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Time-dependent mean-field approximation for nuclear dynamical problems

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A general method for a microscopic description of nuclear dynamical problems is discussed. The method is based on a functional integral representation for the many-body time evolution operator $U(t_f,t_i)$. In the stationary phase limit, a time-dependent mean-field approximation for the matrix elements of U is obtained. Using standard procedures this allows for extraction of quantum mechanical information about bound states, tunneling, or scattering phenomena in a many-nucleon system. The approximation represents a natural generalization of the time-dependent Hartree-Fock method.

[NUCLEAR STRUCTURE, NUCLEAR REACTIONS derived mean-field approximation for matrix elements of exp(−*iHt*) from exact functional integral; discussed relation to static HF, TDHF, and scattering calculations.]

I. INTRODUCTION

During the last few years, there has been considerable interest in the microscopic description of large-scale nuclear dynamics. Rapidly increasing amounts of experimental data from heavy-ion reactions and nuclear fission provide an almost unique opportunity to study the dynamical behavior of large but *finite* collections of fermions undergoing drastic changes.

Recently the time-dependent mean-field approximation has been proposed as a possible candidate for a microscopic theory of these phenomena. Motivated by the successes of the static Hartree-Fock theory and the random-phase approximation, this theory is based on the fact that the mean free path of a nucleon in nuclear matter is quite long for excitations close to the Fermi level.[1] Up to an average excitation energy of about 10 MeV per nucleon, the Pauli principle is an important factor in inhibiting collisions, and each nucleon feels only the average field of the others.

In the discussion of dynamics, the average field is time-dependent and should be self-consistently determined by all the nucleons. One must, in addition, assume that the rate of change of the mean field is small enough so that it does not produce large excitations in a short time. This condition also leads to a limiting figure in the neighborhood of 10 MeV/nucleon for heavy nuclei.[2]

In practical terms these ideas have been employed in the time-dependent Hartree-Fock (TDHF) approximation.[2-4] As in the stationary case, the total wave function of the system in this approach is constrained to be a Slater determinant, and the time evolution of the single-particle wave functions is determined by a time-dependent least-action variational principle.[4]

The TDHF theory has been explored extensively in a simplified slab geometry,[5] light- and heavy-ion systems,[6-8] induced fission,[9] and analytically solvable models.[10,11] Although the results are very encouraging, the whole approach is subject to serious conceptual and practical problems.[12-14] The common nature of these problems is related to the basic difficulty of finding the unambiguous way to extract quantum mechanical information from the results of time-dependent mean-field calculations.

The present investigation is an attempt to overcome this difficulty. We propose to shift the emphasis from the wave function of the many-nucleon systems to the matrix elements of the corresponding time evolution operator and to find a mean-field type of approximation for their calculation. Having done this, we can use standard procedures to extract the quantum mechanical information about bound states, tunneling, or scattering phenomena in the many-nucleon system.

We start here by presenting general ideas and techniques of the approach in a simple form. In the following paper[15] this form will be generalized and used for the explicit description of large amplitude collective states in nuclei. Later on,[16] a mean-field calculational scheme for tunneling processes will be discussed.

The basis of our approach is provided by the recent development of semi-classical functional integral methods in relativistic field theories

(for a review cf. Ref. 17). The relevance of these methods in nuclear physics is obvious, because in the language of second quantization, the nuclear many-body problem is essentially a nonrelativistic field theory of self-interacting field with quartic interaction and nonlocal coupling.

The fermion nature of this theory implies the use of the so-called anticommuting c number representation[17] when the functional integration over the variables of the field is defined. One way to partially avoid this difficulty is described in Ref. 18. We found it insufficient for our purpose and instead use a conceptually related method based on the Hubbard-Stratonovich transformation.[19,20] This is a simple operator identity (2.8) which allows linearization of the exponential of the square of a bounded operator. The application of this identity to the evolution operator $U(t_f, t_i) = \exp[-(i/\hbar)H(t_f - t_i)]$ of a many-nucleon system having two-body interaction leads to a functional integral representation for $U(t_f, t_i)$. In this representation, the operator $U(t_f, t_i)$ is exactly given by another evolution operator for a system in a one-body potential integrated with a certain weight factor over all possible configurations of this potential. Physically, this representation may be considered as the extraction of an effective boson field which is responsible for a *given* fermion-fermion interaction.

We are interested in calculating matrix elements $\langle f | U(t_f, t_i) | i \rangle$ of the time evolution operator for any given states $|f\rangle$ and $|i\rangle$. In the derived functional integral representation, every such matrix element appears as a coherent sum of matrix elements, each corresponding to motion in a different one-body potential.

This representation is most suitable for the derivation of a mean-field approximation. For this purpose one should retain only that configuration of the one-body potential which gives the most significant contribution to the functional integral. This is the mean-field potential. In practical terms, it is found by using the stationary phase approximation (SPA). The SPA condition defines the equation for the mean field. Obviously the latter *depends* on the matrix element which is calculated.

