PHYSICAL REVIEW C VOLUME 24, NUMBER 4 OCTOBER 1981

Path integrals for the nuclear many-body problem

J. P. Blaizot*
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

H. Orland
Service de Physique Theorique, Saclay, 02, 91190 Gif-sur-Yvette, France
(Received 22 December 1980)

We present a general method for constructing path intergrals for the nuclear many-body problem. This method uses continuous and overcomplete sets of vectors in the Hilbert space. The state labels play the role of classical coordinates which are quantized as bosons. The equations of motion for the classical coordinates are obtained by calculating the functional integral in the saddle point approximation. In the particular case where the overcomplete set considered is the set of all Slater determinants, the classical equations of motion are the time-dependent Hartree-Fock equations. The functional integral provides a way of requantizing these classical equations. This quantization involves boson degrees of freedom and is in some cases very similar to the method of boson expansion. It is shown that the functional integral formalism provides a unifying framework to describe various approaches to the nuclear many-body problem.

[NUCLEAR STRUCTURE Functional integrals on continuous overcomplete sets. Time-dependent Hartree and Hartree-Fock theories. Boson representations for fermion systems.]

I. INTRODUCTION

The present work examines the application of path integrals to the nuclear many-body problem. It has been motivated partly by the recent developments in the time-dependent mean field theories which have been applied to the description of large amplitude collective motion or heavy ions reactions.[1-4] One of such theories is the time-dependent Hartree-Fock theory hereafter referred to as TDHF. As is well known, the mean field approximation to the many-body problem leaves out definite effects which are usually interpreted in terms of quantum mechanics. For example the vibrational and rotational modes are not quantized in TDHF. To make connection with quantum spectra, a "requantization" is obviously required. The procedure followed for this requantization is often empirical and mostly unjustified. This originates from the fact that most of the derivations of the time-dependent mean field equations do not allow for a systematic expansion beyond the mean field level. An exception to this criticism is the boson expansion method.[5-7] In this method, the time-dependent mean field equations arise from the replacement of the boson operators by c numbers. Moreover, and this is a major point, it can be shown that the boson expansion retrieves exactly the original many-body problem of interacting fermions. In other words boson expansions provide an exact quantization scheme for the time-dependent mean field equations.

Path integrals provide other possible quantization schemes. The standard procedure is to calculate first the functional integral using the saddle-point approximation. This provides the "classical" approximation of the theory. Knowing the classical solution, one can get a semiclassical expression for the transition amplitudes and apply a generalization of the Wentzel-Kramers-Brillouin (WKB) method to quantize periodic motions. Further quantum effects are recovered by calculating the successive corrections to the saddle-point approximation. In the calculation of these corrections, boson degrees of freedom appear naturally. Actually, as we shall see, the boson expansion method is closely related to the quantization through path integrals.

Path integrals have been extensively used in many different areas of physics, in particular in quantum field theory and statistical mechanics. As is well known they are mathematically ill-defined objects and some of the manipulations one usually performs on ordinary integrals are not necessarily allowed, since they may lead to completely erroneous results. This is an important point which must always be kept in mind. To circumvent part of the mathematical difficulties associated with the definition of the functional integral, one usually identifies the functional integral with the formal perturbation expansion. All the manipulations on the integral which can be interpreted as manipulations on the perturbation expansion are then allowed. Other manipulations should be examined with great care. This does not imply that the use of the functional integral is restricted to perturbative approximations. It only guarantees that the properties of the integral are identical to those of the perturbation expansion.

In this paper, we discuss a general method for constructing path integrals for the nuclear many-body problem. This method, due to Klauder,[8,9] makes use of continuous and overcomplete sets of vectors of the Hilbert space. Among those, coherent states or generalized coherent states are particularly important sets. Thus the vectors of the Hilbert space are parametrized by a set of complex numbers which play the role of classical coordinates in a generalized phase space. According to the choice of the overcomplete set, different "classical approximations" are generated from the functional integral. In the present context one should remember that the word classical does not imply that something is small compared to $\hbar$. For example, choosing the set of all the vectors in the Hilbert space as the overcomplete set, one gets as the classical approximation to the Schrödinger equation, the Schrödinger equation itself. This is certainly an extreme case and most of the interesting approximations leave out genuine quantum effects. One of the purposes of the present work is to analyze these effects in the case of the time-dependent mean field approximations.

Functional integrals have been used recently in nuclear physics by several authors.[10–15] It will be seen that all the methods used by these authors are actually particular cases of the general method presented here which has much more flexibility.

This work is organized as follows. In Sec. II of this paper we discuss the properties of some overcomplete sets which are relevant to the discussion of the nuclear many-body problem. In Sec. III we construct the functional integral. Several specific forms of the functional integral are explicitly given. In Sec. IV we discuss the link between the path integral and the formal perturbation expansion. We analyze the difficulties associated with the quantization of the time-dependent Hartree-Fock theory.

In Sec. V, we analyze the successive corrections to the mean field approximation and discuss the physical nature of the quantum effects which are left out in this approximation. We also briefly discuss the connection between path integrals and the boson expansion methods. Section VI summarizes the conclusions. Let us finally mention that a partial account of this work can be found in Refs. 16–19.

II. OVERCOMPLETE SETS

Let $\{ |\psi(z)\rangle \}$ be an overcomplete set of vectors in the Hilbert space $\mathscr{H}$, depending upon a family of parameters which we denote collectively by z. We shall call the parameters z classical coordinates, and the space of variations of z the generalized phase space. The justification for this will appear in Sec. III. The overcompleteness means that any vector of $\mathscr{H}$ can be expanded on the states $|\psi(z)\rangle$ and that the states $|\psi(z)\rangle$ are linearly dependent. We assume that the parameters z vary continuously and that there exists a measure $\mu(z)$ on the space where z is defined, such that

$$\int d\mu(z)\, |z\rangle\langle z| = 1 \ , \tag{2.1}$$

where 1 denotes the unit operator in $\mathscr{H}$. In (2.1) as well as in the following, we use the abridged notation $|z\rangle$ for the state $|\psi(z)\rangle$. We give below examples of overcomplete sets which are useful in our discussion.

A. Coherent states of the harmonic oscillator

This is a well known and typical example of an overcomplete set. We recall briefly its properties. The coherent states are thus defined:

$$|z\rangle = e^{zc^\dagger}|0\rangle = \sum_n \frac{z^n}{\sqrt{n}\,!}|n\rangle \ , \tag{2.2}$$

where $|0\rangle$ is the oscillator ground state and $|n\rangle$ the state with n quanta. $c^\dagger$ is the raising operator. The closure relation is written in terms of the states

$|z\rangle$ using Bargman's measure[20]:

$$\int \frac{dz\,dz^*}{2\pi i} e^{-z^*z} |z\rangle\langle z| = 1 \ , \tag{2.3}$$

where

$$\frac{dz\,dz^*}{2\pi i} = \frac{d\mathrm{Re}z\,d\mathrm{Im}z}{\pi}$$

and the integration is carried over the whole complex plane. The overlap of two coherent states is given by

$$\langle z|z'\rangle = e^{z^*z'} \ . \tag{2.4}$$

The coherent state $|z\rangle$ is an eigenstate of the lowering operator c with eigenvalue z,

$$c|z\rangle = z|z\rangle \ . \tag{2.5a}$$

The matrix element of an operator $A(c^\dagger,c)$, in which the operators $c^\dagger$ and c are written in normal order (the $c^\dagger$ on the left of the c's) is therefore given by

$$\langle z|A(c^\dagger,c)|z'\rangle = e^{z^*z'} A(z^*,z') \ . \tag{2.5b}$$

B. Bosons coherent states

Let us consider the boson Fock space generated by the repeated action of the creation operators $c_\alpha^\dagger$ on the vacuum $|0\rangle$, the index α running over a complete set of single particle states. The operators $c_\alpha^\dagger$ and their Hermitian conjugates c_α obey boson commutation rules

$$[c_\alpha,c_\beta] = 0, \ [c_\alpha^\dagger,c_\beta^\dagger] = 0, \ [c_\alpha,c_\beta^\dagger] = \delta_{\alpha\beta} \ . \tag{2.6}$$

Boson coherent states are defined by

$$|Z\rangle = \exp\left[\sum_\alpha z_\alpha c_\alpha^\dagger\right]|0\rangle \ . \tag{2.7}$$

The properties of these coherent states generalize those of the preceding section. The closure relation in Fock space can be written

$$\int \prod_\alpha \frac{dz_\alpha^*\,dz_\alpha}{2\pi i} \exp\left[-\sum_\alpha z_\alpha^* z_\alpha\right]|Z\rangle\langle Z| = 1 \ . \tag{2.8}$$

