$\simeq \lim_{t\to\infty} \langle \beta | U_0(0,t)U(t,-t)U_0(-t,0) | \beta'\rangle \qquad (2.59d)$$

$$\simeq S_{\beta\beta'}\,. \qquad (2.59e)$$

In passing from Eqs. (2.59c) to (2.59d), we have used the anti-unitary property of K [Eq. (XV.24) of Ref. 24] and have assumed that β and β' are symmetric under time reversal,

$$K|\beta\rangle \simeq |\beta\rangle \quad K|\beta'\rangle \simeq |\beta'\rangle\,, \qquad (2.60)$$

which can always be chosen to be true for a time-reversal invariant H_0. Time reversal thus implies that the exact S-matrix elements for the direct and reverse process are equal within a phase. We now consider how time reversal symmetry is manifested in the mean-field approximation to S. Specifically, we show that if σ_i, σ, and σ_f are a solution to Eq. (2.52) for the direct process $\beta \to \beta'$, then the fields $\bar\sigma_f$, $\bar\sigma$, and $\bar\sigma_i$ defined by

$$\bar\sigma_i(\tau) = \sigma_f(-\tau) \quad -t<\tau<0\,, \qquad (2.61a)$$

$$\bar\sigma(\tau) = \sigma(-\tau) \quad -t<\tau<t\,, \qquad (2.61b)$$

$$\bar\sigma_f(\tau) = \sigma_i(-\tau) \quad 0<\tau<t\,, \qquad (2.61c)$$

are a stationary solution for the reverse process $\beta' \to \beta$. Furthermore, the approximate S-matrix elements (2.55) are equal, within a phase. To demonstrate these statements, we exploit transformation properties of the U_σ's under time reversal, which are analogous to Eq. (2.58):

$$K^\dagger U_{\sigma_i}^\dagger(-t,\tau)K \simeq U_{\bar\sigma_f}(-\tau,t)\,, \qquad (2.62a)$$

$$K^\dagger U_\sigma^\dagger(\tau,-t)K \simeq U_{\bar\sigma}(t,-\tau)\,, \qquad (2.62b)$$

$$K^\dagger U_{\sigma_f}^\dagger(\tau,t)K \simeq U_{\bar\sigma_i}(-t,-\tau)\,. \qquad (2.62c)$$

The equation defining $\bar\sigma_f(\tau)$ $(0<\tau<t)$ may then be written as

$$\sigma_f(\tau) = \sigma_i(-\tau) = \mathrm{Re}\, \frac{\langle \beta' | U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,-\tau)\rho U_{\sigma_i}(-\tau,0) | \beta\rangle}{\langle \beta' | U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0) | \beta\rangle} \qquad (2.63a)$$

$$= \mathrm{Re}\, \frac{\langle \beta | U_{\sigma_i}(-\tau,0)\rho U_{\sigma_i}(-t,-\tau)U(t,-t)U_{\sigma_f}(0,t) | \beta'\rangle^*}{\langle \beta | U_{\sigma_i}^\dagger(-t,0)U_\sigma^\dagger(t,-t)U_{\sigma_f}^\dagger(0,t) | \beta'\rangle^*}\,. \qquad (2.63b)$$

Upon inserting $KK^\dagger$ between all operators and using $K\rho K^\dagger = \rho$, together with Eqs. (2.60) and (2.62), this becomes

$$\bar\sigma_f(\tau) = \mathrm{Re}\, \frac{\langle \beta | U_{\bar\sigma_f}(0,\tau)\rho U_{\bar\sigma_f}(\tau,t)U_{\bar\sigma}(t,-t)U_{\bar\sigma_i}(-t,0) | \beta'\rangle}{\langle \beta | U_{\bar\sigma_f}(0,t)U_{\bar\sigma}(t,-t)U_{\bar\sigma_i}(-t,0) | \beta'\rangle}\,. \qquad (2.64)$$

Note that any possible phases are canceled exactly between numerator and denominator. This equation and its analogs for $\bar\sigma$ and $\bar\sigma_i$ show that $\bar\sigma_f$, $\bar\sigma$, and $\bar\sigma_i$ are a solution for the reverse process $\beta' \to \beta$. It is then straightforward to verify that $S_{\beta'\beta}$ and $S_{\beta\beta'}$, as given by Eq. (2.55), are the same, within a phase.

For elastic propagation ($\beta' = \beta$), the direct and reverse processes are identical. Consequently, solutions to Eqs. (2.52) must exist in time reversed pairs, or be time reversal invariant. The former case corresponds to Eq. (2.61), while in the later case, $\bar\sigma_f = \sigma_f$, $\bar\sigma = \sigma$, and $\bar\sigma_i = \sigma_i$, so that

$$\sigma_f(\tau) = \sigma_i(-\tau) \text{ for } 0 \le \tau \le t\,, \qquad (2.65a)$$

$$\sigma(\tau) = \sigma(-\tau) \text{ for } |\tau| \le t\,. \qquad (2.65b)$$

In particular, $\sigma_f(0) = \sigma_i(0)$, implying the continuity of σ at the lower midpoint of the loop in Fig. 1. Moreover, $\langle\beta(\tau)| = (K|\beta(-\tau)\rangle)^\dagger$ and $\langle\beta_{i,f}(\tau)| = (K|\beta_{f,i}(-\tau)\rangle)^\dagger$. These properties can be usefully exploited to halve the numerical effort involved in mean field calculations for realistic systems.

Before closing this section, it should be mentioned that, in analogy with the TDHF approximation (2.41), time-local approximations for the σ fields in the interaction picture may also be formulated. For example, the TDHF in the interaction picture might be formulated as

$$\sigma_i^{\mathrm{TDHF}}(x,\tau) = \langle\beta_i(\tau)|\rho(x)|\beta_i(\tau)\rangle, \tag{2.66}$$

where $\langle\beta_i(\tau)| = |\beta_i(\tau)\rangle^\dagger$ [not the state implied by Eqs. (2.49)–(2.51)] and

$$S_{\beta'\beta}^{\mathrm{TDHF}} \equiv \langle\beta'|\beta_f(0)\rangle. \tag{2.67}$$

In other words, all evolution along the loop is governed by time-local equations. Note, however, that in addition to being purely *ad hoc* and without foundation, this scheme treats β and β' unsymmetrically and so violates any time reversal symmetry which may be present in the original problem. Nevertheless, as we show below in our study of the Lipkin model, the TDHF in the interaction picture can sometimes be a fair approximation to the S matrix, and can even be justified rigorously if only inclusive averages of the S matrix are desired.[25]

III. ILLUSTRATIVE APPLICATIONS

The determination of the stationary σ fields defined by Eqs. (2.52) and (2.49)–(2.51) represents a self-consistent, time-dependent problem. Any number of iterative schemes for its solution can be imagined. For example, one may begin by generating wave functions $|\beta_i^0(\tau)\rangle$ by evolving $|\beta\rangle$ clockwise around the loop using the TDHF approximation (2.66). Wave functions $\langle\beta'^1_i(\tau)|$ can then be found by evolving β' counterclockwise around the loop according to Eqs. (2.51b), (2.50b), and (2.49b) using σ fields defined according to Eq. (2.52) with the β^0 and the instantaneous value of $\langle\beta'^1|$. Subsequent iterations proceed by alternately evolving $\beta(\beta')$ clockwise (counterclockwise) around the loop using the σ fields generated from the the previous wave functions and the instantaneous value of the wave function being evolved. The problem is thus made equivalent to a number of TDHF-like calculations. This procedure would, presumably, converge on a solution, although there is no proof that this need be so. There is also no simple way to guarantee that in a given situation all solutions will be found. Such problems must be solved for any successful application of our mean-field methods to a realistic situation.

For a number of nontrivial model Hamiltonians the solution of the mean-field equations can be greatly simplified. These are systems for which the relevant operators form a finite Lie algebra, and hence generate a Lie group composed of all possible evolution operators. In this case, the mean-field equations may be reduced to a set of time-local evolution equations for the group parameters which must be solved self-consistently. This simplification of the time nonlocal evolution of the wave functions represents a substantial computational savings and so allows several nontrivial tests of the mean-field approximation. As examples of our method, we consider below two such group-theoretic Hamiltonians; the forced harmonic oscillator and the forced Lipkin model. Although the former is certainly not a many-body Hamiltonian, it is amenable to a mean-field approximation, since evolution under a Hamiltonian quadratic in the coordinate may be reduced to evolution under a time-dependent linear Hamiltonian through methods analagous to the Hubbard-Stratanovich transformation (2.19). The Lipkin model is a true many-body system: a two-level shell model system with pair-wise interactions which may be formulated in an SU(2) context. We demonstrate that the zeroth order mean-field approximation to the S matrix is exact for the forced oscillator and has a well-defined and substantial range of validity for the Lipkin model.