In the present work we discuss only the lowest order SPA. This means that we approximate the functional integral by the value of its integrand at the mean-field configuration. In general it is possible to derive the complete SPA expansion. However, in practice one can hardly go beyond the first correction to the lowest order result. This includes the small oscillations around the stationary point and will be discussed in (15).

In principle, the derived mean-field expressions for matrix elements $\langle f | U(t_f, t_i) | i \rangle$ can be used to construct the S-matrix mean-field theory of nucleus-nucleus collisions. Our discussion is not limited to any particular form of the initial and final wave functions $|i\rangle$ and $|f\rangle$. However, in a many-nucleon problem one is usually confined to only an approximate knowledge of $|i\rangle$ and $|f\rangle$ in terms of single Slater determinants. As a rule these are found by performing (or assuming to have performed) mean-field calculations for the initial and final states.

Given this limitation one immediately faces a very difficult and well known problem.[12,13,23] The Slater determinant approximation to a wave function gives accurate results only for matrix elements of few-body operators. Can such functions be used to calculate the matrix elements of $U(t_f, t_i)$ which is manifestly an A-body operator? A correct way of handling this problem is by simultaneous mean-field treatment of both the "preparation" of initial and final scattering states and the scattering dynamics. The formalism presented in this work provides a suitable framework for such a treatment.

The organization of this paper is as follows. The functional integral representation for the evolution operator is derived in Sec. II and its formal properties are briefly discussed. Section III is devoted to the stationary phase limit of this representation and the resulting mean-field expressions. The important particular case of the Slater determinant representation and the relation to TDHF and static HF are discussed in Sec. IV. A short summary concludes the paper.

II. FUNCTIONAL INTEGRAL REPRESENTATION FOR THE MANY-BODY EVOLUTION OPERATOR

The A-nucleon system we wish to treat is described by the Hamiltonian

$$H = \sum_{i=1}^{A} K_i + \tfrac{1}{2} \sum_{\substack{i,j \\ i \neq j}} V(x_i - x_j), \tag{2.1}$$

where K is the one-body kinetic energy operator and V is the two-body interaction. We assume here here that V depends only on the relative distances between the nucleons and will later show how to deal with a more general interaction. We shall rewrite (2.1) as

$$H = \sum_{i=1}^{A} K_i - \tfrac{1}{2} V(0) A + \tfrac{1}{2} \int \rho(x) V(x - x') \rho(x') dx\, dx', \tag{2.2}$$

where

$$\rho(x)=\sum_{i=1}^{A}\delta(x-x_i) \tag{2.3}$$

is the density operator and

$$A=\int \rho(x)dx \tag{2.4}$$

is an operator which counts the number of nucleons. It is clear that the term $(\frac{1}{2})V(0)A$ subtracts the self-interaction energy present in the last term of (2.2). We do not consider here problems related to the singular nature of $V(0)$.

We redefine the kinetic energy

$$K'=\sum_{i=1}^{A}K_i', \quad K_i'=K_i-\tfrac{1}{2}V(0)1_i, \tag{2.5}$$

where 1_i is the unit operator for particle i. In the second quantized notation the form (2.2) would correspond to a Hamiltonian with non-normal ordered two-body interaction.

The evolution operator for the system is written in the interaction representation as

$$U(t_f,t_i)=T\exp\left[-\tfrac{1}{2}\int_{t_i}^{t_f}dt\int \rho(x,t)V(x-x')\times\rho(x',t)dx\,dx'\right], \tag{2.6}$$

where T is the time-ordering operator

$$\rho(x,t)=e^{iK't}\rho(x)\,e^{-iK't} \tag{2.7}$$

and we have set $\hbar=1$.

Consider now an auxiliary Hamiltonian

$$h=\sum_{i=1}^{A}K_i'+\sum_{i=1}^{A}W(x_i)=K'+\int \rho(x)W(x)dx,$$

which is obtained from (2.2) replacing the two-body term by an interaction with some external potential $W(x)$. We wish to show how the evolution operator for this auxiliary Hamiltonian can be exactly related to the operator (2.6).

In order to derive this relation, we use the so-called Hubbard-Stratonovich transformation[19,20]

$$e^{\pi\hat{a}^2}=\int_{-\infty}^{\infty}d\chi\,e^{-\pi\chi^2+2\pi\hat{a}\chi} \tag{2.8}$$

which is valid for any bounded operator $\hat{a}$. This simple transformation permits the linearization with respect to ρ of the operator in the exponent (2.6).