The state (2.7) is an eigenstate of the destruction operator c_α with the eigenvalue z_α

$$c_\alpha|Z\rangle = z_\alpha|Z\rangle \ . \tag{2.9}$$

The overlap of two coherent states (2.7) is,

$$\langle Z|Z'\rangle = \exp\left[\sum_\alpha z_\alpha^* z_\alpha'\right] \ . \tag{2.10}$$

Therefore the matrix element of a normal ordered operator $A(c^\dagger,c)$ is

$$\langle Z|A(c^\dagger,c)|Z'\rangle = A(Z^*,Z')\exp\left[\sum_\alpha z_\alpha^* z_\alpha'\right] \ . \tag{2.11}$$

C. Fermions coherent states

The coherent states of fermions are defined by analogy with the coherent states of boson.[21] Let $a_\alpha^\dagger$, a_α be the fermion creation and destruction operators. They satisfy the anticommutation relations

$$[a_\alpha,a_\beta]_+ = 0, \ [a_\alpha^\dagger,a_\beta^\dagger]_+ = 0, \ [a_\alpha,a_\beta^\dagger]_+ = \delta_{\alpha\beta} \tag{2.12}$$

Let us consider the state

$$|Z\rangle = \exp\left[\sum_\alpha z_\alpha a_\alpha^\dagger\right]|0\rangle \ , \tag{2.13}$$

where $|0\rangle$ is the vacuum of the fermion Fock space. Since ${a_\alpha}^2 = 0$, $|z\rangle$ can be an eigenstate of a_α only if ${z_\alpha}^2 = 0$. This can be realized using anticommuting Grassman variables. The rules for calculating with these objects have been widely discussed in the literature. All the formulas of Sec. (II B) hold for the fermion coherent states, provided z is understood as a Grassman variable. Note that fermion coherent states do not belong to the Fock space. However, they allow for a decomposition of the identity in Fock space

$$\int \prod_\alpha dz_\alpha^*\,dz_\alpha \exp\left[-\sum_\alpha z_\alpha^* z_\alpha\right]|Z\rangle\langle Z| = 1 \ . \tag{2.14}$$

D. Boson representation for fermions

Fermion states are usually represented by vectors of a fermion Fock space, constructed from a com-

plete set of single particle states $\{ |\alpha\rangle \}$. It is also possible to represent fermion states as vectors belonging to a subspace (called the physical subspace) of a large boson Fock space. We consider in this section the representation which has been described in Ref. 17, and which is a generalization of that introduced in Ref. 7.

To construct the boson image of an N-fermion state, we consider a large space G, product of N boson Fock spaces B_i, associated with each of the particles i

$$G = \mathscr{B}_1 \otimes \mathscr{B}_2 \otimes \cdots \otimes \mathscr{B}_N \ . \tag{2.15}$$

We call $C_i^\dagger(\alpha)$, $C_i(\alpha)$ the creation and annihilation operators acting in $\mathscr{B}_i$. These operators satisfy the commutation relations

$$\begin{aligned} &[C_i(\alpha),C_j^\dagger(\beta)] = \delta_{ij}\delta_{\alpha\beta} \ , \\ &[C_i(\alpha),C_j(\beta)] = [C_i^\dagger(\alpha),C_j^\dagger(\beta)] = 0 \ . \end{aligned} \tag{2.16}$$

The following states

$$|\psi\rangle = \sum_P (-)^p C_1^\dagger(\alpha_{P_1})...C_N^\dagger(\alpha_{P_N})|0\rangle_B \ , \tag{2.17}$$

where $\sum_P$ is a sum over all the possible permutations of the indices $\alpha_1...\alpha_N$, and $|0\rangle_B$ is the boson vacuum, are in one-to-one correspondence with the N-fermion states of the fermion Fock space. They span the physical subspace. They are characterized by two properties. There is one and only one particle per subspace $\mathscr{B}_i$,

$$\sum_\alpha C_i^\dagger(\alpha)C_i(\alpha)|\psi\rangle = |\psi\rangle \quad (i = 1, \ldots, N) \ . \tag{2.18}$$

The state changes sign in any transposition of the particle indices. The operator which realizes such a transposition is

$$\begin{aligned} P_{ij} &= \sum_{\alpha\beta} C_i^\dagger(\alpha)C_j^\dagger(\beta)C_j(\alpha)C_i(\beta) \\ &= -\sum_\alpha C_i^\dagger(\alpha)C_i(\alpha) \\ &\quad + \sum_\alpha C_i^\dagger(\alpha)C_j(\alpha)\sum_\beta C_j^\dagger(\beta)C_i(\beta) \ . \end{aligned} \tag{2.19}$$

In view of Eqs. (2.18) and (2.19), the condition

$$P_{ij}|\psi\rangle = -|\psi\rangle \tag{2.20}$$

is equivalent to the condition

$$\sum_\alpha C_i^\dagger(\alpha)C_j(\alpha)|\psi\rangle = 0 \quad (i \neq j) \ . \tag{2.21}$$

Thus the states of the physical subspace are characterized by the following set of equations

$$\sum_\alpha C_i^\dagger(\alpha)C_j(\alpha)|\psi\rangle = \delta_{ij}|\psi\rangle \begin{bmatrix} i = 1, \ldots, N \\ j = 1, \ldots, N \end{bmatrix} \ . \tag{2.22}$$

The operators $d_{ij} = \sum_\alpha C_i^\dagger(\alpha)C_j(\alpha)$ satisfy the U(N) algebra,

$$[d_{ij},d_{kl}] = d_{il}\delta_{jk} - d_{kj}\delta_{li} \ . \tag{2.23}$$

They are the generators of the transformation which mixes the various components of a state vector in G. These operators can be used to construct explicitly a projector onto the physical subspace

$$P = \int \prod_{i,j} dA_{ij} e^{-i\,\mathrm{Tr}A} \exp\left[i \sum_{ij} A_{ij}d_{ij} \right] \ , \tag{2.24}$$

where the matrix A may be chosen to be a real matrix and the integration carried from $-\pi$ to π. Other forms are of course possible for P. The Hamiltonian in G takes the following form

$$\begin{aligned} H_B &= \sum_{i=1}^N \sum_{\alpha\beta} T_{\alpha\beta}C_i^\dagger(\alpha)C_i(\beta) \\ &\quad + \tfrac{1}{2}\sum_{i,j}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta)C_i^\dagger(\alpha)C_j^\dagger(\beta)C_j(\delta)C_i(\gamma) \end{aligned} \tag{2.25}$$

where $(\alpha\beta|V|\gamma\delta)$ denotes the nonantisymmetrized matrix element of the two-body interaction V. It is easily verified that H_B has the same matrix element within the physical subspace as the Hamiltonian

$$H = \sum_{\alpha\beta} T_{\alpha\beta}a_\alpha^\dagger a_\beta + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta)a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \tag{2.26}$$

has in the Fermion Fock space. It is also easily checked that H_B commutes with the projector P given by (2.24), that is, H_B has no matrix elements between physical and unphysical states. This follows from the fact that physical and unphysical states belong to different representations of the unitary group, and H_B commutes with the generators d_{ij}.

The closure relation in G is conveniently written

with the help of the coherent states:

$$|Z\rangle = \exp\left[\sum_{k=1}^{N}\sum_{\alpha} Z_k(\alpha)C_k^\dagger(\alpha)\right]|0\rangle_B \ , \tag{2.27a}$$

where the index α runs over all the single particle states and $|0\rangle_B$ is the boson vacuum. We shall also use continuous representation with the notation

$$|\varphi\rangle = \exp\left[\sum_{k=1}^{N}\int dx\, \varphi_k(x)\psi_k^\dagger(x)\right]|0\rangle_B \ . \tag{2.27b}$$

The closure relation in G reads [see Eq. (2.8)]

$$\begin{aligned} 1_G &= \int \prod_{k=1}^{N}\prod_{\alpha}\frac{dZ_k^*(\alpha)dZ_k(\alpha)}{2\pi i} \\ &\quad\times \exp\left[-\sum_k (Z_k\,|\,Z_k)\right]|Z\rangle\langle Z| \\ &= \int \prod_{k=1}^{N}\prod_{x}\frac{d\varphi_k^*(x)d\varphi_k(x)}{2\pi i} \\ &\quad\times \exp\left[-\sum_k (\varphi_k\,|\,\varphi_k)\right]|\varphi\rangle\langle\varphi| \ , \end{aligned} \tag{2.28}$$

where we have used the abridged notations

$$(Z_k\,|\,Z_k) = \sum_{\alpha} Z_k^*(\alpha)Z_k(\alpha) \ , \tag{2.29}$$

$$(\varphi_k\,|\,\varphi_k) = \int dx\, \varphi_k^*(x)\varphi_k(x) \ .$$

The closure relation (2.28) induces a closure relation in the physical subspace of G, obtained by applying the projector P onto the physical subspace on both sides of (2.28),

$$\begin{aligned} P = \int \prod_{k=1}^{N}\prod_{\alpha}\frac{dZ_k^*(\alpha)dZ_k(\alpha)}{2\pi i} \\ \times \exp\left[-\sum_k (Z_k\,|\,Z_k)\right]P\,|\,Z\rangle\langle Z\,|\,P \ . \end{aligned} \tag{2.30}$$