A. Forced harmonic oscillator

We consider a simple harmonic oscillator of unit mass and frequency subject to a real external time-dependent force $f(t)$, with $f(t)\to 0$ as $|t|\to\infty$. The unperturbed Hamiltonian is

$$H_0 = \tfrac{1}{2}p^2 + \tfrac{1}{2}q^2, \tag{3.1}$$

where q is the oscillator coordinate and p the conjugate momentum satisfying $[q,p]=i$ and the perturbation is

$$V(t) = f(t)q. \tag{3.2}$$

The exact S matrix for this problem can be found analytically by familiar algebraic methods.[26,27] If we define

$$\alpha = \frac{-i}{\sqrt{2}}\int_{-\infty}^{\infty} d\tau\, f(\tau)\, e^{i\tau} \tag{3.3}$$

and

$$\mu = -\,\mathrm{Im}\left[\int_{-\infty}^{\infty} d\tau\, f(\tau)\, e^{i\tau}\int_{-\infty}^{\tau} d\tau'\, f(\tau')e^{-i\tau'}\right], \tag{3.4}$$

then

$$S=\exp[\alpha a^\dagger-\alpha^* a+i\mu]\,, \tag{3.5}$$

where $a=(q+ip)/\sqrt{2}$ and $a^\dagger=(q-ip)/\sqrt{2}$ are the annihilation and creation operators. The S-matrix element between oscillator states having n and n' quanta is

$$\begin{aligned}\langle n'|S|n\rangle\equiv S_{n'n}&=e^{i\mu}e^{-|\alpha|^2/2}\left(\frac{n'!}{n!}\right)^{1/2}\\ &\quad\times(-\alpha^*)^{n-n'}L_{n'}^{(n-n')}(|\alpha|^2)\\ &=e^{i\mu}e^{-|\alpha|^2/2}\left(\frac{n!}{n'!}\right)^{1/2}\\ &\quad\times(\alpha)^{n'-n}L_n^{(n'-n)}(|\alpha|^2)\,,\end{aligned} \tag{3.6b}$$

where $L_s^k(z)$ is the associated Laguerre polynomial of integer degree s and integer index k, with $k+s\geq 0$.

To apply our mean-field methods, we consider first the exact Schrödinger propagator,

$$U(t,-t)=T\exp\left\{-i\int_{-t}^{t}d\tau\,[\tfrac{1}{2}p^2+\tfrac{1}{2}q^2+f(\tau)q]\right\}. \tag{3.7}$$

By introducing an auxiliary function of time $\sigma(\tau)$, we can employ the Hubbard-Stratanovich transformation to rewrite Eq. (3.7) as

$$U(t,-t)=\int D[\sigma(\tau)]\exp\left[i/2\int_{-t}^{t}\sigma^2(\tau)d\tau\right]\times U_\sigma(t,-t)\,, \tag{3.8}$$

where

$$U_\sigma(t,-t)=T\exp\left[-i\int_{-t}^{t}d\tau\,H_\sigma(\tau)\right] \tag{3.9}$$

with

$$H_\sigma(\tau)=\tfrac{1}{2}p^2+\sigma(\tau)q+f(\tau)q\,. \tag{3.10}$$

The analogy with the many-body problem may be seen by identifying q^2 with the two-body potential energy, which is quadratic in the density operator. Like Eq. (2.19) for the many-body problem, Eq. (3.8) expresses the exact propagator for the oscillator in terms of the "linearized" propagators (3.9), although for the latter case σ is only a single function of time, not a whole field.

To evaluate S-matrix elements, we work in the interaction picture as in Eq. (2.42):

$$\langle n'|S|n\rangle=\lim_{t\to\infty}\int D[\sigma_i]D[\sigma]D[\sigma_f]\exp\left(i/2\oint d\tau\,\sigma^2\right)\langle n'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|n\rangle\,, \tag{3.11}$$

where each of the U_σ's evolve with the "one-body" Hamiltonian

$$H_{\sigma_l}(\tau)=\tfrac{1}{2}p^2+\sigma_l(\tau)q+\delta_{l0}f(\tau)q\,. \tag{3.12}$$

Here, δ_{l0} is unity when $l=$"no subscript" and zero for $l=$"f" or "i." Note that for the initial and final states we have chosen exact eigenstates of H_0, since the corresponding "static Hartree-Fock" Hamiltonian, $\frac{1}{2}p^2+\sigma q$, has no bound states for any time-independent σ.

The matrix element in Eq. (3.11) is most conveniently evaluated in the interaction picture with respect to the kinetic energy $\frac{1}{2}p^2$. We denote operators and states in this picture by carets (^). For any Schrödinger operator $\mathcal{O}$,

$$\hat{\mathcal{O}}(\tau)\equiv\exp(ip^2\tau/2)\mathcal{O}\exp(-ip^2\tau/2) \tag{3.13}$$

and, specifically,

$$\hat{q}(\tau)=q+p\tau=[(1+i\tau)a^\dagger+(1-i\tau)a]/\sqrt{2}\,,$$
$$\hat{p}(\tau)=p\,.$$

The interaction picture evolution operators are

$$\hat{U}_{\sigma_l}(t_1,t_2)=\exp(+ip^2t_1/2)\,U_{\sigma_l}(t_1,t_2)\exp(-ip^2t_2/2)\,, \tag{3.14}$$

and evolve with

$$\hat{H}_{\sigma_l}(\tau)=\sigma_l(\tau)\hat{q}(\tau)+\delta_{l0}f(\tau)\hat{q}(\tau)\,, \tag{3.15}$$

while the interaction-picture states are

$$|\hat{n}_l(\tau)\rangle=\exp(-ip^2\tau/2)\,|n_l(\tau)\rangle \tag{3.16}$$

and satisfy relations identical to Eqs. (2.49)–(2.51) with all U's replaced by $\hat{U}$'s. Thus in the interaction picture, Eq. (3.11) reads simply

$$\langle n'|S|n\rangle=\lim_{t\to\infty}\int D[\sigma_i]D[\sigma]D[\sigma_f]\exp\left(i/2\oint d\tau\,\sigma^2\right)\times\langle\hat{n}'|\hat{U}_{\sigma_f}(0,t)\hat{U}_\sigma(t,-t)\hat{U}_{\sigma_i}(-t,0)|\hat{n}\rangle\,. \tag{3.17}$$

The stationary points of the integrand in Eq. (3.17) satisfy self-consistent equations analogous to Eq. (2.52):

$$\sigma_l(\tau)=\mathrm{Re}\left[\frac{\langle\hat{n}_l'(\tau)|\hat{q}(\tau)|\hat{n}_l(\tau)\rangle}{\langle\hat{n}_l'(\tau)|\hat{n}_l(\tau)\rangle}\right]. \tag{3.18}$$

This is, of course, the same σ field as would be obtained if we evaluated the matrix elements in Eq. (3.11) directly. To solve these equations, we proceed in four steps: (i) adopt a convenient representation of the evolution operators in terms of two complex time-dependent parameters, $\alpha_l(\tau)$

and $\mu_l(\tau)$; (ii) express the σ fields in terms of these parameters; (iii) demonstrate that the σ fields satisfy time-local differential equations; and (iv) solve these equations self-consistently in order to determine the S matrix. The details of these steps follow below.

(i) For any complex parameters α, μ, we define a unitary operator

$$W[\alpha, \mu] = \exp[\alpha a^\dagger - \alpha^* a + i\mu] \tag{3.19}$$

and parametrize the evolution operators as

$$\hat{U}_{\sigma_i}(\tau, 0) \equiv W[\alpha_i(\tau), \mu_i(\tau)], \quad 0 \geq \tau \geq -t, \tag{3.20a}$$

$$\hat{U}_\sigma(\tau, -t)\,\hat{U}_{\sigma_i}(-t, 0) \equiv W[\alpha(\tau), \mu(\tau)], \quad -t \leq \tau \leq t, \tag{3.20b}$$

$$\hat{U}_{\sigma_f}(\tau, t)\,\hat{U}_\sigma(t, -t)\,\hat{U}_{\sigma_i}(-t, 0) \equiv W[\alpha_f(\tau), \mu_f(\tau)], \quad t \geq \tau \geq 0. \tag{3.20c}$$

Note that $\alpha_i(0) = \mu_i(0) = 0$, and the parametrization is defined so that

$$|\hat{n}_l(\tau)\rangle = W[\alpha_l(\tau), \mu_l(\tau)]\,|n\rangle. \tag{3.21}$$

Since counterclockwise evolution around the loop to a time τ is equivalent to complete counterclockwise evolution followed by clockwise evolution to the same point τ, we also can write

$$\langle \hat{n}'_l(\tau)| = \langle n'|W[\alpha_f(0), \mu_f(0)]W^\dagger[\alpha_l(\tau), \mu_l(\tau)]. \tag{3.22}$$

The parameters α and μ thus specify the evolution of $|n\rangle$ clockwise around the loop or of $\langle n'|$ counterclockwise around the loop. They are, of course, continuous at $\tau = \pm t$.

The evolution of the $\hat{U}$'s through the $\hat{H}_\sigma$'s defined by Eq. (3.15) implies that the parameters α and μ evolve as

$$i\dot{\alpha}_l(\tau) = 1/\sqrt{2}\,[\sigma_l(\tau) + \delta_{l0} f(\tau)](1 + i\tau) \tag{3.23a}$$

and

$$\dot{\mu}(\tau) = \mathrm{Im}(\dot{\alpha}\alpha^*), \tag{3.23b}$$

where the dot denotes $d/d\tau$.