We first rewrite (2.6) as

$$U(t_f,t_i)=\lim_{\substack{\Delta t\to 0\\ M\to\infty}} T\prod_{j=1}^{M}\exp\left[-\frac{i}{2}\Delta t\int \rho(x,t_j)V(x-x')\times\rho(x',t_j)dx\,dx'\right], \tag{2.9}$$

where we divided the time interval (t_i,t_f) into $M+1$ equal subintervals of length Δt and took the limit of $\Delta t\to 0$, $M\to\infty$. To each term in the product we apply the functional integral generalization of the transformation (2.8). As shown in Appendix A,

$$\exp\left[-\frac{i}{2}\Delta t\int \rho(x,t_j)V(x-x')\rho(x',t_j)dx\,dx'\right]=\int \tilde{D}[\sigma(x,t_j)]\left\{\exp\left[\frac{i}{2}\Delta t\int \sigma(x,t_j)V(x-x')\sigma(x',t_j)dx\,dx'\right]\times\exp\left[-i\Delta t\int \rho(x,t_j)V(x-x')\sigma(x',t_j)dx\,dx'\right]\right\}. \tag{2.10}$$

The precise definition of $\tilde{D}[\sigma(x,t_j)]$ is given by Eq. (A10).

Using (2.10) in (2.9) and passing to the limit, we arrive at the result

$$U(t_f,t_i)=\int D[\sigma(x,t)]\left\{\exp\left[\frac{i}{2}\int_{t_i}^{t_f}dt\int \sigma(x,t)V(x-x')\times\sigma(x',t)dx\,dx'\right]U_\sigma(t_f,t_i)\right\}, \tag{2.11}$$

with

$$U_\sigma(t_f,t_i)=T\exp\left[-i\int_{t_i}^{t_f}dt\int \rho(x,t)V(x-x')\times\sigma(x',t)dx\,dx'\right]. \tag{2.12}$$

The symbol $D[\sigma(x,t)]$ is naturally defined by the limit of products of $\tilde{D}[\sigma(x,t_j)]$.

The meaning of (2.11) is clear. The quantity $U_\sigma(t_f,t_i)$ is the evolution operator in the interaction representation for the A-nucleon system with Hamiltonian

$$H_\sigma=\sum_{i=1}^{A}K_i'+\int \rho(x)V(x-x')\sigma(x',t)dx'=\sum_{i=1}^{A}[K_i'+W_\sigma(x_i,t)],$$
$$W_\sigma(x,t)=\int V(x-x')\sigma(x',t)dx. \tag{2.13}$$

The nucleons are moving in the *time-dependent* external potential $W_\sigma(x,t)$, which is a linear

functional of the auxiliary field $\sigma(x,t)$. The total evolution operator $U(t_f,t_i)$ is a coherent sum over the auxiliary fields with the weighting factor

$$\exp\left[\frac{i}{2}\int_{t_i}^{t_f} dt \int \sigma(x,t)V(x-x')\sigma(x',t)dx\,dx'\right]. \tag{2.14}$$

To some extent, the procedure of going from (2.6) to (2.11) may be considered as the recovery of the effective *boson* field acting between the nucleons and producing the given two-body interaction in the Hamiltonian (2.2). From this point of view, the free propagator for the σ field is just the inverse of $V(x-x')$, and the nucleons are coupled to the σ field by the nonlocal coupling $V(x-x')$. The absence of time dependence in the boson propagator is obviously related to the static nature of the two-body interaction which is used.

The derivation of (2.11) is easily generalized to include the internal nuclear variables, spin and isospin. The second quantized form of a general two-body interaction is written

$$\sum_{\alpha,\beta,\gamma,\delta}\int dx\,dx'\psi_\alpha^\dagger(x)\psi_\beta^\dagger(x')V_{\alpha\beta\gamma\delta}(x,x')\psi_\delta(x')\psi_\gamma(x). \tag{2.15}$$

The representation (2.11) corresponds to a particular case, where

$$V_{\alpha\beta\gamma\delta}(x,x')=V(x-x')\delta_{\alpha\gamma}\delta_{\beta\delta}$$

and

$$\rho(x)=\sum_\alpha \psi_\alpha^\dagger(x)\psi_\alpha(x).$$

For a more general interaction, one should consider a nondiagonal density operator $\rho_{\alpha\gamma}(x)=\psi_\alpha^\dagger(x)\psi_\gamma(x)$ and introduce a corresponding auxiliary field $\sigma_{\alpha\gamma}(x)$. At this point we remark that the way of introducing the σ field is by no means unique.[19] Different pairings of the field operators $\psi^\dagger$ and ψ in (2.15) lead to different possibilities of introducing the intermediate σ field. All these possibilities are equivalent as far as the exact evolution operator is considered, but may differ significantly in the approximations they suggest. This feature will be discussed in detail in (15). Here we will proceed with the simple form (2.11) in order to make clear the essential ideas and to avoid cumbersome notation.

As a final remark of this section we notice that the introduction of an auxiliary field to linearize the two-body interaction is extensively used in the calculation of statistical operators in solid state physics[21] and generating functionals in quantum field theory.[17,18] Recently pairing modes in a simple soluble nuclear model were treated by a similar technique.[22]

III. MEAN-FIELD APPROXIMATION

The exact relation (2.11) provides a very convenient basis for deriving mean-field approximations for various physical quantities which are of interest in nuclear dynamical problems. Using the time evolution operator, one can construct exact expressions for these quantities. By virtue of (2.11) they are represented in terms of the corresponding quantities of a system in the external potential $W_\sigma(x,t)$, Eq. (2.13), integrated over all possible σ fields. The mean-field expression can then be obtained by retaining only those σ configurations which give the most significant contribution to the integral.