Now we note that

$$P\,|\,Z\rangle = \det[Z_k(\alpha_i)]C_1^\dagger(\alpha_1)\cdots C_N^\dagger(\alpha_N)|0\rangle \ . \tag{2.31}$$

Thus, in a scale transformation

$$Z(\alpha) = \Lambda Z'(\alpha), \tag{2.32}$$

$P\,|\,Z\rangle$ scales as $\det\Lambda$. This property can be verified using the explicit form of P given by Eq. (2.26). One has indeed

$$P\,|\,\Lambda Z\rangle = \int d\mu(Z')\,|\,Z'\rangle\langle Z'\,|\,P\,|\,\Lambda Z\rangle \tag{2.33}$$

and

$$\langle Z'\,|\,P\,|\,\Lambda Z\rangle = \int dA e^{-i\,\mathrm{Tr}A}\prod_{\alpha} e^{Z'^\dagger(e^{iA}\Lambda)Z} \ , \tag{2.34}$$

where we have used the property

$$e^{C_k^\dagger A_{kl}C_l} = :e^{(e^A-1)_{kl}C_k^\dagger C_l}: \ . \tag{2.35}$$

Changing the integration variable A into A-$i\ln\Lambda$ and using the property $\det\Lambda = \exp\mathrm{tr}\ln\Lambda$, one obtains the desired equation

$$P\,|\,\Lambda Z\rangle = (\det\Lambda)P\,|\,Z\rangle \ . \tag{2.36}$$

Equation (2.30) may then be written as follows

$$\begin{aligned} P = \int \prod_{k=1}^{N}\prod_{\alpha}\frac{dZ_k^*(\alpha)\,dZ_k(\alpha)}{2\pi i} \\ \times \int d\Lambda \prod_{k,l}\delta[\Lambda_{kl} - (Z_k^*\,|\,Z_l)] \\ \times e^{-\mathrm{Tr}\Lambda}P\,|\,Z\rangle\langle Z\,|\,P \ , \end{aligned} \tag{2.37}$$

where the integration over Λ runs over all the positive definite Hermitian matrices. Making the change of variable

$$Z(\alpha) = \Lambda^{1/2}Z'(\alpha), \ \ Z^*(\alpha) = Z'^*(\alpha)\tilde{\Lambda}^{1/2} \ , \tag{2.38}$$

where $\tilde{\Lambda}$ denotes the transpose of the matrix Λ one gets

$$\begin{aligned} P = \left[\int d\Lambda(\det\Lambda)^n e^{-\mathrm{Tr}\Lambda}\right] \\ \times \int \prod_{k=1}^{N}\prod_{\alpha}\frac{dZ_k'^*(\alpha)dZ_k'(\alpha)}{2\pi i} \\ \times \prod_{l=1}^{N}\delta[(Z_k'\,|\,Z_l') - \delta_{kl}] \\ \times P\,|\,Z'\rangle\langle Z'\,|\,P \ , \end{aligned} \tag{2.39}$$

where n is the total number of single particle states. The integral over Λ is just a normalization constant

. I'. We thus arrive at the result

$$P=\mathcal{N}\int\prod_{k=1}^{N}\prod_{\alpha}\frac{dZ_k^*(\alpha)dZ_k(\alpha)}{2\pi i}\prod_{l=1}^{N}\delta[(Z_k\mid Z_l)-\delta_{kl}]P\mid Z\rangle\langle Z\mid P\ . \tag{2.40}$$

This result will be rederived in a different way in the next section.

E. Independent particle states

In this section we consider the overcomplete set formed by all the Slater determinants describing systems with a fixed number of particles N. This set can be parametrized in many ways. We give below some parametrizations which are useful in practice, together with the corresponding closure relations. The derivations are reported in the Appendix.

Let $\mid\phi_0\rangle$ be a particular Slater determinant. $\mid\phi_0\rangle$ is composed of N orthonormalized single particle orbitals, which we call "hole" states,

$$\mid\phi_0\rangle=\prod_h a_h^\dagger\mid 0\rangle\ . \tag{2.41}$$

We call "particle" states the states such that

$$a_p\mid\phi_0\rangle=0\ . \tag{2.42}$$

We assume that the number of single particle states is finite. We call n_h the number of hole states and n_p the number of particle states. It is known that any Slater determinant nonorthogonal to $\mid\phi_0\rangle$ can be written[22]

$$\mid Z\rangle=\exp\sum_{ph}(Z_{ph}a_p^\dagger a_h)\mid\phi_0\rangle\ . \tag{2.43}$$

The states (2.43) are not normalized. The overlap between two of them is

$$\langle Z\mid Z'\rangle=\det(1+Z^\dagger Z')\ , \tag{2.44}$$

where Z denotes the complex $n_p\times n_h$ matrix made out of the Z_{ph} amplitudes. In terms of the states (2.43) the closure relation in the Hilbert space of N-fermions states takes the following form (see the Appendix),

$$\int\prod_{ph}\frac{dZ_{ph}^*\,dZ_{ph}}{2\pi i}[\det(1+Z^\dagger Z)]^{-(n_p+n_{h+1})}\times\mid Z\rangle\langle Z\mid=1\ . \tag{2.45}$$

Using Wick's theorem one can express the matrix elements of any operator between two states Z and Z' in terms of the one-body density matrix defined thus

$$\rho_{\beta\alpha}(Z^\dagger,Z')=\frac{\langle Z\mid a_\alpha^\dagger a_\beta\mid Z'\rangle}{\langle Z\mid Z'\rangle}\ . \tag{2.46}$$

Thus, for example, one has

$$\frac{\langle Z\mid a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta\mid Z'\rangle}{\langle Z\mid Z'\rangle}=\rho_{\delta\alpha}(Z^\dagger,Z')\rho_{\gamma\beta}(Z^\dagger,Z')-\rho_{\delta\beta}(Z^\dagger,Z')\rho_{\gamma\alpha}(Z^\dagger,Z') \tag{2.47}$$

The matrix elements $\rho_{\alpha\beta}(Z^\dagger,Z')$ have the following expressions[6]

$$\begin{aligned}\rho_{ph}&=[Z'(1+Z^\dagger Z')^{-1}]_{ph}\ ,\\ \rho_{hp}&=[(1+Z^\dagger Z')^{-1}Z^\dagger]_{hp}\ ,\\ \rho_{pp'}&=[Z'(1+Z^\dagger Z')^{-1}Z^\dagger]_{pp'}\ ,\\ \rho_{hh'}&=[(1+Z^\dagger Z')^{-1}]_{hh'}\ .\end{aligned} \tag{2.48}$$

Performing the change of variable,

$$\beta_{ph}=Z_{ph'}[(1+Z^\dagger Z)^{-1/2}]_{h'h}\ , \tag{2.49}$$

one can simplify (2.45). In the variables β, the closure relation takes the form

$$\int\prod_{ph}\frac{d\beta_{ph}^*\,d\beta_{ph}}{2\pi i}\mid\tilde{\beta}\rangle\langle\tilde{\beta}\mid=1\ , \tag{2.50}$$

where the states $\mid\tilde{\beta}\rangle$ are obtained from (2.43) by expressing Z in terms of β and normalizing. This parametrization has been used in works on boson expansions.[5] The density matrix elements have the following expressions in terms of the β's

$$\begin{aligned}\rho_{\alpha\beta}&=\langle\tilde{\beta}\mid a_\beta^\dagger a_\alpha\mid\tilde{\beta}\rangle\ ,\\ \rho_{ph}&=[\beta(1-\beta^\dagger\beta)^{1/2}]_{ph},\quad \rho_{hp}=\rho_{ph}^*\ ,\\ \rho_{pp'}&=(\beta\beta^\dagger)_{pp'}\ ,\\ \rho_{hh'}&=\delta_{hh'}-(\beta^\dagger\beta)_{hh'}\ .\end{aligned} \tag{2.51}$$

Note that the measure in (2.50) is extremely simple. This results from the fact that the β_{ph} are the coefficients of the unitary transformation which carries $\mid\phi_0\rangle$ into the state $\mid\tilde{\beta}\rangle$. The domain of integration is complicated, however, since the matrix β must

satisfy

$$1-\beta^{\dagger}\beta\rangle 0 \ , \tag{2.52}$$

while in the parametrization (2.43) the parameters Z_{ph} vary over the whole complex plane. Note also that the expression of the density matrix (2.48) is formally the same, whether Z' differs from Z or not. The density matrix (2.51) has a simple expression only if the bra and the ket in (2.51) are Hermitian conjugates of one another.

