

Mean-field approximation for inclusive observables

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The excitation of a many-body system by a one-body perturbation is considered. The stationary phase approximation to a functional-integral representation of the many-body evolution operator shows that the optimal mean field for describing the final expectation values of one- and two-body operators is that given by the time-dependent Hartree-Fock method. The forced Lipkin model is considered as a test of the mean-field approximation.

[NUCLEAR REACTIONS Mean-field approximation, inclusive observables.]
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I. INTRODUCTION

The time-dependent mean-field approximation has recently been proposed as a framework for the description of large-scale collective motion¹ and excitations² in many-body systems. This latter work showed that it is possible to obtain approximate values for many-body S -matrix elements in terms of matrix elements of an effective one-body evolution operator. This is a significant improvement over the well-known time-dependent Hartree-Fock (TDHF) approximation which, although of a similar one-body nature, cannot be used to compute elements of the many-body S matrix. The mean-field approximation requires the solution of a temporally nonlocal equation for the evolution of the system with boundary conditions in the past *and* in the future. It has been applied to the schematic forced Lipkin model, where it was found to give a very good estimate of the exact S matrix.²

The optimal mean field for a given S -matrix element depends upon the initial and final channels and hence must be calculated anew for every transition of interest. While this might be acceptable for exclusive (or nearly exclusive) measurements, it is evidently a considerable complication in describing any inclusive measurement which averages over a large number of exit channels. In these cases, the full S matrix contains far more information than is needed to describe the experiment. It is therefore appropriate to consider an alternative implementation of the mean-field approximation which calculates directly inclusive observables, i.e., the final expectation values of self-adjoint few-body operators for a given initial channel. This is the subject of the present paper. For a many-body system with two-body interactions perturbed by a time-dependent one-body potential, we shall demonstrate that to approximate the final expectation values of one- and two-body constants of the

unperturbed motion, the appropriate mean field is that determined by the usual TDHF equations.

The balance of our paper is organized as follows: Section II is a review of the Hubbard-Stratonovich representation of the many-body time evolution operator, followed by Sec. III, the derivation of the equations of motion for the mean field in the stationary-phase approximation. In Sec. IV we test the quality of the approximation in the forced Lipkin model by comparing with the exact results. Finally, we offer a brief discussion and conclusion in Sec. V.

II. THE TIME-EVOLUTION OPERATOR

We shall assume that our many-body system is described by a Hamiltonian containing a static two-body interaction v and a time-dependent one-body potential V which vanishes as $|t| \rightarrow \infty$:

$$H(t) = K + \frac{1}{2} \int dx dx' \rho(x) v(x-x') \rho(x') + \int dx V(x, t) \rho(x), \quad (1)$$

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

$$K = \frac{1}{2m} \int dx (\nabla \psi^\dagger)(\nabla \psi) - \frac{v(0)}{2} \int dx \rho(x), \quad (2)$$

and

$$\rho(x) = \psi^\dagger(x) \psi(x) \quad (3)$$

is the density operator. The Hubbard-Stratonovich approach^{1,3,4} represents the many-body time evolution operator

$$U(t, -t) = T \exp \left[-i \int_{-t}^t d\tau H(\tau) \right] \quad (4)$$

by a functional integral over evolution operators for all possible one-body fields

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

with

$$\begin{aligned} U_\sigma(t, -t) &= T \exp \left[-i \int_{-t}^t d\tau H_\sigma(\tau) \right] \\ &= T \exp \left[-i \int_{-t}^t d\tau [K + (\sigma(\tau), v\rho) + (V(\tau), \rho)] \right]. \end{aligned} \quad (6)$$

In these equations T denotes the time-ordering operation and we have introduced the scalar product notation for the integration over coordinate-space variables; e.g.,

$$(\sigma(\tau), v\rho) = \int dx dx' \sigma(x, \tau) v(x - x') \rho(x'). \quad (7)$$