The systematic way of implementing this procedure is provided by the stationary phase method. We will now demonstrate it by calculating the matrix element (transition amplitude) $\langle f|U(t_f,t_i)|i\rangle$ for some given initial and final states.

Using (2.11) we write

$$\langle f|U|i\rangle=\int D[\sigma]\exp[(i/2)(\sigma,V\sigma)]\langle f|U_\sigma|i\rangle$$

$$\equiv\int D[\sigma]\exp(iS_{\rm eff}[\sigma]), \tag{3.1}$$

where we have suppressed the dependence on the time interval. We used in (3.1) the short hand notation

$$(\sigma,V\sigma)=\int_{t_i}^{t_f} dt\int \sigma(x,t)V(x-x')\sigma(x',t)dx\,dx' \tag{3.2}$$

and introduced an effective action of the σ field

$$S_{\rm eff}[\sigma]=\tfrac{1}{2}(\sigma,V\sigma)-i\ln\langle f|U_\sigma|i\rangle. \tag{3.3}$$

This action can be interpreted as describing the dynamics of the σ field and is completely specified by the form of the interaction $V(x-x')$ and given initial and final states.

The stationary phase approximation to the integral (3.1) amounts to solving $\delta S_{\rm eff}[\sigma]=0$, which defines what can be called a classical equation for the σ field. The resulting mean-field expression for the quantum transition amplitude may therefore be viewed as a semiclassical approximation to the many-body problem.

In order to justify this approximation, one should check how fast $S_{\rm eff}$ changes as σ is varied. If $|f\rangle$ and $|i\rangle$ are such that all the nucleons are affected by the transition, it seems reasonable to assume that small changes of the σ field produce large variations in $S_{\rm eff}$ when the number A of nucleons is sufficiently large. One expects therefore that the approximation is valid for the

description of collective dynamical processes in many-nucleon systems. Unfortunately it is very difficult to formulate a more precise quantitative criterion.

The stationary "points" of S_{eff} are found from

$$\delta S_{\text{eff}} = \int_{t_i}^{t_f} dt \int \delta\sigma(x,t)V(x-x')\sigma(x',t)dx\,dx' - i\frac{\delta\langle f|U_\sigma|i\rangle}{\langle f|U_\sigma|i\rangle} = 0 . \tag{3.4}$$

The numerator of the last term is

$$\delta\langle f|U_\sigma|i\rangle = -i\int_{t_i}^{t_f} dt \int \delta\sigma(x,t)V(x-x') \times\langle f|U_\sigma(t_f,t)\rho(x',t)U_\sigma(t,t_i)|i\rangle\,dx\,dx' ,$$

where the appearance of the two operators U_σ in the right-hand side is due to the effect of the time-ordering operator in Eq. (2.12).

The two equations (3.4) and (3.5) lead to the following result for the σ field which satisfies $\delta S_{\text{eff}} = 0$,

$$\sigma(x,t) = \frac{\langle f|U_\sigma(t_f,t)\rho(x,t)U_\sigma(t,t_i)|i\rangle}{\langle f|U_\sigma(t_f,t_i)|i\rangle} = \frac{\langle\Phi_f^{(\sigma)}(t)|\rho(x,t)|\Phi_i^{(\sigma)}(t)\rangle}{\langle\Phi_f^{(\sigma)}(t)|\Phi_i^{(\sigma)}(t)\rangle} , \tag{3.6}$$

where $\rho(x,t)$ is given by (2.7) and we have introduced the following time-dependent wave functions

$$|\Phi_i^{(\sigma)}(t)\rangle = U_\sigma(t,t_i)|i\rangle , \qquad |\Phi_f^{(\sigma)}(t)\rangle = [U_\sigma(t_f,t_i)]^\dagger|f\rangle . \tag{3.7}$$

The field σ appears on both sides of (3.6), which, therefore, represents a functional equation with respect to σ. In general, this equation should be solved self-consistently and we will discuss later how this can be done in particular cases.

Once the solution of Eq. (3.6) for $\sigma(x,t)$ is found, the stationary phase approximation gives the transition amplitude (in the lowest order) as the integrand of (3.1) calculated at this value of $\sigma(x,t)$:

$$\langle f|U|i\rangle \cong \exp[(i/2)(\sigma,V\sigma)]\langle f|U_\sigma|i\rangle = \exp[(i/2)(\sigma,V\sigma)]\langle\Phi_f^{(\sigma)}|\Phi_i^{(\sigma)}\rangle . \tag{3.8}$$

This result corresponds to neglecting second and higher variations of the last term in (3.3). It is clear that $\sigma(x,t)$ and, consequently, the mean-field potential $\int V(x-x')\sigma(x',t)dx'$ depend on both initial and final states $|i\rangle$ and $|f\rangle$. This reflects the general spirit of the present approximation, in which the time-dependent mean field plays an auxiliary role and differs for different physical quantities which are calculated.