Using a further change of variable, one arrives at a parametrization in which the coordinates are the single particle wave functions which build up the determinant. The closure relation can be written (see Appendix), with respect to a normalization constant,

$$\int \prod_{k=1}^{N}\prod_{x}\frac{d\varphi_k^*(x)d\varphi_k(x)}{2\pi i}\prod_{l=1}^{N}\delta[(\varphi_k\,|\,\varphi_l)-\delta_{kl}] \times |\varphi\rangle\langle\varphi| \sim 1 \ , \tag{2.53}$$

which is identical to the relation (2.40).

III. PATH INTEGRALS

In this section we give functional integral representations for the matrix elements of the evolution operator e^{-iHt} between some initial state $|Z_i\rangle$ and some final state $\langle Z_f|$,

$$\langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle \ , \tag{3.1}$$

where $|Z_f\rangle$ and $|Z_i\rangle$ belong to the class of states described in the previous section. The general procedure for constructing path integrals is quite standard. First one factorizes the operator $e^{-iH(t_f-t_i)}$ into N terms $e^{-i\epsilon H}$, where $\epsilon=(t_f-t_i)/N$. Then one inserts the closure relation (2.1) between each of the factors and gets

$$\langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle=\int\prod_{k=1}^{N}d\mu(Z_k)\langle Z_f|Z_N\rangle\langle Z_N|e^{-i\epsilon H}|Z_{n-1}\rangle\cdots\langle Z_{k+1}|e^{-i\epsilon H}|Z_k\rangle\cdots\langle Z_1|e^{-i\epsilon H}|Z_i\rangle. \tag{3.2}$$

In the limit $N\to\infty$, $\epsilon\to 0$ and

$$\frac{\langle Z_{k+1}|e^{-i\epsilon H}|Z_k\rangle}{\langle Z_{k+1}|Z_k\rangle}=\exp\left[-i\epsilon\frac{\langle Z_{k+1}|H|Z_k\rangle}{\langle Z_{k+1}|Z_k\rangle}\right]+0(\epsilon^2) \ . \tag{3.3}$$

One then arrives at

$$\langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle=\lim_{N\to\infty}\int\prod_{k=1}^{N}d\mu(Z_k)\prod_{k=0}^{N}\langle Z_{k+1}|Z_k\rangle\exp\left[-i\epsilon\sum_{k=0}^{N-1}\frac{\langle Z_{k+1}|H|Z_k\rangle}{\langle Z_{k+1}|Z_k\rangle}\right] \ , \tag{3.4}$$

where $|Z_0\rangle\equiv|Z_i\rangle$ and $\langle Z_{N+1}|\equiv\langle Z_f|$. One defines

$$|\delta Z_{k+1}\rangle=|Z_{k+1}\rangle-|Z_k\rangle \ , \tag{3.5}$$

so that (3.3) may be rewritten as follows:

$$\langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle=\lim_{N\to\infty}\int\prod_{k=1}^{N}[d\mu(Z_k)\langle Z_k|Z_k\rangle]\langle Z_f|Z_N\rangle \times\exp\left\{\sum_{k=1}^{N}\left[\ln\left[1-\frac{\langle Z_k|\delta Z_k\rangle}{\langle Z_k|Z_k\rangle}\right]-i\epsilon\frac{\langle Z_k|H|Z_{k-1}\rangle}{\langle Z_k|Z_{k-1}\rangle}\right]\right\} . \tag{3.6}$$

A further simplification is achieved if one admits that the major contribution to the integral comes from those "paths" for which $|\delta Z_k\rangle$ is of order ϵ for almost all k, that is, assuming that only piecewise continuous paths contribute in (3.6). Setting $d|Z\rangle/dt=|\delta Z\rangle/\epsilon$ and keeping only lowest order terms in ϵ, one finally ends up with the continuous expression

$$\langle Z_f | e^{-iH(t_f-t_i)} | Z_i \rangle = \int_{\substack{\langle Z(t_f)| = \langle Z_f| \\ |Z(t_i)\rangle = |Z_i\rangle}} \mathscr{D}(Z^*(t),Z(t)) e^{iS[Z^*,Z]} , \tag{3.7}$$

where the action S is given by

$$S[Z^*,Z] = \int_{t_i}^{t_f} dt \frac{\langle Z(t) | i\partial_t - H | Z(t)\rangle}{\langle Z(t) | Z(t)\rangle} - i \ln\langle Z_f | Z(t_f)\rangle , \tag{3.8}$$

and the integration measure is

$$\mathscr{D}(Z^*,Z) = \prod_{t_i<t<t_f} d\mu[Z^*(t),Z(t)]\langle Z(t) | Z(t)\rangle . \tag{3.9}$$

The integration in (3.7) is carried over all the paths $\langle Z(t)|$ and $|Z(t)\rangle$ in the overcomplete set, subject to the boundary conditions

$$|Z(t_i)\rangle = |Z_i\rangle, \quad \langle Z(t_f)| = \langle Z_f| . \tag{3.10}$$

Note that in this formulation $\langle Z(t)|$ and $|Z(t)\rangle$ have to be considered as independent variables, e.g., there are no constraints on $|Z(t_f)\rangle$ and $\langle Z(t_i)|$. It is important to keep this point in mind when applying the saddle-point approximation. (See Sec. V and Refs. 9 and 23.)

The action (3.8) may be given a more symmetrical form with respect to the boundary conditions by an integration by parts

$$S[Z^*,Z] = \int_{t_i}^{t_f} dt \frac{\langle Z(t) | i\overleftrightarrow{\partial}_t - H | Z(t)\rangle}{\langle Z(t) | Z(t)\rangle} - \frac{i}{2} \ln\langle Z(t_i) | Z_i\rangle\langle Z_f | Z(t_f)\rangle , \tag{3.8'}$$

where we have used the notation

$$\langle Z(t) | \overleftrightarrow{\partial}_t | Z(t)\rangle = \tfrac{1}{2}\left[\left\langle Z(t)\middle|\frac{dZ}{dt}\right\rangle - \left\langle\frac{dZ}{dt}\middle|Z\right\rangle\right] .$$

It is worth emphasizing that the expression (3.7) has gotten no rigorous mathematical meaning from its derivation. This is known to lead to difficulties when some "unallowed" manipulations are performed on the functional integral. An example of such difficulties will be encountered in Sec. IV.

We examine now various explicit forms of the functional integral (3.8) obtained with some of the overcomplete sets described in Sec. II.

Let us first consider the form of the functional integral obtained when one uses coherent states as an overcomplete set. Due to the special form of the overlap (2.10), the integration measure simplifies into

$$\mathscr{D}(Z^*,Z) = \prod_t \frac{dZ^*(t)dZ(t)}{2\pi i} . \tag{3.11}$$

The action reads

$$S[Z^*,Z] = \int_{t_i}^{t_f} dt \left\{ \frac{i}{2}(Z^*\dot{Z} - \dot{Z}^*Z) - H(Z^*,Z) - \frac{i}{2}[Z_f^*Z(t_f) + Z^*(t_i)Z_i] \right\} , \tag{3.12}$$

where $H(Z^*,Z)$ is the normal form of the second quantized Hamiltonian, with the creation and annihilation operators $a^\dagger$ and a replaced by Z^* and Z, respectively. The formulas above hold for bosons and fermions. In the latter case, the variable Z has to be understood as a Grassman variable. This formulation has been used in Refs. 11 and 13. The formulas (3.11) and (3.12) hold also for the coherent states (2.27) described in Sec. II D. However, in this latter case, special attention must be given to the boundary conditions. Indeed, one is not interested in the matrix element of the evolution operator between two coherent states (2.27), but rather in this matrix element between two physical states. Let $|\phi\rangle$ and $\langle\psi|$ be two coherent states (2.27) and $|\Phi\rangle$ and $\langle\Psi|$ the Slater determinants built from the same single particle orbitals; that is,

$$|\Phi\rangle = \sum_P (-)^r |\phi_{P_1}\phi_{P_2}\cdots\phi_{P_N}\rangle = P|\phi) , \tag{3.13}$$

$$\langle\Psi| = \sum_P (-)^r \langle\psi_{P_1}\psi_{P_2}\cdots\psi_{P_N}| = (\psi|P ,$$