(ii) Using the representations (3.21) and (3.22) for $|\hat{n}(\tau)\rangle$ and $\langle \hat{n}'(\tau)|$, (3.18) can be expressed as a relation between σ and α, μ. Choosing to evaluate the τ-independent denominator at $\tau = 0$ on the final part of the loop, and using standard commutation relations to effect the unitary transformation of $\hat{q}(\tau)$ by W, we have

$$\sigma_l(\tau) = \mathrm{Re}\,[\langle n'|W[\alpha_f(0), \mu_f(0)]W^\dagger[\alpha_l(\tau), \mu_l(\tau)]\hat{q}(\tau)\,W[\alpha_l(\tau), \mu_l(\tau)]\,|n\rangle / \langle n'|W[\alpha_f(0), \mu_f(0)]\,|n\rangle] \tag{3.24a}$$

$$= \sqrt{2}\,\mathrm{Re}\,[(1 - i\tau)\alpha_l(\tau)](1/\sqrt{2})\mathrm{Re}\,[(1 + i\tau)\xi + (1 - i\tau)\eta], \tag{3.24b}$$

where the complex parameters ξ and η are functions of $\alpha_f(0)$ and are defined by

$$\xi = \frac{\langle n'|W[\alpha_f(0), 0]a^\dagger|n\rangle}{\langle n'|W[\alpha_f(0), 0]|n\rangle} = -\alpha_f^*(0)\frac{L_{n'}^{(n-n'+1)}(|\alpha_f(0)|^2)}{L_{n'}^{(n-n')}(|\alpha_f(0)|^2)} = \frac{n+1}{\alpha_f(0)}\,\frac{L_{n+1}^{n'-n-1}(|\alpha_f(0)|^2)}{L_n^{n'-n}(|\alpha_f(0)|^2)}, \tag{3.25a}$$

$$\eta = \frac{\langle n'|W[\alpha_f(0), 0]a|n\rangle}{\langle n'|W[\alpha_f(0), 0]|n\rangle} = -\frac{n}{\alpha_f^*(0)}\,\frac{L_{n'}^{(n-n'-1)}(|\alpha_f|^2)}{L_{n'}^{(n-n')}(|\alpha_f|^2)} = \alpha_f(0)\frac{L_{n-1}^{n'-n-1}(|\alpha_f(0)|^2)}{L_n^{n'-n}(|\alpha_f(0)|^2)}. \tag{3.25b}$$

Both Eqs. (3.24) and (3.25) are independent of all of the overall phases μ. In deriving Eq. (3.25) we have also exploited relations similar to (3.6).

(iii) The closed algebra of the harmonic oscillator has allowed us to express the σ fields at any time τ in terms of the instantaneous values of the parameter α and only two parameters, ξ and η, which are determined in terms of only $\alpha_f(0)$ through Eq. (3.25). Since (3.23a) determines $\alpha_f(0)$ for a given σ field, the self-consistency of σ at all times, expressed through Eq. (3.18), has been reduced to a single consistency condition on $\alpha_f(0)$.

Rather than solving the coupled equations (3.23)–(3.25), it is more convenient to eliminate α and solve for σ directly. By taking the second time derivative of Eq. (3.24b) and using (3.23a) and its first time derivative, we find that the σ fields satisfy

$$\ddot{\sigma}_l(\tau) = -\sigma_l(\tau) - \delta_{l0} f(\tau), \tag{3.26}$$

i.e., the σ fields satisfy differential equations equivalent to a forced classical harmonic oscillator. Equations (3.26) could also have been derived directly from the second derivative of Eq. (3.18) using the commutation rules for $\hat{q}(\tau)$ and $\hat{H}_\sigma(\tau)$.

(iv) The solutions to Eq. (3.26) may be written as

$$\sigma_i(\tau) = \sigma_i(0)\cos\tau + \dot{\sigma}_i(0)\sin\tau, \tag{3.27a}$$

$$\sigma(\tau) = C\cos\tau + D\sin\tau - \int_{-t}^{\tau} d\tau'\, f(\tau')\sin(\tau - \tau'), \tag{3.27b}$$

$$\sigma_f(\tau)=\sigma_f(0)\cos\tau+\dot\sigma_f(0)\sin\tau\,, \tag{3.27c}$$

with coefficients $\sigma_i(0)$, $\dot\sigma_i(0)$, C, D, $\sigma_f(0)$, and $\dot\sigma_f(0)$ to be determined. The quantities $\sigma_{i,f}(0)$ and $\dot\sigma_{i,f}(0)$ can be determined from Eq. (3.24b), its first derivative, and (3.23a), using $\alpha_i(0)=0$. One finds

$$\sigma_i(0)=\frac{1}{\sqrt{2}}\operatorname{Re}(\xi+\eta)\,, \tag{3.28a}$$

$$\dot\sigma_i(0)=-\frac{1}{\sqrt{2}}\operatorname{Im}(\xi-\eta)\,, \tag{3.28b}$$

$$\sigma_f(0)=\sqrt{2}\operatorname{Re}\alpha_f(0)+\frac{1}{\sqrt{2}}\operatorname{Re}(\xi+\eta)\,, \tag{3.28c}$$

$$\dot\sigma_f(0)=\sqrt{2}\operatorname{Im}\alpha_f(0)-\frac{1}{\sqrt{2}}\operatorname{Im}(\xi-\eta)\,. \tag{3.28d}$$

To determine C and D, we require that σ_i and $\dot\sigma_i$ at time $-t$ match with σ and $\dot\sigma$, recalling that $f(-t)=0$. This continuity follows from the general discussion of the continuity of the σ fields given in the previous section. Thus,

$$C=\sigma_i(0)=1/\sqrt{2}\operatorname{Re}(\xi+\eta)\,, \tag{3.29a}$$

$$D=\dot\sigma_i(0)=-1/\sqrt{2}\operatorname{Im}(\xi-\eta)\,. \tag{3.29b}$$

This determines all the coefficients. Final self-consistency, i.e., the determination of $\alpha_f(0)$, is imposed by smoothly joining σ and σ_f at time $+t$. One finds

$$\alpha_f(0)=-\frac{i}{\sqrt{2}}\int_{-t}^{t}d\tau\, f(\tau)e^{-i\tau}\,. \tag{3.30}$$

Note that $\alpha_f(0)$ is independent of both n and n', which is not the usual situation (see the Lipkin model below). However, as can be seen from Eqs. (3.27) and (3.28), the σ field does depend upon the matrix element being considered.

Having determined $\alpha_f(0)$, we may now evaluate the zeroth order approximation to the S matrix:

$$S_{n'n}=\exp\left(i/2\oint\sigma^2 d\tau\right)\langle n'|W[\alpha_f(0),\mu_f(0)]|n\rangle \tag{3.31a}$$

$$=\exp\left[\frac{i}{2}\int_0^{-t}d\tau\,\sigma_i^{\,2}(\tau)+\int_{-t}^{t}d\tau\,\sigma^2(\tau)+\int_t^0 d\tau\,\sigma_f^{\,2}(\tau)\right]e^{i\mu_f(0)} \tag{3.31b}$$

$$\times\left(\frac{n'!}{n!}\right)^{1/2}\exp[-|\alpha_f(0)|^2][-\alpha_f^*(0)]^{n-n'}L_{n'}^{(n-n')}[|\alpha_f(0)|^2]\,.$$

The phase $\mu_f(0)$ can be found from Eq. (3.23b) to be simply $\frac{1}{2}|\alpha_f(0)|^2$, while the time integrals can be done explicitly using Eqs. (3.27)–(3.29). After some algebra, one recovers Eq. (3.3).

The implications of time-reversal symmetry for our solution are straightforward. When $f(\tau)=f(-\tau)$, Eq. (3.30) shows that $\alpha_f(0)$ is purely imaginary $[\alpha_f(0)^*=-\alpha_f(0)]$. The alternate forms of $S_{n'n}$ given in Eqs. (3.6a) and (3.6b) then show that $S_{n'n}=S_{nn'}$. The relations between the σ fields for $S_{n'n}$ and $S_{nn'}$ are readily demonstrated by realizing that ξ and η are real, so that from Eq. (3.28) $\sigma_i(0)=\sigma_f(0)=0$, and $\dot\sigma_i(0)=-1/\sqrt{2}\operatorname{Im}(\xi-\eta)$, $\dot\sigma_f(0)=\sqrt{2}\operatorname{Im}\alpha_f(0)-1/\sqrt{2}\operatorname{Im}(\xi-\eta)$. The alternate forms for ξ and η given in Eqs. (3.25) then establish the symmetry. For elastic propagation $(n'=n)$, the requirement $\dot\sigma_f(0)=\dot\sigma_i(0)$ implies $\alpha_f(0)=\xi-\eta$, which leads by Eqs. (3.25) to a demonstrable recursion relation satisfied by the associated Laguerre polynomials, and it is then simple to verify that $\sigma_f(\tau)=\sigma_i(-\tau)$ and $\sigma(\tau)=\sigma(-\tau)$.

It is interesting to examine the behavior of our solutions as $f(t)\to 0$, corresponding to free propagation. Of course, in this limit, $S_{n'n}\to\delta_{n'n}$. Nevertheless, the σ fields are, in general, nonzero. For $n'=n$, Eq. (3.25) shows $\xi,\eta\to 0$, so by (3.28), (3.29), all σ fields are zero. However, for $n'\geq n+1$, $\eta\to 0$, but $\xi\sim 1/\alpha_f(0)$. Similarly, for $n'\leq n-1$, $\xi\to 0$, but $\eta\sim 1/\alpha_f^*(0)$. Thus, the σ fields diverge, even though they cause no net transitions around the loop.

It is simple to demonstrate the relation of our mean-field approach to the TDHF approximation in the interaction picture. According to Eq. (2.66), the latter implies putting $\alpha_f(0)=0$ in Eq. (3.24a) and setting the denominator there to unity. The quantities ξ and η are then zero by formulas similar to Eq. (3.25) and the solution for the σ fields follows from Eqs. (3.27)–(3.29), with (3.30) still being valid. One can then show that $S_{n'n}$ is as given by the exact or mean-field evolutions, but with a very different set of σ fields than the latter case. Thus, for the special case of the oscillator, the mean-field TDHF approximations in the interaction picture give the same (exact) S matrix, although this is not generally true (see the Lipkin model below).