The auxiliary field $\sigma(x, \tau)$ is a scalar c -number function, and the functional integral in Eq. (5) runs over all possible σ fields with the measure¹

$$\int \mathcal{D}[\sigma] = \lim_{\substack{N \rightarrow \infty \\ \Delta x, \Delta t \rightarrow 0}} \int \frac{(\det v)^{1/2}}{(2\pi i)^{N/2}} \prod_{i=1}^N [\Delta x \Delta t d\sigma(x_i, t_i)]. \quad (8)$$

In the mean-field approach to the many-body S matrix, the matrix elements of Eq. (5) (or expressions similar to it) between given initial and final states ($|i\rangle$ and $|f\rangle$) are evaluated in the stationary phase approximation, where an optimal field $\sigma_0(x, t)$ is determined by making the phase of the integrand stationary as a functional of σ . Thus, in the case of Eq. (5), one demands $\delta\phi/\delta\sigma = 0$, with

$$\phi[\sigma] = \frac{1}{2} \int_{-t}^t d\tau (\sigma, v\sigma) + \arg \langle f | U_\sigma | i \rangle. \quad (9)$$

No exchange (Fock) term is obtained in this formulation.¹ However, a straightforward rem-

edy can be had by introducing a nonlocal mean field $\sigma(x, x', t)$ for the nonlocal density operator $\rho(x, x') = \psi^\dagger(x)\psi(x')$. Since this is merely a formal complication and does not change the essence of our arguments, we shall work throughout with only the local mean-field representation.

III. EXPECTATION VALUES IN THE STATIONARY PHASE APPROXIMATION

Let

$$A = \int dy \psi(y) \rho(y) \equiv (a, \rho) \quad (10a)$$

and

$$B = \int dy d\bar{y} \rho(y) b(y, \bar{y}) \rho(\bar{y}) \equiv (\rho, b\rho) \quad (10b)$$

by one- and two-body operators, respectively, in the Schrödinger picture, which commute with the Hamiltonian as $|t| \rightarrow \infty$ and are therefore asymptotic constants of the motion. If the many-body system was initially prepared in state $|i\rangle$ at time $t = T_0 \rightarrow -\infty$ the constant expectation values of A and B at a late time $T \rightarrow +\infty$ are given by

$$\langle A \rangle_T = \int dy a(y) \langle i | U^\dagger(T, T_0) \rho(y) U(T, T_0) | i \rangle, \quad (11a)$$

$$\begin{aligned} \langle B \rangle_T &= \int dy d\bar{y} b(y, \bar{y}) \langle i | U^\dagger(T, T_0) \rho(y) \rho(\bar{y}) \\ &\quad \times U(T, T_0) | i \rangle. \end{aligned} \quad (11b)$$

It is thus sufficient to know the expectation value of the density operator, ρ , and its correlation $\rho\rho$. With the functional integral representation of $U(T, T_0)$, as given by Eq. (5), we can express these as

$$\langle \rho(y) \rangle_T = \int \mathcal{D}[\sigma] \mathcal{D}[\sigma'] \exp \left\{ \frac{i}{2} \int_{T_0}^T d\tau [(\sigma, v\sigma) - (\sigma', v\sigma')] \right\} \langle i | U_\sigma^\dagger(T, T_0) \rho(y) U_\sigma(T, T_0) | i \rangle, \quad (12a)$$

$$\langle \rho(y) \rho(\bar{y}) \rangle_T = \int \mathcal{D}[\sigma] \mathcal{D}[\sigma'] \exp \left\{ \frac{i}{2} \int_{T_0}^T d\tau [(\sigma, v\sigma) - (\sigma', v\sigma')] \right\} \langle i | U_\sigma^\dagger(T, T_0) \rho(y) \rho(\bar{y}) U_\sigma(T, T_0) | i \rangle. \quad (12b)$$