where P denotes the projector on the physical subspace (see Sec. II D). We are interested in the matrix elements

$$\langle\Psi| e^{-iH(t_f-t_i)} |\Phi\rangle , \tag{3.14}$$

which can be written

$$\int d\mu(\phi^*,\phi) d\mu(\psi^*,\psi) \times \langle\Psi|\psi)(\psi| e^{-iH_B(t_f-t_i)} |\phi)(\phi|\Phi\rangle , \tag{3.15}$$

where H_B is the boson image of H, given by Eq. (2.25). $(\psi| e^{-iH_B(t_f-t_i)} |\phi)$ may be represented by

the functional integral

$$\int \mathcal{D}(\varphi^*,\varphi)e^{iS[\varphi^*,\varphi]} ,$$

where the measure and the action are given, respectively, by (3.11) and (3.12), except for an obvious change of notation. The overlaps $\langle \Psi \mid \psi \rangle$ and $\langle \phi \mid \Phi \rangle$ determine the boundary condition

$$\varphi_k(t_i) = \phi_{P(k)}, \quad \varphi_k^*(t_f) = \psi_{P'(k)}^* ,$$

where $p(k)$ and $p'(k)$ denote two permutations of the particle indices $1,2,\ldots,N$. The expression (3.15) thus contains an obvious summation over all such permutations. An alternative way of calculating (3.14) is to use the explicit form (2.24) for the projector P onto the physical subspace. Furthermore, since P commutes with H, it needs to be inserted only once. One then arrives at the expression

$$\begin{aligned}\langle \Psi \mid e^{-iH(t_f-t_i)} \mid \Phi \rangle &= (\psi \mid Pe^{-iH_B(t_f-t_i)} \mid \phi) \\ &= \int dA e^{-i\,\mathrm{Tr}A}(\psi \mid e^{-i(t_f-t_i)\{H_B-[A/(t_f-t_i)]\}} \mid \phi) ,\end{aligned} \tag{3.16}$$

where A is the following operator

$$A = \sum_{kl}\sum_{\alpha} C_k^\dagger(\alpha)A_{kl}C_l(\alpha) . \tag{3.17}$$

The matrix element $(\psi \mid e^{-it[H_B-(A/t)]} \mid \varphi)$ has the following functional integral representation

$$(\psi \mid e^{-it[H_B-(A/t)]} \mid \phi) = \int \mathcal{D}(\varphi^*,\varphi)e^{iS[\varphi^*,\varphi;A]} \tag{3.18}$$

with

$$S[\varphi^*,\varphi;A] = S[\varphi^*,\varphi] - \frac{i}{t}\sum_{kl} A_{kl}(\varphi_k \mid \varphi_l) , \tag{3.19}$$

where $S[\varphi^*,\varphi]$ is the action (3.12), except for an obvious change of notations. The expression (3.18) describes the evolution of a system of bosons subject to special constraints represented by the "external" field A. When Fourier transformed [see Eq. (3.16)] with respect to A this expression retrieves the original fermion dynamics.

In the two formulations above [cf. Eqs. (3.15) and (3.18)], the paths are allowed to lie outside the physical subspace; the projection onto the physical subspace is done by the overall integral over A in the case of (3.18), or by the summation over specific boundary conditions in the case of (3.15). Now it is possible to constrain the path at each time t so that it lies entirely within the physical subspace. This is achieved by inserting the projector P at each time step in the construction of the path integral. One then arrives at the following expression

$$\begin{aligned}\langle \Psi \mid e^{-iH(t_f-t_i)} \mid \Phi \rangle &= \int \mathcal{D}(\varphi^*,\varphi)\prod_t \langle \varphi \mid P \mid \varphi \rangle e^{iS[\varphi^*,\varphi]} \\ S[\varphi^*,\varphi] &= \int_{t_i}^{t_f} \frac{\langle \varphi \mid (i\overleftrightarrow{\partial}_t - H_B)P \mid \varphi \rangle}{\langle \varphi \mid P \mid \varphi \rangle} \\ &\quad - \frac{i}{2}\mathrm{Tr}\ln\langle \Psi \mid \varphi(t_f)\rangle\langle \varphi(t_i) \mid \Phi \rangle .\end{aligned} \tag{3.20, 3.21}$$

Now let us perform the same change of variable as in Sec. II D, namely, $\varphi = \Lambda^{1/2}\varphi'$ [see Eq. (2.38)]. In this change of variable, $\langle \varphi \mid P \mid \varphi \rangle$ scales as $\det\Lambda$, as $\langle \varphi \mid HP \mid \varphi \rangle$ and $\langle \varphi \mid \overleftrightarrow{\partial}_t P \mid \varphi \rangle$ do. In this later case, it is easily verified that the possible time derivative of Λ cancel. Thus Eq. (3.21) can be rewritten as follows (with respect to an overall constant, namely, the integral over Λ; see Sec. II D)

$$\langle \Psi \mid e^{-iH(t_f-t_i)} \mid \Phi \rangle = \int \mathcal{D}(\varphi^*,\varphi)\delta[(\varphi_k \mid \varphi_l) - \delta_{kl}]e^{iS[\varphi^*,\varphi]} , \tag{3.22}$$

where, ignoring the boundary term

$$S[\varphi^*,\varphi] = \sum_k (\varphi_k \mid i\overleftrightarrow{\partial}_t \mid \varphi_k) - \sum_k (\varphi_k \mid T \mid \varphi_k) - \tfrac{1}{2}\sum_{kl}\langle \varphi_k\varphi_l \mid V \mid \varphi_k\varphi_l \rangle , \tag{3.23}$$

where now the *antisymmetrized* matrix element of the two-body interaction occurs. In contrast, the action (3.19) involves only the direct matrix elements of the two-body interaction. One recognizes in the expression (3.22) the functional integral one would have obtained working directly with Slater determinants and the measure (2.53).

The functional integrals (3.18) and (3.22) are *a priori* equivalent, i.e., they correspond to the same Schrödinger equation. However, we shall see in the next section that they have actually very different structures. Let us remark here that they differ essentially by the way the constraints are handled. In (3.18) the constraints are imposed in a global way while in (3.22) they are imposed locally (in time). One may also notice that the constraints

$(\varphi_k \mid \varphi_l)$ are constants of motion for the classical equations of motion. This situation is very much reminiscent of what happens in gauge theory; here the gauge group is the group $U(N)$ which mixes the single particle orbitals. We shall not further develop this point of view here. There is still another way to take care of the constraints, namely, choose a system of coordinates in which the constraints are automatically satisfied. This is realized by the parametrizations (2.43) and (2.49) of Slater determinants. We give below the explicit form of the functional integrals in these two representations.

For the representation (2.43) the integration measure reads

$$\mathscr{D}(Z^\dagger,Z) = \prod_t \prod_{ph} \frac{dZ^*_{ph}(t)\,dZ_{ph}(t)}{2\pi i} \times \det[1 + Z^\dagger(t)Z(t)]^{-(n_p+n_h)} \quad , \tag{3.24}$$

and the action is

$$S[Z^\dagger,Z] = \int_{t_i}^{t_f} dt \frac{i}{2}\mathrm{Tr}(1 + Z^\dagger Z)^{-1}(Z^\dagger \dot{Z} - \dot{Z}^\dagger Z) - E[\rho(Z^\dagger,Z)] - \frac{1}{2}\mathrm{Tr}\ln[1 + Z_f^\dagger Z(t_f)][1 + Z^\dagger(t_i)Z_i] \, , \tag{3.25}$$

where ρ is the density matrix (2.48) and $E[\rho]$ is the HF energy calculated with this density matrix

$$E[\rho] = \sum_{\alpha\beta} T_{\alpha\beta}\rho_{\beta\alpha} + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle \alpha\beta \mid V \mid \gamma\delta\rangle \rho_{\gamma\alpha}\rho_{\delta\beta} \tag{3.26}$$

and $\langle \alpha\beta \mid V \mid \gamma\delta\rangle$ is the antisymmetrized matrix element of the two-body interaction V. For later purposes, we write $E[\rho]$ using the following matrix notation

$$E[\rho] = T\cdot\rho + \tfrac{1}{2}\rho\cdot V\cdot\rho \quad , \tag{3.27}$$

where V is the (symmetrical) matrix,

$$V_{\alpha\gamma,\beta\delta} = \langle \alpha\beta \mid V \mid \gamma\delta\rangle = V_{\beta\delta,\alpha\gamma} \quad . \tag{3.28}$$

The action (3.25) is the one used in Ref. 14, except for the boundary term.