Some useful insights can also be obtained by considering the mean-field approximation to the Schrödinger picture evolution, which can be simply formulated using the methods discussed above. In the general case, the approximate

$\langle n'|U(t,-t)|n\rangle$ is time dependent, since no linear field $\sigma(t)q$ can prevent the initial state n from spreading in coordinate space due to the free kinetic energy. Unfortunately, the self-consistency conditions determining the parameter analogous to $\alpha_f(0)$ above are complicated nonlinear equations involving the Laguerre polynomials, and so cannot be solved in the general case. One interesting specific case to consider, however, is free propagation of the ground state, i.e., $f(\tau)=0$. In this case, apart from a discrete set of values of t determined by $\tan t=-1/t$ (where the stationary σ field is undefined), the stationary σ field is $\sigma(\tau)=0$, yielding $\langle 0|U(t,-t)|0\rangle=1/(1+it)^{1/2}$, which makes explicit the dispersion of the wave function. This then graphically illustrates the correcting power of the additional U_0's in the interaction picture, which act to cancel this spread.

B. The forced Lipkin model

As a second nontrivial application of our mean-field techniques, we consider the S matrix for the Lipkin model[28,29] under the influence of an external, one-body perturbation. The unperturbed system consists of N fermions with pairwise interactions. These fermions are labeled by a quantum $p=1,\ldots,N$, and each can occupy an upper (denoted by $s=+1$) or lower ($s=-1$) single-particle level having energy $+\epsilon/2$ and $-\epsilon/2$, respectively. For convenience, we henceforth measure all energies in units of ϵ and all times in units of $1/\epsilon$.

If $a^\dagger_{ps}$ is the creation operator for a fermion of type p in level s, then the unperturbed Hamiltonian of the model may be written as

$$H_0=\tfrac{1}{2}\sum_{s=\pm1} s a^\dagger_{ps}a_{ps}+\tfrac{1}{2}v\sum_{pp's} a^\dagger_{ps}a^\dagger_{p's}a_{p'-s}a_{p-s}\,, \quad (3.32)$$

where v is a real parameter specifying the strength of the two-body interaction.

This Hamiltonian can be discussed in terms of an SU(2) algebra by defining quasi-spin operators

$$J_\pm=\sum_p a^\dagger_{p\pm1}a_{p\mp1}\equiv\sum_p j_\pm^{(p)}\,, \quad (3.33a)$$

$$J_z=\tfrac{1}{2}\sum_{ps} s a^\dagger_{ps}a_{ps}\equiv\sum_p j_z^{(p)}\,. \quad (3.33b)$$

Using the anticommutation rules for the $a^\dagger$ and a, it is straightforward to show that these operators satisfy the usual SU(2) commutation rules: $[J_\pm,J_z]=\mp J_\pm$, $[J_+,J_-]=2J_z$, as do each of the $j^{(p)}$'s individually. In terms of the quasi-spin operators,

$$H_0=J_z+\tfrac{1}{2}v(J_+{}^2+J_-{}^2)=J_z+v(J_x{}^2-J_y{}^2)\,. \quad (3.34)$$

The general time dependent Hermitian one-body perturbation of this Lipkin model can be written as

$$V(t)=\vec{f}(t)\cdot\vec{J}=f_x(t)J_x+f_y(t)J_y+f_z(t)J_z\,. \quad (3.35)$$

We take $\vec{f}$ real, with $|\vec{f}|\to 0$ as $|t|\to\infty$.

Since H_0 commutes with $\vec{J}^2$, to find its exact eigenstates one need only diagonalize it within each subspace of well-defined J, the eigenvalue of J^2 being $J(J+1)$. We shall confine the discussion to the ground state multiplet, which has $J=\frac{1}{2}N$. When $v=0$, the eigenstates of H_0 are simply $|J=\frac{1}{2}N,M\rangle$, $-J\le M\le J$, with energies M. The lowest member of this multiplet is the state with $M=-J$, which corresponds to all particles occupying the lower level, $s=-1$. When $v\ne0$, one has to diagonalize the $(N+1)\times(N+1)$ matrix $\langle J,M'|H_0|J,M\rangle$, and the eigenstates $|\beta\rangle$, with eigenvalues E_β, will be real linear combinations of the $|J,M\rangle$:

$$|\beta\rangle=\sum_{M=-J}^{J}|J,M\rangle\langle J,M|\beta\rangle\,. \quad (3.36)$$

Note that one can effectively halve the numerical work by exploiting the invariance of H_0 under the "parity" transformation $\exp(i\pi J_z)$, so that the diagonalization can be carried out separately for even and odd M.

Since the perturbation $V(t)$ also commutes with $\vec{J}^2$, the wave function will evolve continuously within the subspace $J=\frac{1}{2}N$ if the initial state was within this subspace. The exact excitation problem can thus be solved by expanding in the ground-state multiplet:

$$|\psi(t)\rangle=\sum_\beta C_\beta(t)\exp(-iE_\beta t)|\beta\rangle\,. \quad (3.37)$$

The (interaction picture) amplitudes C_β satisfy first order linear equations:

$$\begin{aligned}i\dot{C}_\beta&=\sum_{\beta'}\langle\beta|V(\tau)|\beta'\rangle\exp(i(E_\beta-E_{\beta'})\tau)C'_\beta\\&=\sum_{\beta'MM}\langle M|V(\tau)|M'\rangle\langle M|\beta\rangle\langle M'|\beta'\rangle\\&\quad\times\exp[i(E_\beta-E_{\beta'})\tau]C_{\beta'}\,,\end{aligned} \quad (3.38)$$

where $\langle M|\beta\rangle\equiv\langle J=\frac{1}{2}N,M|\beta\rangle$ are the real transformation coefficients from the quasi-spin basis $|J,M\rangle$ to the exact eigenstates $|\beta\rangle$ as defined in Eq. (3.36). Note that the perturbation $\langle M|V(t)|M'\rangle=\vec{f}(t)\cdot\langle M|\vec{J}|M'\rangle$ has nonvanishing matrix elements only for $M'=M,M\pm1$. To find $S_{\beta'\beta}$, we start at time $\tau=-t$ [when $V(-t)=0$] with $C_{\beta''}=\delta_{\beta''\beta}$, integrate the set (3.38) to $\tau=+t$, and then $S_{\beta'\beta}=C_{\beta'}(t)$.

The Lipkin model has a new feature not present in the harmonic oscillator: a Hartree-Fock approximation to the ground state. If one assumes a variational many-body wave function which is the direct product of N identical single-particle wave functions (one for each type of particle), minimization of the expectation value of H_0 shows the following to be true.[30] In the weak coupling limit, $|\chi| \equiv |(N-1)v| < 1$, the Hartree-Fock ground state, $|0_{\rm HF}\rangle$, is given simply by $|M=-J\rangle$; i.e., all particles are in the lower level $s=-1$. Thus,

$$|0_{\rm HF}\rangle \equiv \prod_p |s_p=-1\rangle = |M=-J\rangle \,. \tag{3.39}$$

In the strong coupling limit $|\chi|>1$, there are two degenerate, deformed HF minima:

$$\begin{aligned}|0_{\rm HF}\rangle &= |\pm\varphi_{\rm HF}\rangle = \exp[\mp i\varphi J_y]\,|-J\rangle \\ &= \prod_p \exp[\mp i\varphi j_y^{(p)}]\,|s_p=-1\rangle\end{aligned}$$

$$\text{for } \chi < -1\,, \tag{3.40a}$$

$$\begin{aligned}|0_{\rm HF}\rangle &= |\pm\varphi_{\rm HF}\rangle = \exp[\pm i\varphi J_x]\,|-J\rangle \\ &= \prod_p \exp[\pm i\varphi j_x^{(p)}]\,|s_p=-1\rangle\end{aligned}$$

$$\text{for } \chi > 1\,, \tag{3.40b}$$

where the angle φ is given by $\cos\varphi = 1/|\chi|$. In these states, each single particle wave function is mixed between the lower and upper levels, and the mixing is the same for all particles. Note that the degeneracy can be lifted[30] by taking the combinations $|\varphi_{\rm HF}\rangle \pm |-\varphi_{\rm HF}\rangle$. There is then a parity doublet where the ground and first excited states are nearly degenerate.

Our primary interest in this paper is testing the mean-field approximation to the S matrix, and not the HF approximation for the initial and final states. We shall therefore concentrate on the S-matrix elements for exact Lipkin states. Nevertheless, it is also interesting to consider the exact and mean-field S-matrix elements for elastic propagation between static HF states. The former may be computed exactly by taking $C_\beta(\tau=-t) = \langle\beta|0_{\rm HF}\rangle$ in Eq. (3.38), integrating these equations from $-t$ to $+t$, and then forming the S-matrix element as $\langle 0_{\rm HF}|S|0_{\rm HF}\rangle = \Sigma_{\beta'}\langle 0_{\rm HF}|\beta'\rangle \times C_{\beta'}(+t)$.