If we were to make the stationary phase approximation at this point, the variation of $U_\sigma, U_\sigma^\dagger$ with respect to σ, σ' would result in stationary equations containing matrix elements having an additional factor of ρ . Thus, we would have to evaluate expectation values of a two-body operator for Eq. (12a) and of a three-body operator for Eq. (12b). This complication is avoided by the well-known technique⁵ of replacing U_σ by the evolution operator in the presence of an external source function $\mathcal{F}(x, t)$

$$\begin{aligned} U_\sigma^\mathcal{F}(T, T_0) &= T \exp \left\{ -i \int_{T_0}^T d\tau [K + (\sigma, v\rho) + (V, \rho) + (\mathcal{F}(\tau), \rho)] \right\} \end{aligned} \quad (13)$$

and introducing factors of ρ in the matrix elements by functional variation with respect to $\mathcal{F}(x, \tau)$. Note that this procedure produces a simple result only if the variation is made with respect to \mathcal{F} taken at time T or T_0 , otherwise

$$\frac{\delta}{\delta \mathcal{F}(y, t)} U_\sigma^\mathcal{F}(T, T_0) = -i U_\sigma^\mathcal{F}(T, t) \rho(y) U_\sigma^\mathcal{F}(t, T_0). \quad (14)$$

With this method we find

$$\langle i | U_{\sigma_0}^\dagger(T, T_0) \rho(y) U_{\sigma_0}(T, T_0) | i \rangle = \lim_{\mathfrak{F}, \mathfrak{F}' \rightarrow 0} \frac{1}{2i} \left[\frac{\delta}{\delta \mathfrak{F}(y, t)} - \frac{\delta}{\delta \mathfrak{F}'(y, T)} \right] \langle i | U_{\sigma_0}^{\mathfrak{F}\mathfrak{F}'}(T, T_0) U_{\sigma_0}^{\mathfrak{F}}(T, T_0) | i \rangle. \quad (15)$$

The symmetrization in \mathfrak{F} and \mathfrak{F}' is not really required for the expectation value of ρ but we shall need it for $\rho\rho$, as will be seen below. If we now make a linear change in the functional integration variables of Eqs. (12(a)), $\sigma \rightarrow \sigma - v^{-1}\mathfrak{F}$ and similarly for σ' , the influence of the source is shifted from the evolution operators $U_{\sigma_0}^{\mathfrak{F}}$ to the Gaussian weight functional. The functional differentiation required in Eq. (15) is then easily performed and upon letting $\mathfrak{F}, \mathfrak{F}' \rightarrow 0$, we obtain

$$\begin{aligned} \langle \rho(y) \rangle_T = & \int \mathcal{D}[\sigma] \mathcal{D}[\sigma'] \exp \left\{ \frac{i}{2} \int_{T_0}^T dt [(\sigma, v\sigma) - (\sigma', v\sigma')] \right\} \\ & \times \frac{1}{2} [\sigma(y, T) + \sigma'(y, T)] \\ & \times \langle i | U_{\sigma_0}^\dagger(T, T_0) U_{\sigma_0}(T, T_0) | i \rangle. \end{aligned} \quad (16)$$

The stationary phase approximation in lowest order requires that the phase of the integrand be stationary with respect to small variations in σ and σ' , and takes the value of the integral to be the integrand at the stationary point. The calculation proceeds in the same way as that for the S-matrix elements^{1,2} and yields the two coupled equations of motion

$$\begin{aligned} \sigma_0(x, t) = & \text{Re} \frac{\langle i | U_{\sigma_0}^\dagger(T, T_0) U_{\sigma_0}(T, t) \rho(x) U_{\sigma_0}(t, T_0) | i \rangle}{\langle i | U_{\sigma_0}^\dagger(T, T_0) U_{\sigma_0}(T, T_0) | i \rangle}, \\ \sigma'_0(x, t) = & \text{Re} \frac{\langle i | U_{\sigma'_0}^\dagger(t, T_0) \rho(x) U_{\sigma'_0}^\dagger(T, t) U_{\sigma'_0}(T, t_0) | i \rangle}{\langle i | U_{\sigma'_0}^\dagger(T, T_0) U_{\sigma'_0}(T, T_0) | i \rangle}. \end{aligned} \quad (17)$$