For the representation (2.49) the measure is simply

$$\mathscr{D}(\beta^\dagger,\beta) = \prod_t \prod_{ph} \frac{d\beta^*_{ph}(t)d\,\beta_{ph}(t)}{2\pi i} \tag{3.29}$$

and the action reads

$$S[\beta^\dagger,\beta] = \int_{t_i}^{t_f} dt \left\{ \frac{i}{2}(\beta^\dagger\dot{\beta} - \dot{\beta}^\dagger\beta) - E[\rho(\beta^\dagger,\beta)] \right\} - \tfrac{1}{2}\,\mathrm{tr}\ln(1 - \beta_f^\dagger\beta(t_f)(1 - \beta^\dagger(t_i)\beta_i) \tag{3.30}$$

Almost all the functional integrals described in this section describe boson theories with particular constraints. Indeed, the elementary fields, or coordinates, are represented by complex numbers which are quantized as boson. This boson structure has been explicitly analyzed in Sec. (II D) for the representation (3.18). The representations underlying (3.25) and (3.30) are familiar in nuclear physics for their intimate connection with perturbative boson expansions.[24,7] The method we have used to generate path integrals clearly generate at the same time boson expansions, or more precisely boson representations. In these representations, the bosons are just the quantum version of the classical parameters which label the quantum states of the overcomplete set used in the functional integral. The role of the bosons in the functional integrals, and in particular of coherent state of bosons, will be seen in the next sections.

IV. PERTURBATION EXPANSION

In this section we compare the structure of the path integrals described in the preceding section with that of the formal perturbation expansion. Let us consider the expression

$$\langle Z_f \mid e^{-iH(t_f-t_i)} \mid Z_i\rangle = \int_{\substack{Z^*(t_f)=Z_f^* \\ Z(t_i)=Z_i}} \mathscr{D}(Z^*,Z)\exp\left\{ i\int_{t_i}^{t_f} L[Z^*,Z]dt + \ln\langle Z_f \mid Z(t_f)\rangle \right\} \quad , \tag{4.1}$$

where

$$L[Z^*,Z]=\frac{\langle Z\,|\,i\partial_t-H\,|\,Z\rangle}{\langle Z\,|\,Z\rangle}\ . \tag{4.2}$$

We can rewrite L as follows

$$\begin{aligned}L[Z^*,Z]&=\frac{\langle Z\,|\,i\partial_t-H_0\,|\,Z\rangle}{\langle Z\,|\,Z\rangle}-\frac{\langle Z\,|\,V\,|\,Z\rangle}{\langle Z\,|\,Z\rangle}\\&\equiv L_0[Z^*,Z]-\frac{\langle Z\,|\,V\,|\,Z\rangle}{\langle Z\,|\,Z\rangle}\end{aligned}$$

and expand $\exp[-i\int\langle Z\,|\,V\,|\,Z\rangle/\langle Z\,|\,Z\rangle]$ in (4.1) in powers of V. One gets

$$\begin{aligned}\langle Z_f\,|\,e^{-iH(t_f-t_i)}\,|\,Z_i\rangle&=\sum_n\frac{(-i)^n}{n!}\int_{t_i}^{t_f}dt_1\ldots dt_n\int\mathscr{D}(Z^*,Z)\exp\left\{i\int_{t_i}^{t_f}L_0[Z^*,Z]+\ln\langle Z_f\,|\,Z(t_f)\rangle\right\}\\&\quad\times\frac{\langle Z(t_n)\,|\,V\,|\,Z(t_n)\rangle}{\langle Z(t_n)\,|\,Z(t_n)\rangle}\cdots\frac{\langle Z(t_1)\,|\,V\,|\,Z(t_1)\rangle}{\langle Z(t_1)\,|\,Z(t_1)\rangle}\\&=\sum_n\frac{(-i)^n}{n!}\int_{t_i}^{t_f}dt_1\ldots dt_n\int\mathscr{D}(Z^*,Z)\langle Z_f\,|\,Z(t_f)\rangle\\&\quad\times e^{i\int_{t_n}^{t_f}L_0}\frac{\langle Z(t_n)\,|\,V\,|\,Z(t_n)\rangle}{\langle Z(t_n)\,|\,Z(t_n)\rangle}e^{i\int_{t_{n-1}}^{t_n}L_0}\frac{\langle Z(t_{n-1}\,|\,V\,|\,Z(t_{n-1})\rangle}{\langle Z(t_{n-1})\,|\,Z(t_{n-1})\rangle}\cdots\\&\quad\times e^{i\int_{t_1}^{t_2}L_0}\frac{\langle Z(t_1)\,|\,V\,|\,Z(t_1)\rangle}{\langle Z(t_1)\,|\,Z(t_1)\rangle}e^{i\int_{t_i}^{t_1}L_0}\ .\end{aligned}\tag{4.3}$$

By going back to the discretized form of the functional integral (Sec. III), one easily shows that (4.3) can be rewritten as follows

$$\begin{aligned}\langle Z_f\,|\,e^{-iH(t_f-t_i)}\,|\,Z_i\rangle&=\sum_n\frac{(-i)^n}{n!}\int_{t_i}^{t_f}dt_1\ldots dt_n\int d\mu(Z_n)\ldots d\mu(Z_1)d\mu(Z_n')\ldots d\mu(Z_1')\\&\quad\times\langle Z_f\,|\,e^{-iH_0(t_f-t_n)}\,|\,Z_n\rangle\langle Z_n\,|\,V\,|\,Z_n'\rangle\\&\quad\times\langle Z_n'\,|\,e^{-iH_0(t_n-t_{n-1})}\,|\,Z_{n-1}\rangle\ldots\\&\quad\times\langle Z_1'\,|\,e^{-iH_0(t_1-t_i)}\,|\,Z_i\rangle\ ,\end{aligned}\tag{4.4}$$

where we have used the expression

$$\langle Z_n\,|\,e^{-iH_0(t_n-t_{n-1})}\,|\,Z_{n-1}\rangle=\int_{\substack{Z^*(t_n)=Z_n^*\\Z(t_{n-1})=Z_{n-1}}}\mathscr{D}(Z^*,Z)\exp\left[i\int_{t_{n-1}}^{t_n}L_0+\ln\langle Z_n\,|\,Z(t_n)\rangle\right]\ .\tag{4.5}$$

The closure relations over $|\,Z_n\rangle\langle Z_n\,|$ can now be removed. One then ends up with

$$\begin{aligned}\langle Z_f\,|\,e^{-iH(t_f-t_i)}\,|\,Z_i\rangle&=\sum_n\frac{(-i)^n}{n!}\int_{t_i}^{t_f}dt_1\ldots dt_n\langle Z_f\,|\,e^{-iH_0t_f}T[V(t_n)\ldots V(t_1)]e^{iH_0t_i}\,|\,Z_i\rangle\\&=\langle Z_f\,|\,e^{-iH_0t_f}T\exp\left[-\int_{t_i}^{t_f}V(t)dt\right]e^{iH_0t_i}\,|\,Z_i\rangle\ ,\end{aligned}\tag{4.6}$$

where $V(t)$ is the interaction representation of V,

$$V(t) = e^{iH_0 t} V e^{-iH_0 t} \quad . \tag{4.7}$$

One recognizes in the expression (4.6) the standard perturbation expansion in powers of V. This shows that the functional integral preserves the structure of the formal perturbation expansion. This follows from the fact that the functional integral, by construction, preserves the structure of the T product, and that we have the following identity[25]:

$$e^{-iHt} = \lim_{N\to\infty} (e^{-i(t/N)H_0} e^{-i(t/N)V})^N \quad , \tag{4.8}$$

that is, in the continuous limit, one can neglect the noncommutation of the operators V and H_0. Had one started from the expression (4.8) instead of using

$$e^{-iHt} = \lim_{N\to\infty} (e^{-iHt/N})^N$$

for constructing the path integral, one would have obtained directly (4.6).

It should be stressed that the identification of the perturbation series obtained with the functional integral and operator methods has made explicit reference to the discretized form, which was needed to disentangle the integration over Z and Z' at different times. This is therefore not a check of the continuous limit.

In the remaining part of this section, we are going to rearrange the perturbation expansion using operator identities. The rearrangement which will be performed can be interpreted as a change of variable in the functional integral. We shall see that this change of variable is not always allowed.

Let us first notice that the T exponential may be written

$$\begin{aligned} T\exp -i \int_{t_i}^{t_f} V(t)dt &= \lim_{N\to\infty} T \prod_{k=1}^{N} [1 - i\epsilon V(t_k)] \\ &= \lim_{N\to\infty} T \prod_{k=1}^{N} :e^{-i\epsilon V(t_k)}: \quad \left[\epsilon = \frac{t_i - t_f}{N}\right] \quad . \end{aligned} \tag{4.9}$$

The second line differs from the first one by terms which are negligible in the limit $\epsilon \to 0$. We shall keep them, however, for reasons which will become clear soon. Note that the second line defines the T product of two operators at equal times as their normal product:

$$T[A(t)B(t)] = :A(t)B(t): \quad . \tag{4.10}$$

This refinement clearly does not affect the preceding discussion. But it is going to be of crucial importance in the following.