To construct the mean-field approximation to the S matrix, we follow Eq. (2.42) and introduce an auxiliary field $\sigma_{x,y}^{(p)}$ for each one-body operator $j_{x,y}^{(p)}$ appearing in the two-body term of H_0. Thus

$$\begin{aligned}\langle\beta'|S|\beta\rangle = \lim_{t\to\infty} \int &\mathfrak{D}[\sigma_f]\mathfrak{D}[\sigma]\mathfrak{D}[\sigma_i] \\ &\times \exp\Big[iv\sum_{p'\neq p}\oint d\tau(\sigma_x^{(p)}\sigma_x^{(p')} - \sigma_y^{(p)}\sigma_y^{(p')})\Big] \\ &\times \langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle\,,\end{aligned} \tag{3.41}$$

where

$$\mathfrak{D}[\sigma_l] \equiv \prod_{p=1}^{N} \mathfrak{D}[\sigma_{lx}^{(p)}]\mathfrak{D}[\sigma_{ly}^{(p)}] \tag{3.42}$$

and each of the U_{σ_l} evolves with the one-body Hamiltonian

$$H_{\sigma_l} = \sum_p \Big[j_z^{(p)} + \delta_{l0}\vec{\mathrm{f}}\cdot\vec{\mathrm{j}}^{(p)} + 2v\sum_{p'\neq p}\Big(\sigma_{lx}^{(p')}j_x^{(p)} - \sigma_{ly}^{(p')}j_y^{(p)}\Big)\Big]\,. \tag{3.43}$$

The terms $p'=p$ are omitted since $j_x^{(p)2} = j_y^{(p)2}$ for spin-$\frac{1}{2}$ operators. The stationary field configurations of Eq. (3.41) correspond to

$$\sigma_{l\,x,y}^{(p)}(\tau) = \mathrm{Re}\,\frac{\langle\beta_l'(\tau)|j_{x,y}^{(p)}|\beta_l(\tau)\rangle}{\langle\beta_l'(\tau)|\beta_l(\tau)\rangle}\,. \tag{3.44}$$

If $|\beta\rangle$ and $|\beta'\rangle$ belong to the $J=\frac{1}{2}N$ multiplet, they are symmetric under any permutation of the particle labels p, a symmetry which is then also true of the integrand in Eq. (3.41). Consequently, we may search for stationary points where the $\sigma_{x,y}^{(p)} = \sigma_{x,y}$ are the same for all p. The zeroth order contribution of such points to the S matrix is then

$$\begin{aligned}\langle\beta'|S|\beta\rangle \sim &\exp\Big[iN\chi\oint d\tau(\sigma_x^2 - \sigma_y^2)\Big] \\ &\times \langle\beta'|U_{\sigma_f}(0,t)U_\sigma(t,-t)U_{\sigma_i}(-t,0)|\beta\rangle\end{aligned} \tag{3.45}$$

and each of the U_{σ_l} evolve with

$$H_{\sigma_l}(\tau) = \sum_p \Big[j_z^{(p)} + \delta_{l0}\vec{\mathrm{f}}\cdot\vec{\mathrm{j}}^{(p)} + 2\chi(\sigma_{lx}j_x^{(p)} - \sigma_{ly}j_y^{(p)})\Big] \tag{3.46a}$$

$$= J_z + \delta_{l0}\vec{\mathrm{f}}\cdot\vec{\mathrm{J}} + 2\chi(\sigma_{lx}J_x - \sigma_{ly}J_y) \tag{3.46b}$$

$$\equiv \vec{\mathrm{F}}_l(\tau)\cdot\vec{\mathrm{J}}\,, \tag{3.46c}$$

where

$$(F_{lx}, F_{ly}, F_{lz}) = (2\chi\sigma_{lx} + \delta_{l0}f_x, -2\chi\sigma_{ly} + \delta_{l0}f_y, 1 + \delta_{l0}f_z)\,. \tag{3.47}$$

For such symmetric solutions, we can also use Eq. (3.33) to average (3.44) over all p and obtain

$$\sigma_{l\,x,y}(\tau) = \frac{1}{N}\mathrm{Re}\left[\frac{\langle\beta_l'(\tau)\,|\,J_{x,y}\,|\,\beta_l(\tau)\rangle}{\langle\beta_l'(\tau)\,|\,\beta_l(\tau)\rangle}\right]. \tag{3.48}$$

The symmetric solutions are only one class of possible stationary points of the integrand in Eq. (3.41). We expect that these will be the most important ones and retain only them in our subsequent treatment. Nevertheless, there may exist other solutions in which the $\sigma^{(p)}$ depend upon p. The symmetry of Eq. (3.41) then guarantees that for each such solution there exist "mirror" solutions, corresponding to permutations of the p labels, whose contributions to S add coherently.

A simpler, alternative implementation of the Hubbard-Stratanovich representation of the Lipkin propagator would introduce p-independent auxiliary fields directly in the Hamiltonian (3.34). In this case, χ in Eqs. (3.45)–(3.47) would be replaced by $N\chi/(N-1)$, the difference, of course, corresponding to Hartree-Fock. Beginning the formulation with p-dependent σ fields correctly removes the spurious self-interaction present in the Hartree treatment.

We solve the mean-field equations by following methods analogous to steps (i)–(iii) used for the forced harmonic oscillator above, but differ from the previous step (iv) by solving evolution equations for the group parameters rather than for the σ fields.

(i) In analogy with Eq. (3.19), for any real $\vec{\alpha} \equiv (\alpha_x, \alpha_y, \alpha_z)$ we define the unitary operator

$$W[\vec{\alpha}] = \exp[-2i\vec{\alpha}\cdot\vec{\mathrm{J}}]\,. \tag{3.49}$$

Since $[\vec{\mathrm{j}}^{(p)}, \vec{\mathrm{j}}^{(p')}] = 0$ for $p \neq p'$, W can be factored into a product of one-body unitary operators:

$$W[\vec{\alpha}] = \prod_p w^{(p)}[\vec{\alpha}]\,, \tag{3.50}$$

where

$$w^{(p)}[\vec{\alpha}] = \exp[-2i\vec{\alpha}\cdot\vec{\mathrm{j}}^{(p)}]\,. \tag{3.51}$$

Since each of the operators in the H_σ's are elements of the SU(2) algebra, we can parametrize the evolution operators in analogy with Eq. (3.20) as

$$U_{\sigma_i}(\tau, 0) \equiv W[\vec{\alpha}_i(\tau)] \quad 0 \geq \tau \geq -t\,, \tag{3.52a}$$

$$U_\sigma(\tau, -t)U_{\sigma_i}(-t, 0) \equiv W[\vec{\alpha}(\tau)] \quad -t \leq \tau \leq t\,, \tag{3.52b}$$

$$U_{\sigma_f}(\tau, t)U_\sigma(t, -t)U_{\sigma_i}(-t, 0) \equiv W[\vec{\alpha}_f(\tau)] \quad 0 \leq \tau \leq t\,. \tag{3.52c}$$

At time $\tau = 0$ on the initial part of the loop, we must have $\vec{\alpha}_i(0) \equiv 0$ and the parameters must be continuous at the endpoints $\pm t$: $\vec{\alpha}_i(-t) = \vec{\alpha}(-t)$, $\vec{\alpha}(t) = \vec{\alpha}_f(t)$.

With this notation, the initial and final states along the loop are

$$|\beta_l(\tau)\rangle = W[\vec{\alpha}_l(\tau)]\,|\beta\rangle\,, \tag{3.53a}$$

$$\langle\beta_l'(\tau)| = \langle\beta'|\,W[\vec{\alpha}_f(0)]W^\dagger[\vec{\alpha}_l(\tau)]\,. \tag{3.53b}$$

Equations of motion for the parametrization can be found from the evolution equation for the U_{σ_l}'s. These lead to

$$i\frac{\partial W}{\partial\tau}[\vec{\alpha}_l(\tau)] = H_{\sigma_l}(\tau)W[\vec{\alpha}_l(\tau)]\,, \tag{3.54}$$

where H_{σ_l} is given by Eq. (3.46). Since the evolution of the $\vec{\alpha}_l$ implied by Eq. (3.54) is independent of which particular SU(2) irreducible representation is being used (i.e., independent of $J = \frac{1}{2}N$), it is simplest to choose $J = \frac{1}{2}$ and exploit the properties of the Pauli matrices. Defining $\alpha = (\alpha_x^2 + \alpha_y^2 + \alpha_z^2)^{1/2}$, we obtain

$$2\dot{\vec{\alpha}} = \left(\frac{1}{\alpha^2} - \frac{\mathrm{ctg}\alpha}{\alpha}\right)(\vec{\mathrm{F}}\cdot\vec{\alpha})\vec{\alpha} + (\alpha\,\mathrm{ctg}\alpha)\vec{\mathrm{F}} + \vec{\mathrm{F}}\times\vec{\alpha}\,, \tag{3.55}$$

where both $\vec{\alpha}$ and $\vec{\mathrm{F}}$ [defined by Eq. (3.47)] may be along any part of the loop. This is the analog of Eq. (3.23) for the oscillator. Note that at $\tau = 0$ on the initial part of the loop, where $\alpha_i \to 0$, there is no singularity in these equations. This is not true of the conventional Euler-angle parametrization.

The contribution to the S matrix from a given stationary solution may be written simply in terms of our parametrization. From Eqs. (3.45) and (3.52c) we have

$$\langle\beta'|S|\beta\rangle \sim \exp\left[iN\chi\oint d\tau(\sigma_x^2 - \sigma_y^2)\right]\langle\beta'|\,W[\vec{\alpha}_f(0)]\,|\beta\rangle\,. \tag{3.56}$$

The final matrix element $\langle\beta'|\exp[-2i\vec{\alpha}_f(0)\cdot\vec{\mathrm{J}}]\,|\beta\rangle$ is given in terms of the rotation matrix for spin J,

$$D^J_{M'M}[\vec{\alpha}_f(0)] = \langle M'|\exp[-2i\alpha_f(0)\cdot\vec{\mathrm{J}}]\,|M\rangle$$

as

$$\langle\beta'|\,W[\vec{\alpha}_f(0)]\,|\beta\rangle = \sum_{M'M}\langle\beta'|M'\rangle D^J_{M'M}[\vec{\alpha}_f(0)]\langle M|\beta\rangle\,. \tag{3.57}$$

For large values of J, D^J can be conveniently generated from

$$D^{1/2}_{m'm}[\vec{\alpha}] = \delta_{m'm}\cos\alpha - 2i\,\frac{\sin\alpha}{\alpha}\,\vec{\alpha}\cdot\langle m'|\vec{j}\,|m\rangle \tag{3.58}$$

by the usual Clebsch-Gordan series.