In general, these equations may have many different solutions with $\sigma_0 \neq \sigma'_0$ which will depend upon T and are therefore ignored in the following. However, for a well-behaved interaction V the T -independent solution

$$\sigma_0(x, t) = \sigma'_0(x, t) = \langle i | U_{\sigma_0}^\dagger(t, T_0) \rho(x) U_{\sigma_0}(t, T_0) | i \rangle \quad (18)$$

will always exist, since Eq. (18) is local in time with a boundary condition only at $t = T_0$. This is precisely the TDHF equation of motion (the exchange term is absent, as discussed above). Substituting this relation into Eqs. (11a) and (16) we obtain the TDHF expression for the expectation value of the one-body observable A_T :

$$\begin{aligned} \langle A \rangle_T^{\text{SPA}} = & \int dV a(V) \sigma_0(V, T) \\ = & \int dV a(V) \langle i | U_{\sigma_0}^\dagger(T, T_0) \rho(V) U_{\sigma_0}(T, T_0) | i \rangle. \end{aligned} \quad (19)$$

For the expectation value of $\rho\rho$, Eq. (12b), a second variation in \mathfrak{F} is required. The calculation proceeds in precisely the same way, but now explicit symmetrization in \mathfrak{F} and \mathfrak{F}' is required, lest terms such as $iv^{-1}(y - \bar{y})\delta(T - T)$ appear which violate self-adjointness of the operators. One finds

$$\begin{aligned} \langle \rho(y) \rho(\bar{y}) \rangle_T = & \int \mathcal{D}[\sigma] \mathcal{D}[\sigma'] \exp \left\{ \frac{i}{2} \int_{T_0}^T d\tau [(\sigma, v\sigma) - (\sigma', v\sigma')] \right\} \\ & \times \frac{1}{2} [\sigma(y, T) \sigma(\bar{y}, T) + \sigma'(y, T) \sigma'(\bar{y}, T)] \langle i | U_{\sigma_0}^\dagger(T, T_0) U_{\sigma_0}(T, T_0) | i \rangle. \end{aligned} \quad (20)$$

The phase is the same as in the one-body case and the stationary phase approximation yields Eqs. (17) for σ_0, σ'_0 . Again we always have the solution (18) with $\sigma_0 = \sigma'_0$, yielding

$$\langle B \rangle_T^{\text{SPA}} = \int dV d\bar{V} b(V, \bar{V}) \sigma_0(V, T) \sigma_0(\bar{V}, T). \quad (21)$$

Note that this is *not* the same as the expectation value of B taken with the state $U_{\sigma_0}(T, T_0) | i \rangle$. The difference is, of course, the neglected exchange terms, which cannot be expressed solely in terms of the local single-particle density $\rho(y)$.

The derivation above does not apply to the Hamiltonian, because H cannot be written in the form (10b). One alternative is to introduce the nonlocal mean field $\sigma(x, x', t)$, but there exists another, simpler method which we shall employ. Making use of the equation of motion for the time-evolution operator U ,

$$i \frac{\partial}{\partial t} U(t, T_0) = H(t) U(t, T_0), \quad (22)$$

we can write

$$\langle H \rangle_T = \lim_{t, t' \rightarrow T} \frac{i}{2} \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial t'} \right) \langle i | U^\dagger(t', T_0) U(t, T_0) | i \rangle. \quad (23)$$

Representing each operator in the matrix element by the functional integral (5), we arrive at the expression

$$\begin{aligned} \langle H \rangle_T = & \int \mathcal{D}[\sigma] \mathcal{D}[\sigma'] \exp \left\{ \frac{i}{2} \int_{T_0}^T dt [(\sigma, v\sigma) - (\sigma', v\sigma')] \right\} \langle i | U_\sigma^\dagger(T, T_0) U_\sigma(T, T_0) | i \rangle \\ & \times \left\{ \frac{1}{2} \frac{\langle i | U_\sigma^\dagger(T, T_0) [H_\sigma(T) + H_\sigma(T)] U_\sigma(T, T_0) | i \rangle}{\langle i | U_\sigma^\dagger(T, T_0) U_\sigma(T, T_0) | i \rangle} - \frac{1}{4} [(\sigma, v\sigma) + (\sigma', v\sigma')]_{t=T} \right\}. \end{aligned} \quad (24)$$