If the solution of (3.6) is not unique, one should include the summation over different solutions in Eq. (3.8). As an example of such a situation let us consider the case when the initial and the final wave functions $|i\rangle$ and $|f\rangle$ are eigenfunctions of the total momentum. Then, as shown in Appendix B, any (x-dependent) solution of Eq. (3.6) is not unique, and shifting this solution by an arbitrary vector a produces another solution. This is a usual property of a mean-field approximation which breaks a certain symmetry of the exact Hamiltonian (space translational symmetry in this case). In evaluating the integral (3.1) by SPA, one must sum over all solutions with different values of the shifting vector a, i.e., to integrate over a. We discuss in Appendix B how this results in momentum conservation for the approximate matrix element (3.8). There we also show a similar treatment of time translation invariance and the consequent energy conservation.

The self-consistent σ-field solution of Eq. (3.6) is, in general, not real. This is a direct consequence of our exponentiation of the complex valued quantity $\langle f|U_\sigma|i\rangle$ to obtain the effective action (3.3). In order to avoid this complication one can use instead

$$S_{\text{eff}}[\sigma] = \tfrac{1}{2}(\sigma,V\sigma) + \arg\langle f|U_\sigma|i\rangle = \tfrac{1}{2}(\sigma,V\sigma) - \tfrac{1}{2}i\ln\langle f|U_\sigma|i\rangle + \tfrac{1}{2}i\ln\langle f|U_\sigma|i\rangle^* . \tag{3.9}$$

The integrand of (3.1) is then written as $|\langle f|U_\sigma|i\rangle|\exp iS_{\text{eff}}[\sigma]$, and the SPA is defined by the real phase of this expression. Repeating the steps which led to Eq. (3.6), one obtains in this case

$$\sigma(x,t) = \mathrm{Re}\frac{\langle\Phi_f^{(\sigma)}(t)|\rho(x,t)|\Phi_i^{(\sigma)}(t)\rangle}{\langle\Phi_f^{(\sigma)}(t)|\Phi_i^{(\sigma)}(t)\rangle} , \tag{3.10}$$

and the self-consistent σ field is real.

It is easy to understand the origin of the difference between Eqs. (3.6) and (3.10). It follows from the fact that different parts of the integrand in (3.1) were used to define the stationary phase conditions. In obtaining (3.6), the whole integrand was assumed to oscillate rapidly with the variation of σ whereas the derivation of (3.10) is based on the rapid oscillations of the real part of the phase.

As a final remark, we notice that expression (3.8) represents the lowest order term of an SPA expansion for the transition amplitude $\langle f|U|i\rangle$. In principle, one can derive all higher order terms of this expansion, but in practice, only the first correction is considered. This

correction is related to the second variation $\delta^2 S_{\text{eff}}$ of the effective action (3.3) and will be discussed in (15).

IV. SLATER DETERMINANT REPRESENTATION

We now discuss an important particular case in which the initial and the final states are Slater determinants:

$$|i\rangle = (A!)^{-1/2} \sum_P (-1)^P \prod_{j=1}^A \psi_{Pj}^{(i)}(j), \tag{4.1a}$$

$$|f\rangle = (A!)^{-1/2} \sum_P (-1)^P \prod_{l=1}^A \phi_{Pl}^{(f)}(l), \tag{4.1b}$$

where P stands for all possible permutations. Using the relation (3.1) we write the transition amplitude

$$\langle f|U|i\rangle = \sum_P (-1)^P \int D[\sigma]\{\exp[(i/2)(\sigma, V\sigma)]\} \times \prod_{j=1}^A \langle \phi_j^{(f)}|U_\sigma^{(j)}|\psi_{Pj}^{(i)}\rangle \equiv \sum_P (-1)^P \langle f|U|i\rangle_P . \tag{4.2}$$

Here we used the fact that U_σ in Eq. (3.1) is a product of one-body evolution operators

$$U_\sigma = \prod_{j=1}^A U_\sigma^{(j)} \tag{4.3}$$

commuting between themselves, and is therefore symmetric in nucleon coordinates.

In each term of the sum (4.2), the motion of a single nucleon is correlated to the others through the common σ field. The exclusion principle is taken into account by the usual antisymmetrization *after* the partial transition amplitudes $\langle f|U|i\rangle_p$ are calculated.

In order to evaluate a particular term in Eq. (4.2) we follow (3.9) and construct

$$S_{\text{eff}}[\sigma] = \tfrac{1}{2}(\sigma, V\sigma) - \frac{i}{2}\sum_{j=1}^A (\ln\langle\phi_j^{(f)}|U_\sigma^{(j)}|\psi_{Pj}^{(i)}\rangle - \ln\langle\phi_j^{(f)}|U_\sigma^{(j)}|\psi_{Pj}^{(i)}\rangle^*). \tag{4.4}$$

The solution of $\delta S_{\text{eff}}[\sigma] = 0$ is

$$\sigma(x,t) = \sum_{j=1}^A \text{Re}\frac{\phi_j^{(\sigma)*}(x,t)\psi_{Pj}^{(\sigma)}(x,t)}{\langle\phi_j^{(\sigma)}|\psi_{Pj}^{(\sigma)}\rangle}, \tag{4.5}$$

where

$$|\psi_j^{(\sigma)}(t)\rangle = U_\sigma^{(j)}(t,t_i)|\psi_j^{(i)}\rangle, \tag{4.6a}$$

$$|\phi_j^{(\sigma)}(t)\rangle = [U_\sigma^{(j)}(t_f,t_i)]^\dagger|\phi_j^{(f)}\rangle, \tag{4.6b}$$

in analogy with (3.7).