Of course, the entire discussion above remains valid when β and β' are replaced by the HF ground state. In this case, Eq. (3.56) may be simplified further using the factorization of W, Eq. (3.50), and the product nature of $|0_{\rm HF}\rangle$ as in Eqs. (3.39) and (3.40):

$$\langle 0_{\rm HF}|S|0_{\rm HF}\rangle = \left\{\exp\left[i\chi\oint d\tau(\sigma_x{}^2-\sigma_y{}^2)\right]\langle s=-1\,|w[\alpha_f(0)]\,|s=-1\rangle\right\}^N,\quad |\chi|\le 1. \tag{3.59}$$

For strong coupling situations, the single particle states $|s=-1\rangle$ should be replaced by rotated states as in Eq. (3.40). Thus, the zeroth order mean-field approximation to the S-matrix element for elastic propagation of the HF ground state depends very simply upon N for fixed χ.

(ii) Using Eqs. (3.48) and (3.53) we can derive an expression for σ in terms of $\vec{\alpha}$ similar to Eq. (3.24) for the oscillator. The unitary transformation of $\vec{J}$, $W^\dagger\vec{J}W$, can be simply evaluated using the SU(2) commutation rules to obtain

$$\sigma_{iy} = \left[(\cos2\alpha_i)\hat{y} - 2\,\frac{\sin2\alpha_i}{2\alpha_i}(\vec{\alpha}_i\times\hat{y}) + 2\left(\frac{\sin\alpha_i}{\alpha_i}\right)^2\alpha_{iy}\vec{\alpha}_i\right]\cdot\vec{\sigma}_i(0)\,, \tag{3.60}$$

where $\hat{y}$ is the unit vector in the y direction. A similar expression determines σ_{ix}.

The parameters $\vec{\sigma}_i(0)$ are analogous to ξ and η for the oscillator in Eq. (3.25) and depend only upon $\vec{\alpha}_f(0)$:

$$\vec{\sigma}_i(0) = \frac{1}{N}\mathrm{Re}\left[\frac{\langle\beta'|\exp[-i2\vec{\alpha}_f(0)\cdot\vec{J}]\vec{J}\,|\beta\rangle}{\langle\beta'|\exp[-i2\vec{\alpha}_f(0)\cdot\vec{J}]\,|\beta\rangle}\right] \tag{3.61a}$$

$$= \frac{1}{N}\mathrm{Re}\left[\frac{\Sigma\langle\beta'|M'\rangle D^J_{M'M''}[\vec{\alpha}_f(0)]\langle M''|\vec{J}\,|M\rangle\langle M|\beta\rangle}{\Sigma\langle\beta'|M'\rangle D^J_{M'M}[\vec{\alpha}_f(0)]\langle M|\beta\rangle}\right], \tag{3.61b}$$

where the sums run over all M indices appearing in the summand. When $|\beta\rangle$ and $|\beta'\rangle$ are replaced by $|0_{\rm HF}\rangle$, this can be simplified by using Eq. (3.44) rather than Eq. (3.48):

$$\vec{\sigma}_i(0) = \mathrm{Re}\left[\frac{\langle s=-1\,|\exp[-2i\vec{\alpha}_f(0)\cdot\vec{j}\,]\vec{j}\,|s=-1\rangle}{\langle s=-1\,|\exp[-2i\vec{\alpha}_f(0)\cdot\vec{j}\,]\,|s=-1\rangle}\right],\quad |\chi|<1\,. \tag{3.62}$$

(iii) Equations (3.55) and (3.60) can now be solved for $\vec{\alpha}_i(\tau)$, where the full self-consistency requirement on the time-dependent σ fields has been reduced to one on the three parameters $\vec{\sigma}_i(0)$. That is, the $\vec{\sigma}_i(0)$ in Eq. (3.60) used to evolve $\vec{\alpha}$ must be the same determined by $\vec{\alpha}_f(0)$ through Eqs. (3.61).

As in the oscillator, we can eliminate $\vec{\alpha}$ and obtain closed equations for the σ fields. We introduce another auxiliary field $\sigma_z(\tau)$ defined analogously to Eq. (3.48). Taking the first time derivative of this equation and simply evaluating $[H_\sigma,\vec{J}]$, we obtain

$$\dot{\vec{\sigma}}_i(\tau) = \vec{F}_i(\tau)\times\vec{\sigma}_i(\tau)\,. \tag{3.63}$$

These equations are analogous to Eq. (3.26) for the oscillator, but are nonlinear since $\vec{F}$ is a function of $\vec{\sigma}$. Note also that it follows immediately from Eq. (3.63) that $\sigma^2\equiv\vec{\sigma}\cdot\vec{\sigma}$ is conserved around the loop.

(iv) In contrast to the forced oscillator, Eq. (3.63) alone is not sufficient to find the stationary solutions. One might hope to guess $\vec{\sigma}_i(0)$, integrate Eq. (3.63) around the loop to find $\vec{\sigma}_f(0)$, and then demand self-consistency on $\vec{\sigma}_f(0)$ through Eq. (3.60). Unfortunately, this latter explicitly involves $\vec{\alpha}_f(0)$, and it is impossible to invert Eq. (3.61) to find $\vec{\alpha}_f(0)$ in terms of $\vec{\sigma}_i(0)$. Hence, self-consistency can be assured only by also integrating the $\vec{\alpha}$ equation (3.55) together with (3.60).

The unperturbed Lipkin Hamiltonian (3.34) is not time reversal invariant due to the term linear in J_z. Consequently, the mean fields will not possess this symmetry either. For example, for elastic propagation ($\beta'=\beta$), it is easy to show that $\vec{\sigma}_i$ and $\vec{\sigma}_f$ are not continuous at $\tau=0$, but instead suffer a discontinuity

$$\sigma_{fx,y}(0) - \sigma_{ix,y}(0) = \frac{1}{N}\mathrm{Re}\left\{\frac{\langle\beta|[J_{x,y}, W[\vec{\alpha}_f(0)]]|\beta\rangle}{\langle\beta|W[\vec{\alpha}_f(0)]|\beta}\right\}. \tag{3.64}$$

However, other symmetries of the problem are preserved by the mean-field approximation to the S matrix. In particular, by methods analogous to those used to discuss time-reversal symmetry in Sec. II, the following two symmetries can be shown.

(i) H_0 is invariant under the transformation $(x,y)\to(y,x)$ and $v\to -v$ (i.e., a 90° rotation about the z axis followed by a reflection through the $y-z$ plane and a change in sign of the two-body interaction). If $V(t)$ also has this symmetry [i.e., $f_x(t)=f_y(t)$], then the exact and mean-field S matrices for the original and transformed problems also have this symmetry, and if (σ_x,σ_y) is a self-consistent solution of the original problem, (σ_y,σ_x) is a solution of the transformed problem.

(ii) Since H_0 is invariant under a rotation by π about the z axis (i.e., $J_{x,y}\to -J_{x,y}$), each of its exact eigenstates $|\beta\rangle$ has a definite parity $(-)^\beta$ under this transformation. The exact and mean-field S-matrix elements $S_{\beta'\beta}$ for the perturbation (f_x,f_y,f_z) are related to those for $(-f_x,-f_y,f_z)$ by the phase factor $(-)^{\beta+\beta'}$. If (σ_x,σ_y) is a solution of the original problem, then $(-\sigma_x,-\sigma_y)$ is a solution of the transformed problem. When $f_x=f_y=0$, transitions can be induced only between states of the same parity. In this case, the original and transformed problems are identical and either $\sigma_x=\sigma_y=0$ or the mean-field solutions occur in conjugate pairs, $(\pm\sigma_x,\pm\sigma_y)$. In the former instance, it is evident that $S_{\beta'\beta}$ will vanish unless β' and β have the same parities, while in the latter case, the conjugate solutions give equal and opposite contributions to S to satisfy the parity selection rule.

The model defined above is specified by the number of particles N, the coupling constant χ, and the driving field $\vec{f}(t)$. Since it is not possible to explore the full range of these parameters here, we have chosen to present some representative studies where $\vec{f}(t)$ has a Gaussian time dependence on a time scale τ.

$$\vec{f}(t)=e^{-(t/\tau)^2}(f_x,f_y,f_z)\,. \tag{3.65}$$

Here, the amplitudes $f_{x,y,z}$ are time independent. Unless stated otherwise, we assume the "standard" parameters $\tau=f_x=f_y=f_z=1$. Throughout, we focus on the moduli of the various S-matrix elements, but note that results for the phases are of a similar quality.

In Fig. 2, we show several approximations to the elastic S-matrix element $|S_{00}|$ as a function of N. The standard parameters are assumed in a typical weak coupling situation $\chi=0.5$. The mean field is seen to be a good approximation to propagation of the exact ground state and an even better approximation to that of the (undeformed) HF ground state. Note that in this latter case, an exponential N dependence is predicted by (3.59). Also shown in Fig. 2 is the interaction-picture TDHF approximation defined by (2.66)–(2.67), which is seen to be a rather poor approximation to the S-matrix element for the HF ground state, although it is (accidentally) a fair approximation to that for the exact ground state.