The symmetrization in t and t' is necessary here to retain the explicit self-adjointness of the operator at every stage of the derivation. As a consequence the term in curly brackets is real for real σ fields and does not contribute to the phase of the integrand. Going through the same steps as before, we find the same equation of motion for the σ fields in the stationary phase approximation, and for $\sigma_0 = \sigma'_0$ the energy expectation value reads

$$\begin{aligned} \langle H \rangle_T^{\text{SPA}} = & \langle i | U_\sigma^\dagger(T, T_0) H_\sigma(T) U_\sigma(T, T_0) | i \rangle \\ & - \frac{1}{2} [\sigma_0(T), v\sigma_0(T)]. \end{aligned} \quad (25)$$

This is precisely the Hartree-Fock expression for the total energy, without the exchange term as discussed in Sec. II.

IV. THE LIPKIN MODEL

To illustrate and test these ideas, we consider the forced Lipkin model,⁶ which was previously treated as an example of the mean-field approximation to the S matrix.² The Lipkin model is particularly interesting in that it exhibits a phase transition from a "spherical" to a "deformed" ground state when the coupling parameter χ is ± 1 (see below), and the Hartree-Fock approximation may be expected to provide a poor description in this region. We shall only state the necessary equations here and refer to the treatment of Ref. 2 for all details.

The Hamiltonian for the forced Lipkin model can be expressed in terms of $SU(2)$ quasispin operators \tilde{J} :

$$H(t) = J_x + \frac{\chi}{N-1} (J_x^2 - J_y^2) + \tilde{f}(t) \cdot \tilde{J}. \quad (26)$$

Here $\tilde{f}(t)$ is an arbitrary vector function defining the one-body perturbation and will be assumed to vanish for $|t| \rightarrow \infty$. Without the external perturbation, the Hartree-Fock ground state is given by $|0_{\text{HF}}\rangle = |J = \frac{1}{2}N, J_x = -\frac{1}{2}N\rangle$ when $|\chi| \leq 1$.

If $|\chi| > 1$, there are two degenerate Hartree-Fock ground states which are obtained from $|0_{\text{HF}}\rangle$ by rotation in opposite directions around the x axis (for $\chi > 1$) or y axis (for $\chi < -1$) by an angle $\varphi = \cos^{-1}(1/|\chi|)$.

The mean field is conveniently defined as

$$\tilde{\sigma}(t) = \frac{1}{N} \langle i | U_\sigma^\dagger(t, T_0) \tilde{J} U_\sigma(t, T_0) | i \rangle \quad (27)$$

which is independent of N if $|i\rangle$ is a Hartree-Fock state. The effective Hamiltonian is

$$H_\sigma = J_x + 2\chi(\sigma_x J_x - \sigma_y J_y) + \tilde{f}(t) \cdot \tilde{J} \equiv \tilde{F}(t) \cdot \tilde{J}. \quad (28)$$

It is easy to show that the mean field evolves through

$$\frac{d}{dt} \tilde{\sigma}(t) = \tilde{F}(t) \times \tilde{\sigma}(t) \quad (29)$$

with the initial condition $\tilde{\sigma}(T_0) = \langle i | \tilde{J} | i \rangle / N$. The final expectation value of the Hamiltonian, Eq. (25), is given by

$$\langle H \rangle_T^{\text{SPA}} = N \{ \sigma_x(T) + \chi [\sigma_x^2(T) - \sigma_y^2(T)] \}, \quad (30)$$

where we have assumed that $\tilde{f}(T) = 0$. Of course, Eqs. (28) and (29) guarantee that Eq. (30) is independent of T when $\tilde{f}(T) = 0$.

We have solved numerically Eqs. (28)–(30) for excitation of the HF ground state by the perturbation $\tilde{f}(t) = \exp(-t^2)(1, 1, 1)$. The figure shows the mean-field approximation for the initial and final expectation values of the energy per particle, $\langle H \rangle / N$, over a range of coupling strength $-0.1 \geq \chi \geq -10$, covering both the weak and strong coupling regions. These results are independent of N . For weak coupling ($\chi \geq -1$) we compare these results with the exact treatment starting from the exact ground state. As can be seen, the agreement is excellent for $N=30$ particles. In the strong coupling region, $\chi < -1$, we consider the following three cases