We now consider an alternative form of the perturbation expansion which relies on the following identity

$$T\exp -\frac{i}{2}\int_{t_i}^{t_f} V(t)dt = N \int \mathscr{D}W \exp\left[\frac{i}{2}\int_{t_i}^{t_f} W(t)\cdot V^{-1}\cdot W(t)dt\right] T\exp\left[-i\int_{t_i}^{t_f} W_{\alpha\beta}(t) a_\alpha^\dagger(t) a_\beta(t) dt\right] \tag{4.11}$$

where the normalization constant N is given by

$$N^{-1} = \int \mathscr{D}W \exp\left[\frac{i}{2}\int_{t_i}^{t_f} dt\; W(t)\cdot V^{-1}\cdot W(t)\right] \tag{4.12}$$

and V^{-1} is the inverse of the matrix

$$V_{\alpha\gamma,\beta\delta} = (\alpha\beta \mid V \mid \gamma\delta) \quad . \tag{4.13}$$

$(\alpha\beta \mid V \mid \gamma\delta)$ is the nonantisymmetrized matrix element of V and in (4.11) $\frac{1}{2}V(t)$ stands for $\frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta \mid V \mid \gamma\delta) a_\alpha^\dagger(t) a_\beta^\dagger(t) a_\delta(t) a_\gamma(t)$. The identity (4.11) is easily proved. It is very similar to the identity used in Ref. 26. Let us simply remark here that the Gaussian integration over W operates like a Wick's theorem, the elementary contraction being

$$\begin{aligned} \langle W_{\alpha\beta}(t_1) W_{\gamma\delta}(t_2)\rangle &= N \int \mathscr{D}W \exp\left[\frac{i}{2}\int_{t_i}^{t_f} W(t)\cdot V^{-1}\cdot W(t)dt\right] W_{\alpha\beta}(t_1) W_{\gamma\delta}(t_2) \\ &= -\delta(t_1 - t_2) V_{\alpha\beta,\gamma\delta} \quad . \end{aligned} \tag{4.14}$$

Thus the integration over W reconstructs the original two-body potential. Now it is important to realize that the integration over W involves two W at the same time, and therefore, depends crucially upon the way the T product at equal time has been defined. The formula (4.4) follows then from the application of the two identities

$$T\exp -i\int_{t_i}^{t_f} V(t)dt = \lim_{N\to\infty} T\prod_{k=1}^{N} :e^{-i\epsilon V(t_k)}: , \tag{4.15}$$

$$:e^{-i\epsilon V}: = N\int \mathscr{D}w e^{i/2\epsilon WV^{-1}W} :e^{-i\epsilon Wa^{\dagger}a}: \ . \tag{4.16}$$

Let us now consider the functional integral representation of $\langle Z_f | e^{-iH(t_f-t_i)} | Z_i\rangle$ in the overcomplete set of Slater determinants. To avoid complications with the constraints, let us use for example the parametrization (3.25) or (3.30). Using the identity

$$\exp\left[-\frac{i}{2}\int \rho\cdot V\cdot\rho\, dt\right] = N\int \mathscr{D}W \exp\left[\frac{i}{2}\int W\cdot V^{-1}\cdot W\, dt - i\int W\cdot\rho\, dt\right]$$

one obtains the following expression

$$\langle Z_f | e^{-iH(t_f-t_i)} | Z_i\rangle = \int_{\substack{Z^*(t_f)=Z_f^* \\ Z(t_i)=Z_i}} \mathscr{D}W \exp\left[\frac{i}{2}\int W(t)\cdot V^{-1}\cdot W(t)dt\right] \times \exp\left[i\int_{t_i}^{t_f} \frac{\langle Z | i\partial_t - H_0 - W | Z\rangle}{\langle Z | Z\rangle} + \ln\langle Z_f | Z(t_f)\rangle\right] . \tag{4.17}$$

Note that in the above formula, the matrix V is constructed with antisymmetrized matrix elements of the two-body interaction. It is extremely tempting at this stage to interchange the orders of the integrations over W and Z. Writing

$$\langle Z_f | e^{-iH(t_f-t_i)} | Z_i\rangle = \int \mathscr{D}W \exp\left[\frac{i}{2}\int W(t)\cdot V^{-1}\cdot W(t)dt\right] \times \int \mathscr{D}(Z^*,Z) \exp\left[i\int_{t_i}^{t_f} \frac{\langle Z | i\partial_t - H_0 - W | Z\rangle}{\langle Z | Z\rangle} + \ln\langle Z_f | Z(t_f)\rangle\right] . \tag{4.18}$$

Now the integral over Z is the matrix element between $|Z_i\rangle$ and $\langle Z_f|$ of the evolution operator for noninteracting particles in the fluctuating field $W(t)$. It is, therefore, equal to

$$\langle Z_f | e^{-iH_0 t_f}\left[T\exp -i\int_{t_i}^{t_f} W(t)\right] e^{iH_0 t_i} | Z_i\rangle \ . \tag{4.19}$$

However, a careful analysis of the first terms of the perturbation expansion reveals overcounting, a signal that nonallowed manipulations have been performed. The origin of the trouble can be traced back to the fact that the contributions to the integral over W in (4.8) comes from terms which are of order $(dt)^2$, or ϵ^2 in the discretized version. Thus the integral over Z in (4.18) contains terms like

$$e^{-\epsilon W\langle a^{\dagger}a\rangle} \sim 1 - \epsilon W\langle a^{\dagger}a\rangle + \frac{\epsilon^2}{2} W\langle a^{\dagger}a\rangle W\langle a^{\dagger}a\rangle \ . \tag{4.20}$$

If one replaces this integral by the expression (4.19) one gets instead terms of the form

$$\langle e^{-\epsilon W a^\dagger a}\rangle \sim 1-\epsilon W\langle a^\dagger a\rangle + \frac{\epsilon^2}{2}W_{\alpha\beta}W_{\gamma\delta}\langle a_\alpha^\dagger a_\beta\rangle\langle a_\gamma^\dagger a_\delta\rangle + \frac{\epsilon^2}{2}W_{\alpha\beta}W_{\gamma\delta}\langle a_\alpha^\dagger a_\delta\rangle\langle a_\beta a_\gamma^\dagger\rangle \ , \tag{4.21}$$

that is, one obtains two terms corresponding to the two possible contractions, and this is the origin of the overcounting. Thus one cannot replace the integral over Z by the expression (4.19) which is really troublesome, since the integral over Z in (4.18) is really the one which in our formalism represents (4.19). Another way of stating the difficulty is to consider that the change of variable involved in (4.17) is not allowed for the integral over Slater determinants, or more precisely that one is not allowed to interchange the order of integration over Z and W in (4.17).

It is easily seen that all these difficulties disappear when one is working with a path integral constructed with coherent states. Indeed taking the matrix element of Eq. (4.16) between two coherent states yields

$$\langle :e^{-i\epsilon V}:\rangle = e^{-i\epsilon\langle V\rangle} = N\int \mathscr{D}W e^{i/2\epsilon W V^{-1}W} e^{-i\epsilon W\langle a^\dagger a\rangle} \ , \tag{4.22}$$

that is, the functional integral preserves exactly the operator identities. In this particular case, the change of variable involved in (4.17) is therefore perfectly allowed. Note that this holds for any kind of coherent states, of boson or fermions. It holds in particular for the coherent states (2.27).

V. MEAN FIELD THEORIES AND BEYOND

In the preceding section, we made explicit the similarities in the structures of the functional integral and the formal perturbation expansion. However, the most interesting feature of the functional integral is to suggest approximation schemes which are different from those of conventional perturbation theory. In this section, we examine in particular the saddle-point approximation and its successive corrections. As well known, this approximation, when performed on the standard Feynman path integral, retrieves classical mechanics. In the many-body problem, the classical approximation obtained depends on the choice of the overcomplete set of states which have been chosen to construct the functional integral. If independent particle wave functions are used, the classical equations are the time-dependent mean field equations. It turns out that these nonlinear equations have definite classical features which we analyze. We also discuss in this section the connection between path integrals and perturbative boson expansions.