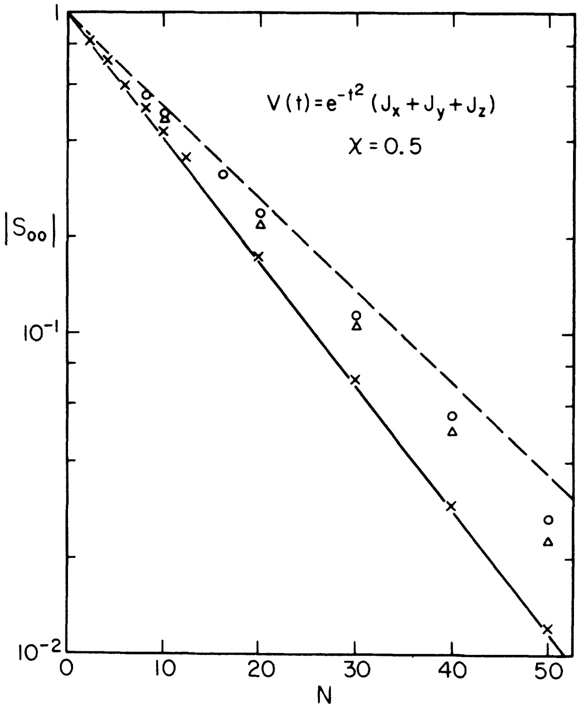

FIG. 2. Modulus of the ground-state elastic propagation amplitude $|S_{00}|$ in the forced Lipkin model for various ground states and evolution methods. Plotted as a function of the number of particles N are the results for o—exact evolution of the exact ground state; △—mean-field evolution of the exact ground state; × —exact evolution of the HF ground state; —— —mean-field evolution of the HF ground state; --- —interaction-picture TDHF for the HF ground state.

The moduli of the amplitudes to excite the exact nth excited state from the exact ground state $|S_{n0}|$ are shown in Figs. 3–5 for various cases. The exact propagation is compared with both the mean field and interaction picture TDHF results for $\chi=0.5$. Figure 3, a typical case of intermediate excitation, shows that the zeroth order mean-field approximation well reproduces the exact results, though somewhat underestimates the excitation of those states which are strongly excited. The approximation gets better with increasing N, since the phase of the functional integrand, which is assumed to be varying rapidly, is roughly proportional to N, as in (3.56). The interaction picture TDHF, although unitary, generally predicts

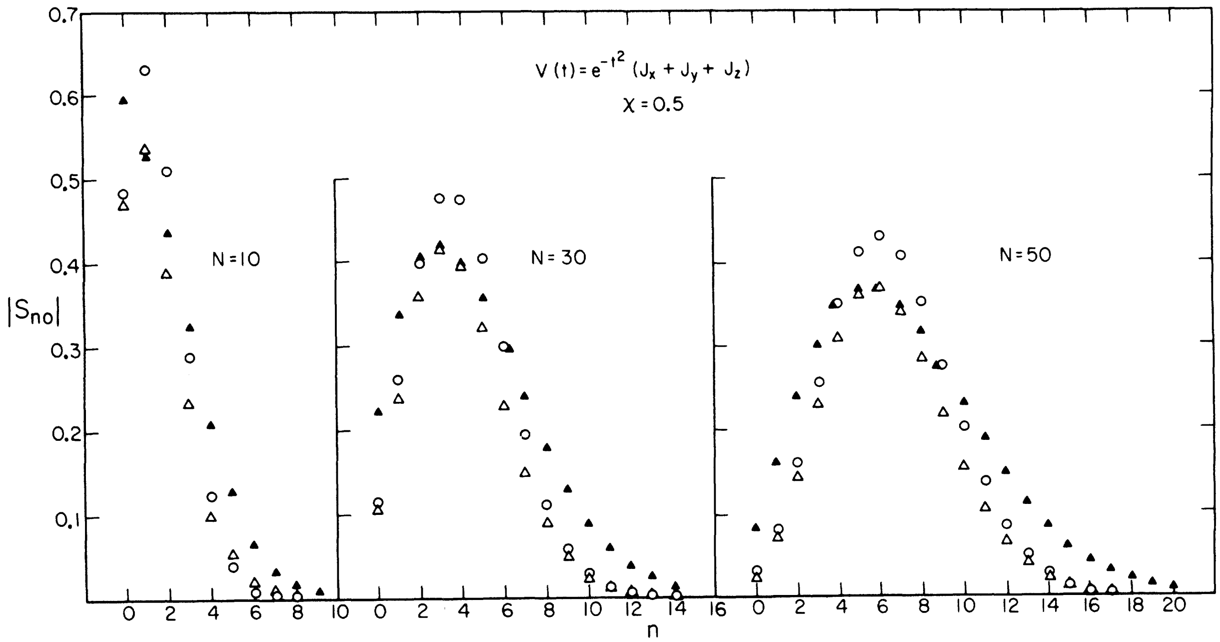

FIG. 3. Moduli of the amplitudes to excite the exact nth excited state from the exact ground state $|S_{n0}|$ in the forced Lipkin model. Shown for several values of N are the exact amplitudes (o), their mean-field approximation (△), and their interaction-picture TDHF approximation (▲).

too broad an excitation spectrum. Figure 4 is a case of strong excitation (short time-scale $\tau=\frac{1}{4}$ and large amplitude $f_{x,y,z}=4$) where both approximations agree very well with the exact result, although again the mean field is slightly better. Such agreement is to be expected, since the strong external field makes the treatment of the two-body interaction less important, which is how the two approximations differ. Figure 5 is a case of weak excitation.

The stationary mean field $\sigma_{x,y}(\tau)$ is shown in Fig. 6 for a weak coupling situation. When $V(\tau)\approx 0$, the fields oscillate and, of course, $\sigma_{i,f}(\tau)$ coincide with $\sigma(\tau)$. Since the Lipkin Hamiltonian is not time-reversal invariant, the mean fields are not symmetric about $\tau=0$, even though $V(\tau)$ is.

To explore the strong coupling limit $|\chi|>1$, we consider the elastic propagation of the positive-

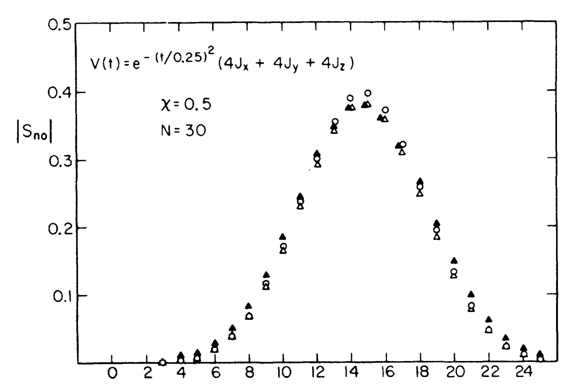

FIG. 4. Similar to Fig. 3, but for a case of stronger excitation.

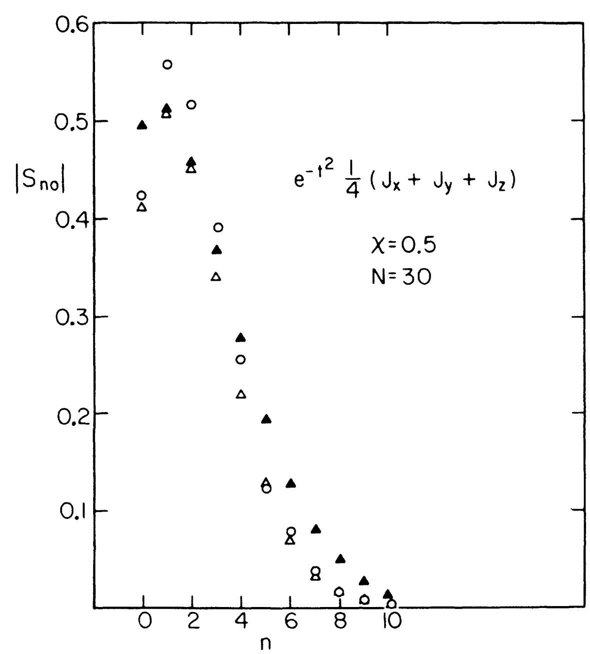

FIG. 5. Similar to Fig. 3, but for a case of weaker excitation.

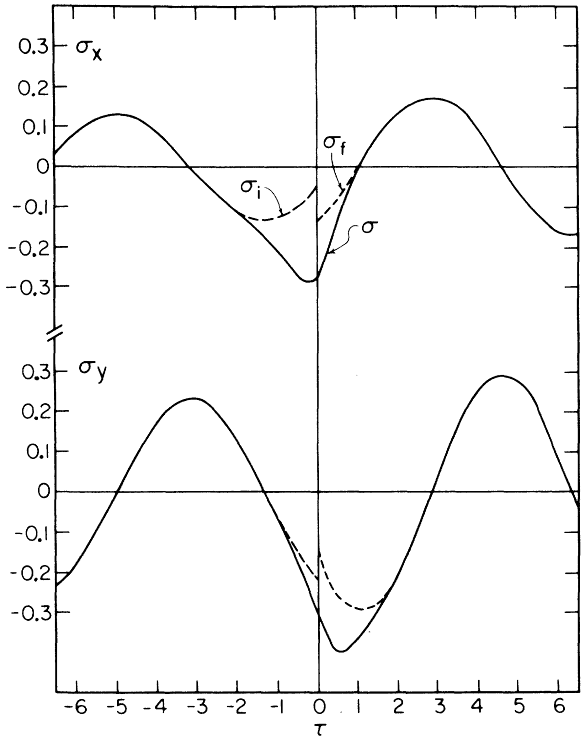

FIG. 6. The mean fields $\sigma_{x,y}(\tau)$ for the evolution of the HF ground state with $\chi = 0.5$ under the standard perturbation. Note that $\sigma_{i,f}(\tau)$ coincide with $\sigma(\tau)$ when $V(\tau) \approx 0$ (i.e., $|\tau| \gg 1$).