(1) and (2) The mean-field calculation and the exact treatment starting from both deformed HF

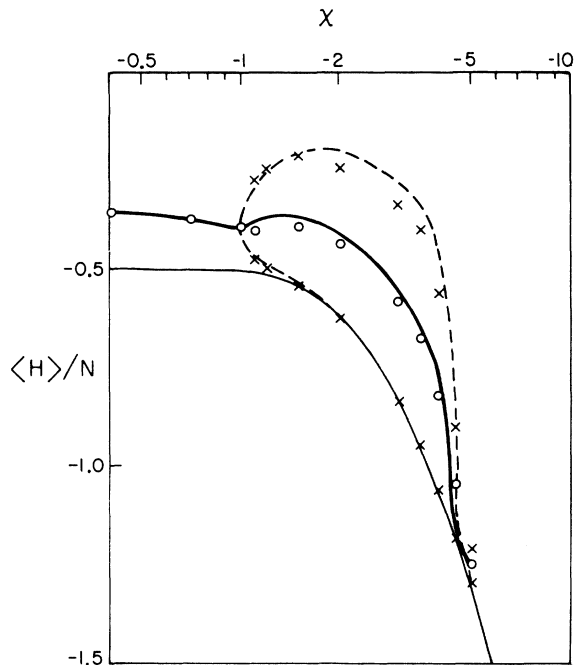


FIG. 1. The expectation value of the final total energy per particle, $\langle H \rangle / N$, of the forced Lipkin model with perturbation $f(t) = e^{-t^2} (1, 1, 1)$. Plotted as functions of the coupling parameter are the results for the following cases: \circ , exact evolution of the exact ground state for $N=30$. \times (in the strong coupling region $\chi < -1$, exact evolution of each of the two deformed HF ground states $|1\rangle$ and $|2\rangle$ for $N=30$. ---, TDHF evolution of each of the above states $|1\rangle$ and $|2\rangle$. —, in the weak coupling region ($-1 < \chi < 0$), TDHF evolution of the HF ground state. In the strong coupling region ($\chi < -1$), TDHF evolution of the symmetrized HF ground state (the average of the two dashed lines). The light solid line describes the HF ground state energy.

ground states $|1\rangle$ and $|2\rangle$. Depending on the orientation of the deformation with respect to the external perturbation the amount of excitation is quite different. Nevertheless, the agreement is within $\sim 10\%$.

(3) The exact evolution of the exact ground state in comparison with the mean-field evolution of the initial state with positive parity, $|+\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$. Here we neglected all matrix elements of the type $\langle 1|2\rangle$ and $\langle 1|U^\dagger H U|2\rangle$, which should be a good approximation (of order $|\chi|^{-N}$)

except in the immediate vicinity of $\chi = -1$. Thus, the mean-field result is the average of cases (1) and (2) above. We find also here, that the mean-field calculation is able to reproduce the exact results quite well. This also holds true in the region $\chi \sim -1$, where fluctuations in σ might have been expected to induce a larger error.

V. CONCLUSIONS

We have obtained expressions for one- and two-body inclusive observables in the framework of the time-dependent mean-field approximation. For excitation by a time-dependent one-body operator, we found that the mean field which defines the stationary point of the full functional integral over auxiliary fields obeys the time-dependent Hartree (-Fock) equations. Expectation values of one- and two-body operators, in particular of the total energy, can be expressed solely in terms of the mean field. For the forced Lipkin model with 30 particles we found excellent agreement between the mean-field expression for the excitation energy and the exact solution, even in the region of coupling parameters where the phase transition to a deformed ground state occurs.

Although we have considered only a schematic model, our results have implications for more realistic situations. This work is the first step toward a rigorous justification of the TDHF method for computing inclusive observables in heavy-ion collisions, although a number of the difficulties discussed in Ref. 2 prevent us from making a direct statement about the full many-body scattering problem. However, it may be plausibly surmised that TDHF is the correct mean-field theory for such one-body observables as fragment changes, masses, angular momenta, and kinetic energies, although the accurate evaluation of the dispersions in these quantities will most likely require consideration of the fluctuations of the field about its mean value.

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