It is convenient to write the relations (4.5) and (4.6) in a differential form. The functions $\phi_j^{(\sigma)}$ and $\psi_j^{(\sigma)}$ obey the following equations (in the Schrödinger representation):

$$i\frac{\partial\psi_j^{(\sigma)}}{\partial t} = (K + w_\sigma)\psi_j^{(\sigma)}, \tag{4.7a}$$

$$i\frac{\partial\phi_j^{(\sigma)}}{\partial t} = (K + w_\sigma)\phi_j^{(\sigma)}, \tag{4.7b}$$

where

$$K = p^2/2m - (\tfrac{1}{2})V(0), \tag{4.7c}$$

$$w_\sigma(x,t) = \int V(x-x') \times \text{Re}\sum_{l=1}^A \frac{\phi_l^{(\sigma)*}(x',t)\psi_{Pl}^{(\sigma)}(x',t)}{\langle\phi_l^{(\sigma)}|\psi_{Pl}^{(\sigma)}\rangle}dx', \tag{4.7d}$$

and

$$\psi_j^{(\sigma)}(x,t_i) = \psi_j^{(i)}(x), \tag{4.8a}$$

$$\phi_j^{(\sigma)}(x,t_f) = \phi_j^{(f)}(x). \tag{4.8b}$$

The set of equations (4.7) and (4.8) can be solved by the usual self-consistent procedure: Guessing $\sigma(x,t)$, one calculates the mean-field potential

$$W_\sigma(x,t) = \int V(x-x')\sigma(x',t)dx',$$

solves the Eqs. (4.7) subject to (4.8), and constructs an improved $\sigma(x,t)$ by Eq. (4.5). However, at this moment it seems to be premature to apply this scheme in practical calculations of, say, nucleon-nucleon scattering amplitude. One should first resolve the conceptual problems of defining the proper initial and final states which were mentioned in the Introduction.

It is useful to discuss the relation of the present mean-field approach to the conventional TDHF theory. For this purpose, we try to answer the question of how a given initial state $|i\rangle$ develops in time. It is clear that this is equivalent to finding the final wave function which for any $t_f > t_i$ will satisfy $|\langle f|U(t_f,t_i)|i\rangle|^2 = 1$. In terms of the wave functions (3.7) this means

$$|\Phi_f^{(\sigma)}(t)\rangle = U_\sigma(t,t_i)|i\rangle = |\Phi_i^{(\sigma)}(t)\rangle .$$

(We have omitted here an irrelevant time-dependent phase factor.) Under this condition, instead of two wave functions, one has only one which gives the development in time of the state $|i\rangle$.

The set of equations (4.7) and (4.8) reduces in this case to

$$i\frac{\partial\psi_j}{\partial t} = \left(\frac{p^2}{2m} - \tfrac{1}{2}V(0) + \int V(x-x')\sum_{l=1}^A |\psi_l(x',t)|^2 dx'\right)\psi_j, \tag{4.9a}$$

with initial condition

$$\psi_j(x,t)=\psi_j^{(i)}(x)\,. \tag{4.9b}$$

The result exhibits a close similarity to the usual TDHF equation but without the exchange term in the potential. This is often referred to as a Hartree approximation.

The absence of the exchange term in (4.9a) presents a serious difficulty if one tries to apply the present formalism to the nuclear dynamical problems. The origin of this difficulty can be ultimately related to the particular way of pairing the field operators ψ in (2.15) which we have used. It will be shown in (15) how to pair the ψ operators in order to recover the exchange term in the mean-field potential. At the same time it will be possible to eliminate the trivial but unpleasant term $-\frac{1}{2}V(0)$ from Eq. (4.9a).

Finally we consider what happens in the static limit of our formalism. To obtain this limit, we take the final state identical to the initial state and require it to be an eigenstate of the Hamiltonian, i.e.,

$$\langle i|\,U(t_f,t_i)\,|i\rangle=e^{-iE(t_f-t_i)}\,. \tag{4.10}$$

In the Slater determinant representation, we require in addition that the time dependence of the single-particle wave functions is

$$\psi_j^{(\sigma)}(t)=e^{-i\epsilon_j(t-t_i)}\psi_j\,, \tag{4.11a}$$

$$\phi_j^{(\sigma)}(t)=e^{-i\epsilon_j(t-t_f)}\psi_j\,, \tag{4.11b}$$

where ϵ_j plays the role of the single-particle energy, and ψ_j is independent of time and is normalized.