parity HF ground state obtained by symmetrizing the states (3.40):

$$|0_{\mathrm{HF}}\rangle \equiv \frac{1}{\sqrt{\mathfrak{N}}}[|+\varphi_{\mathrm{HF}}\rangle + |-\varphi_{\mathrm{HF}}\rangle], \tag{3.66}$$

where the normalization is

$$\mathfrak{N} = 2(1 + \mathrm{Re}\langle +\varphi_{\mathrm{HF}}|-\varphi_{\mathrm{HF}}\rangle). \tag{3.67}$$

As $|\chi| \to \infty$, the HF minima became increasingly better defined and $|\pm\varphi_{\mathrm{HF}}\rangle$ became orthogonal to each other. The S-matrix element for the elastic propagation of (3.66) is

$$\langle 0_{\mathrm{HF}}|S|0_{\mathrm{HF}}\rangle = \frac{1}{\mathfrak{N}}[\langle +\varphi_{\mathrm{HF}}|S|+\varphi_{\mathrm{HF}}\rangle + \langle +\varphi_{\mathrm{HF}}|S|-\varphi_{\mathrm{HF}}\rangle + \langle -\varphi_{\mathrm{HF}}|S|+\varphi_{\mathrm{HF}}\rangle + \langle -\varphi_{\mathrm{HF}}|S|-\varphi_{\mathrm{HF}}\rangle]. \tag{3.68}$$

If we separately evaluate each of these four terms in the mean-field approximation, each becomes exponentially dependent on N (as in 3.59) and, in an obvious notation,

$$\langle 0_{\mathrm{HF}}|S|0_{\mathrm{HF}}\rangle = \frac{1}{\mathfrak{N}}[s_{++}^N + s_{+-}^N + s_{-+}^N + s_{--}^N], \tag{3.69}$$

where the s's are N independent. Interference phenomena as a function of N or χ are expected from this form. Often, only two of the four terms contribute significantly. In our standard case, for $|\chi| \gtrsim 1$, s_{++} dominates, and s_{-+} is the second largest contribution. However, for $|\chi| \gtrsim 2$, s_{--} becomes larger as s_{-+} decays. For very large $|\chi|$, $|s_{++}| = |s_{--}| = 1$ and $s_{+-} \approx s_{-+} \approx 0$. This is to be expected, since for the extreme strong coupling limit, the deep and narrow HF minima make it difficult to excite states in the wells at $\pm\varphi$ and the excitation problem essentially reduces to one involving only two channels, the nearly degenerate symmetrized and antisymmetrized ground and first excited states, as in (3.66). In Fig. 7, we show the rather amazing agreement of the exact and mean-field approximations for $|S_{00}|$ over the entire range of $|\chi|$. Again, the improvement with increasing N is evident.

IV. SUMMARY AND DISCUSSION

In this paper, we have developed a mean-field approximation to the many-body S matrix. For a many-body system with pairwise interactions perturbed by a time-dependent one-body field, we have shown that the first-order mean-field equations reduce to a set of temporally nonlocal TDHF-

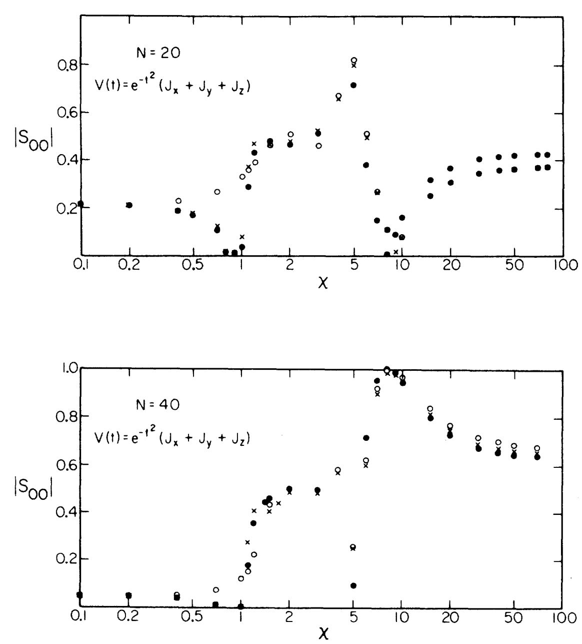

FIG. 7. Elastic propagation amplitudes $|S_{00}|$ as a function of χ for $N = 20$ and $N = 40$; ○—exact evolution of the exact ground state; ×—exact evolution of the symmetrized HF ground state; ●—mean-field evolution of the symmetrized HF ground state.

like equations which must be solved self-consistently to determine the excitation amplitudes. Applications of this method to the forced harmonic oscillator and Lipkin model have shown that it can well reproduce the exact S matrix in a variety of situations.

Our studies naturally raise a number of questions concerning both the mean-field method itself and its future utility in realistic calculations. Some of these will be given detailed consideration in future publications while others are currently being investigated. We briefly summarize some of the more relevant points below.

To generate the zeroth-order mean-field approximation basic to our method, we have chosen one particular stationary-phase approximation to the Hubbard-Stratonovich representation of the many-body evolution operator, i.e., that in which the *phase* of the integrand is assumed to vary much more rapidly with σ-field configuration than does it magnitude. As discussed in Ref. 14 relaxing this assumption leads to generally complex σ fields and a steepest-descent approximation to the functional integral. Although such mean-fields imply a nonunitary one-body evolution through (2.21), the extra freedom they introduce may result in better approximations to the exact integrand with little additional complications. The complex-time (instanton) technique useful in bound-state problems[18] may also be applicable to the S matrix. Such questions can, of course, be readily investigated in the force Lipkin problem discussed above.

We have not considered any quadratic corrections to the lowest-order mean-field approximation, although we discussed in Sec. II why such corrections would generally be expected to be small. Indeed, this proved to be the case in most of the examples considered. This is fortunate, since the evaluation of such corrections requires the practically intractable computation of a functional determinant similar to (2.32). When several solutions contribute coherently to a given S-matrix element, larger errors might be introduced by the neglect of these corrections. To what extent the situation might be corrected by complex σ fields remains to be investigated. All of these issues must be considered case by case, since they clearly depend on the particular problem and coupling strengths being studied.

Although we have given a mean-field approximation to the S matrix, we have emphasized in Sec. II that the choice of initial and final states is quite a separate and independent issue. This point was demonstrated explicitly in our Lipkin studies in Sec. III. Although Slater determinants are the most natural and tractable states to use, more sophisticated wave functions may be necessary to achieve the desired accuracy in any particular situation. One attractive possibility deserving further study is to use the bound-state mean-field techniques[17] to furnish these wave functions. In a sense, this would make the description of the channel states commensurate with the approximate mean-field evolution.

We have not, as yet, been able to generate a tractable mean-field approximation to the complete time-independent many-body scattering problem, in large part due to difficulties in the choice of these channel states. Consider, for example, the elastic scattering of a single nucleus from a spatially localized one-body potential $V(x)$. The channel states should be chosen as approximate eigenstates of H_0 describing the many-body ground state boosted with a total momentum $\vec{P}$, the quantities of interest then being $\langle \vec{P}' | S | \vec{P} \rangle$, where S is given as in (2.8). One possible choice for these eigenstates can be written in terms of the zero-momentum component of the static HF solution. Specifically,

$$| \vec{P} \rangle \approx e^{i\vec{P}\cdot\vec{X}} \left(\mathfrak{N}^{-1/2} \int d\vec{R} | \vec{R} \rangle \right) , \qquad (4.1)$$

where $\vec{X}$ is the nuclear center-of-mass coordinate, $| \vec{R} \rangle$ is the ground-state HF determinant with $\langle \vec{R} | \vec{X} | \vec{R} \rangle = \vec{R}$, and $\mathfrak{N} = \int d\vec{R} \, d\vec{R}' \langle \vec{R}' | \vec{R} \rangle$ is the normalization. Note that $| \vec{P} \rangle$ is not a determinant. The many-body S matrix is then

$$\langle \vec{P}' | S | \vec{P} \rangle = \mathfrak{N}^{-1} \int d\vec{R} \, d\vec{R}' \langle \vec{R}' | e^{-i\vec{P}'\cdot\vec{X}} S e^{i\vec{P}\cdot\vec{X}} | \vec{R} \rangle , \qquad (4.2)$$

i.e., a linear combination of elements of S evaluated between determinantal states. It is, of course, natural to attempt to treat the center-of-mass motion semiclassically and make a stationary phase approximation to the $\vec{R}, \vec{R}'$ integrals, exploiting the fact that $\langle \vec{R}' | \vec{R} \rangle$ is sharply peaked near $\vec{R}' \approx \vec{R}$. The stationary conditions which result require that $\vec{R}$ and $\vec{R}'$ be chosen so that the mixed-time expectation value of the total momentum [analogous to (2.36) for the density] be $\vec{P}$ along the initial part of the loop and $\vec{P}'$ along the final part of the loop. The practical implementation of these conditions appears to be difficult. Other practical problems exist in a real two-nucleus collision as far as properly defining the channel Hamiltonians and the interaction $V = H - H_0$.

Despite the rather discouraging prospects for a completely quantal treatment, the formalism we have developed here is immediately applicable to situations where a separation coordinate $\vec{R}$ can be isolated and treated classically. In this case, the remaining intrinsic coordinates x can be treated via the mean-field methods. The motion $\vec{R}(t)$ then generates an effective time-dependent potential perturbing the x degrees of freedom. A scheme can also be developed to allow the intrinsic excitation to feed-back on the separation trajectory.[21] These approximations are applicable to electronic excitation and charge transfer in atomic collisions, and indeed appear quite tractable in practice.[31] The same scheme for nuclear collisions would allow optical model transmission functions and elastic and inelastic scattering amplitudes to be computed in a microscopic, nonperturbative manner.

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