The two sets of Eqs. (4.7a) and (4.7b) again reduce to one:

$$[p^2/2m-(\tfrac{1}{2})V(0)+w_\sigma]\psi_j=\epsilon_j\psi_j\,, \tag{4.12}$$

with

$$w_\sigma(x)=\int V(x-x')\sigma(x')dx' \tag{4.13}$$

and

$$\sigma(x)=\sum_{i=1}^{A}|\psi_i(x)|^2\,. \tag{4.14}$$

As expected, σ is independent of time and is just the single-particle density.

Using the condition (4.10) for the left-hand side of Eq. (4.2) and evaluating the right-hand side by SPA we obtain

$$e^{-iE(t_f-t_i)}=e^{(i/2)(\sigma,V\sigma)}\prod_{j=1}^{A}\langle\phi_j^{(\sigma)}|\psi_j^{(\sigma)}\rangle \tag{4.15}$$

so that

$$E=\sum_{j=1}^{A}\epsilon_j-\tfrac{1}{2}(\sigma,V\sigma)/(t_f-t_i)\,. \tag{4.16}$$

Here we used the explicit form (4.11) for the functions $\psi_j^{(\sigma)}(t)$ and $\phi_j^{(\sigma)}(t)$. It is clear that only the direct term (with $P=1$) is not zero in the sum of Eq. (4.2).

Substituting in (4.16) the expression (4.14) for σ and recalling the definition (3.2) of $(\sigma,V\sigma)$, we obtain for the energy eigenvalue the static Hartree result

$$E=\sum_{j=1}^{A}\epsilon_j-\tfrac{1}{2}\sum_{i,j=1}^{A}\langle i,j|\,V\,|i,j\rangle \tag{4.17}$$

with the usual notation.

V. SUMMARY

In this work, a mean-field approximation for the many-nucleon time evolution operator $U(t_f,t_i)$ has been described. The stationary phase method was used to obtain this approximation from the exact functional integral representation. This emphasizes the semiclassical nature of the mean field.

One of the main advantages of the approach is the possibility to derive a mean-field approximation for a specific physical quantity which one wants to calculate. One should expect to obtain different mean fields and even different mean-field equations for different quantities. This will be demonstrated in the forthcoming publications.

When the matrix elements of U are calculated between the Slater determinant states, one finds the relation to the conventional TDHF and static HF theories, but without the exchange term. This deficiency is not inherent in the present formalism and is in fact remedied by the judicious derivation of the exact functional integral for U.[15]

The presented formalism is particularly suited for the discussion of the nucleus-nucleus S matrix. However, this discussion cannot be completed without proper understanding of how to consistently define the scattering channels in the mean-field theory. This definition should be done simultaneously with the treatment of the scattering dynamics and further research in this direction is required.

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APPENDIX A

Changing the variables in (2.8),

$$\chi = (\lambda \Delta t/2\pi i)^{1/2}\xi , \tag{A1}$$

$$\hat{a} = (\lambda \Delta t/2\pi i)^{1/2}\hat{b} , \tag{A2}$$

where λ is an arbitrary real constant, we transform (2.8) into

$$e^{-(i/2)\lambda \hat{b}^2 \Delta t} = \int_{-\infty}^{\infty} \frac{d\xi}{(2\pi i/\lambda \Delta t)^{1/2}} e^{i\lambda(\xi^2/2 - \hat{b}\xi)\Delta t} . \tag{A3}$$

Consider a product of such expressions

$$\prod_{i=1}^{N} e^{-i/2\lambda_i \hat{b}^2{}_i \Delta t} = \int \prod_{i=1}^{N} \frac{d\xi_i}{(2\pi i/\lambda_i \Delta t)^{1/2}} e^{i\Delta t \lambda_i (\xi_i^2/2 - \hat{b}_i \xi_i)} \tag{A4}$$

with different operators $\hat{b}_i$ and constants λ_i and assume that

$$[\hat{b}_i, \hat{b}_j] = 0 . \tag{A5}$$

This condition is superfluous in the subsequent limit $\Delta t \to 0$. Because of (A5), the product of exponents in (A4) can be replaced by the exponent of the corresponding sum. This sum represents a diagonal quadratic form and our next step is to make it nondiagonal by a transformation to new variables σ_k and d_k.

We have

$$\xi_i = \sum_{k=1}^{N} A_{ik}\sigma_k , \tag{A6}$$

$$\hat{b}_i = \sum_{k=1}^{N} A_{ik}\hat{d}_k , \tag{A7}$$

where $\{A_{ik}\}$ is some orthogonal matrix.

With the definition

$$V_{jk} = \sum_{i=1}^{N} A_{ij}A_{ik}\lambda_i , \tag{A8}$$

it is a matter of simple algebra to transform (A4) into

$$\exp\left[-(i/2)\Delta t \sum_{j,k=1}^{N} V_{jk}\hat{d}_j\hat{d}_k\right] = (\det V)^{1/2} \int \prod_{k=1}^{N} \frac{d\sigma}{(2\pi i/\Delta t)^{1/2}} \exp\left\{i\left[\tfrac{1}{2}\sum_{j,k=1}^{A} V_{jk}(\sigma_j\sigma_k - \sigma_j\hat{d}_k)\right]\Delta t\right\} . \tag{A9}$$

The proof of the relation (2.10) is now clear. We replace σ_j by $\sigma(x_j, t_i)\Delta x_j$, $\hat{d}_j$ by $\rho(x_j, t_i)\Delta x_j$, and V_{jk} by $V(x_j - x_k)$. Passing now to the limit of $N \to \infty$, $\Delta x \to 0$, we get (2.10), where the precise meaning of the right-hand side is given by

$$\lim_{\substack{N\to\infty \\ \Delta x\to 0}} J_N \int \prod_{j=1}^{N} d\sigma(x_j, t_i) \exp\left\{\frac{i}{2}\Delta t \sum_{k,j=1}^{N} V(x_k - x_j)[\sigma(x_k, t_i)\sigma(x_j, t_i) - 2\rho(x_k, t_i)\sigma(x_j, t_i)]\Delta x_k \Delta x_j\right\} \tag{A10}$$

with

$$J_N = \frac{\Pi_{j=1}^{N} \Delta x_j [\det V(x_k - x_j)]^{1/2}}{(2\pi i/\Delta t)^{N/2}} . \tag{A11}$$

APPENDIX B

We first discuss translational invariance and assume that the initial and the final wave functions $|i\rangle$ and $|f\rangle$ are eigenfunctions of the total momentum P:

$$P|i\rangle = P_i|i\rangle , \quad P|f\rangle = P_f|f\rangle . \tag{B1}$$

Suppose now that under these conditions we have found a solution $\sigma(x)$ to Eq. (3.6). Then for an arbitrary vector a, the function $\sigma_a(x) = \sigma(x - a)$ is also a solution of (3.6). Indeed, replacing x by $x - a$ in (3.6) and omitting the dependence on time variables, which is irrelevant for the moment, we get

$$\sigma_a(x) \equiv \sigma(x - a) = \frac{\langle f|D_a D_a^{-1} U_\sigma D_a \rho(x) D_a^{-1} U_\sigma D_a D_a^{-1}|i\rangle}{\langle f|D_a D_a^{-1} U_\sigma D_a D_a^{-1}|i\rangle} , \tag{B2}$$

where we used

$$\rho(x - a) = D_a \rho(x) D_a^{-1} , \tag{B3}$$

$$D_a = \exp(iPa) \quad (\hbar = 1) . \tag{B4}$$

It is a simple matter to show that

$$D_a^{-1} U_\sigma D_a = U_{\sigma_a} . \tag{B5}$$

Now combining (B5) with (B2), and using (B1), we obtain that $\sigma_a(x)$ satisfies

$$\sigma_a(x) = \frac{\langle f|U_{\sigma_a}\rho(x)U_{\sigma_a}|i\rangle}{\langle f|U_{\sigma_a}|i\rangle} , \tag{B6}$$

and is a solution of Eq. (3.6).

Hence, translational invariance implies that

any stationary point σ of the integral (3.1) belongs to a continuous set of stationary points σ_a. The evaluation of (3.1) by SPA requires that the sum is taken over all stationary points. For the set σ_a this means that one should integrate over the vector a, representing thus the transition amplitude by a coherent sum of contributions (3.8) with different $\sigma_a(x)$.

Since $(\sigma, V\sigma)$, Eq. (3.2) is invariant under translations and becuase of (B5) we obtain that the contribution of a solution σ_a equals

$$e^{-i(P_f - P_i)a} \times (\text{contribution with } a = 0)\,. \qquad \text{(B7)}$$

Therefore, the above mentioned integral over a gives the momentum conserving δ function.

Along the same lines, one discusses the time translation invariance and the consequent energy conservation. Let us denote by $A_{fi}(t_f, t_i)$ the approximate expression for the transition matrix element $\langle f | U(t_f, t_i) | i \rangle$. This is given by the right-hand side of (3.8).

Let us consider a time shifted $A_{fi}(t_f + \Delta t; t_i + \Delta t)$ where Δt is any time interval. It is easy to show that if $\sigma(t)$ is a solution of Eq. (3.6) in the interval $t_i \leq t \leq t_f$ then $\sigma_{\Delta t}(t) = \sigma(t - \Delta t)$ is a solution for $t_i + \Delta t < t < t_f + \Delta t$. Once this is done, it follows that

$$A_{fi}(t_f, t_i) = A_{fi}(t_f + \Delta t\,,\ t_i + \Delta t)\,,$$

i.e., A_{fi} depend only on $t_f - t_i$ and

$$\int dt_i dt_f\, e^{i(E_f t_f - E_i t_i)} A_{fi}(t_f - t_i) = \delta(E_f - E_i) \int dT\, e^{iE_f T} A_{fi}(T)\,. \qquad \text{(B8)}$$

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