Let us then apply the saddle-point approximation and its successive corrections to the calculation of the functional integral

$$\int_{\substack{Z^*(t_f)=Z_f^* \\ Z(t_i)=Z_i}} \mathscr{D}(Z^*,Z)e^{iS[Z^*,Z]} = \langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle \ . \tag{5.1}$$

The saddle points are given by the following equations, with their boundary condition

$$\frac{\delta S}{\delta Z}=0, \ Z^*(t_f)=Z_f^* \ , \tag{5.2a}$$

$$\frac{\delta S}{\delta Z^*}=0, \ Z(t_i)=Z_i \ . \tag{5.2b}$$

We call $Z_C^{(+)^*}$ and $Z_C^{(-)}$ the solutions of Eqs. (5.2a) and (5.2b), respectively. Note that $Z_C^{(+)^*}(t)$ and $Z_C^{(-)}(t)$ are not, in general, complex conjugates of each other. We then expand the action $S[Z^*,Z]$ around the classical solution $(Z_C^{(+)^*}, Z_C^{(-)})$:

$$S = S_C + \sum_{n\geq 2} S_n[Z^*,Z] \ , \tag{5.3}$$

where we have set

$$S_C \equiv S[Z_C^{(+)^*},Z_C^{(-)}] \ ,$$

$$S_n[Z^*,Z] = \frac{1}{n!}\sum_{p=1}^{N} C_N^p (Z^*)^p \frac{\delta^n S}{\delta Z^{*p}\delta Z^{n-p}}\bigg|_C Z^{n-p} \ , \tag{5.4}$$

and the functional derivatives are evaluated for $Z^*=Z_C^{(+)^*}$, $Z=Z_C^{(-)}$. The functional integral (5.1) then takes the form

$$\langle Z_f|e^{-iH(t_f-t_i)}|Z_i\rangle = e^{iS_C}\int_{\substack{Z^*(t_f)=0 \\ Z(t_i)=0}} \mathscr{D}(Z^*,Z)\exp\left[i\sum_{n\geq 2}S_n(Z^*,Z)\right] \ . \tag{5.5}$$

Note that the boundary conditions are now independent of Z_i and Z_f^*. That is, all the dependence of the expression (5.5) on Z_i and Z_f^* is contained in S_C and the possible boundary terms which subsist in S_n.

It is interesting to notice that Eqs. (5.2a) and (5.2b) correspond to the time-dependent variational principle (very similar to the ones developed in Ref. 27):

$$\delta S[Z^*,Z] = 0 \ , \tag{5.6}$$

where $S[Z^*,Z]$ reads explicitly:

$$S[Z^*,Z] = \int_{t_i}^{t_f} \frac{\langle Z \,|\, i\partial_t - H \,|\, Z\rangle}{\langle Z \,|\, Z\rangle} - i\ln\langle Z_f \,|\, Z(t_f)\rangle \ . \tag{5.7}$$

It is easily verified that Eq. (5.6) leads back to the time-dependent Schrödinger equation if $|Z\rangle$ is assumed to represent any state of the Hilbert space, i.e., in the case of unrestricted variations. When $|Z\rangle$ is chosen in a given class of states, the solution of the Eq. (5.6) provides an approximation for the transition amplitude $\langle Z_f \,|\, e^{-iH(t_f-t_i)} \,|\, Z_i\rangle$. This is given by e^{iS_C}. The usefulness of this expression lies in the fact that it is a stationary quantity. It appears then clearly that the choice of an overcomplete set for the construction of the functional integral is equivalent to the choice of a class of trial states in the use of the time-dependent variational principle. Therefore the separation into a classical motion and quantum corrections, implied by Eq. (5.3) does not require that some quantity is small compared to $\hbar$. The nature of the classical approximation discussed here, or the type of quantum effects which are left out in this approximation, are entirely determined by the specific choice of an overcomplete set in the Hilbert space. In particular, if the overcomplete set is the Hilbert space itself, the classical equations of motion are identical with the Schrödinger equation.

The limitation of the time-dependent variational principle (5.6) is that it does not provide a way of estimating the error associated with a given choice of trial states. This is precisely what the functional integral (5.5) does. Although the corrections to the classical approximation would be in most cases hard to evaluate, the functional integral provides the possibility of analyzing them, and therefore, allows for a better understanding of the classical approximation itself. We shall illustrate these considerations in the case of the mean field approximations to the many-body problem.

Let us then consider that the coordinates $\{Z\}$ represent a Slater determinant, that is, $\{Z\}$ denotes any of the sets of coordinates discussed in Sec. II E. [Actually the equations of motion given below only hold if the action (3.30) or (3.23) are used. If the action (3.25) is used, extra kinematical terms appears in front of the time derivatives.] The classical equations of motion are the time-dependent Hartree-Fock equations

$$i\dot{Z} - \frac{\delta H(Z^*,Z)}{\delta Z^*} = 0 \ , \tag{5.8}$$

$$i\dot{Z}^* + \frac{\delta H(Z^*,Z)}{\delta Z} = 0 \ , \tag{5.9}$$

where $H(Z^*,Z) = \langle Z \,|\, H \,|\, Z\rangle / \langle Z \,|\, Z\rangle$ is given explicitly in Sec. II E. The state vectors $|Z(t)\rangle$ which make the action (5.7) stationary are of the form

$$|Z(t)\rangle = |Z_0(t)\rangle \exp\left[-i\int_{t_i}^{t} f(t')dt'\right] \ , \tag{5.10}$$

where $f(t)$ is an arbitrary function of time and $Z_o(t)$ is a solution of the Eq. (5.8). This arbitrariness in the phase of $|Z(t)\rangle$ reflects the invariance of the action (5.7) with respect to the choice of phase of the state vectors. Equations (5.8) and (5.9) can be easily transformed into an equation for the one-body density matrix

$$i\dot{\rho} = [h,\rho] \tag{5.11}$$

with

$$\rho_{\alpha\beta}(t) = \frac{\langle Z_C^{(+)}(t) \,|\, a_\alpha^\dagger a_\beta \,|\, Z_C^{(-)}(t)\rangle}{\langle Z_C^{(+)}(t) \,|\, Z_C^{(-)}(t)\rangle} \ , \tag{5.12}$$

and $h = \delta E/\delta\rho$ is the usual Hartree-Fock Hamiltonian calculated with the density matrix (5.12). Note that the density matrix is not Hermitian, so that the Hartree-Fock Hamiltonian is in general not real. Equation (5.11) is a generalization of the ordinary time-dependent Hartree-Fock equation, appropriate to the calculation of scattering amplitudes. This equation has already been considered in Ref. 12. Note that the standard TDHF equations are recovered if one chooses the boundary conditions such that $Z(t_f) = Z_f$. Then $Z_C^{(-)}(t)$ and $Z_C^{(+)*}(t)$ are complex conjugates of each other and the density matrix, as well as the Hartree-Fock Hamiltonian are Hermitian. The classical solutions $[Z_C^{(+)}(t), Z_C^{(-)}(t)]$ can be used to get a sem-

iclassical approximation to the transition amplitude $\langle Z_f t_f \mid Z_i t_i \rangle$. It can also be used to obtain semiclassical approximations to the bound state energies of the system, applying a generalization of the WKB method developed in Ref. 28. Typically one arrives at semiclassical quantization rules for the periodic trajectories of the time-dependent mean-field equations. This method has already been applied in different ways to several simple cases.[13,12,29–31]

Let us now calculate the corrections to the mean field theory. This is obtained by expanding the action S around the classical solution $[Z_C^{(+)*}(t), Z_C^{(-)}(t)]$, as indicated by Eq. (5.3). We shall limit ourselves first to the quadratic corrections, and to simplify the discussion, we shall consider the fluctuations around a static solution of Eq. (5.8). We call $\mid \phi_0 \rangle$ the corresponding state and we calculate

$$\langle \phi_0 \mid e^{-\beta H} \mid \phi_0 \rangle \approx e^{-\beta E_{\mathrm{HF}}} \int_{\substack{Z^*(\beta)=0 \\ Z(0)=0}} \mathscr{D}(Z^*,Z) \exp\left\{ - \int_0^\beta [Z^* \dot{Z} + H_2(Z^*,Z)] dt \right\} , \tag{5.13}$$

where E_{HF} is the Hartree-Fock energy of the state $\mid \phi_0 \rangle$ and we have assumed $\langle \phi_0 \mid \phi_0 \rangle = 1$. $H_2(Z^*,Z)$ is the quadratic form obtained by expanding $H(Z^*,Z)$ around $Z = 0$ ($\equiv \mid \phi_0 \rangle$). In terms of the amplitudes Z_{ph}, $H_2(Z^*,Z)$ have the explicit form

$$H_2(Z^*,Z) = \tfrac{1}{2}(Z_{ph}^*, Z_{ph}) \begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} \begin{bmatrix} Z_{ph} \\ Z_{ph}^* \end{bmatrix} , \tag{5.14}$$

where the matrices A and B are the usual matrices of the random phase approximation. Note that at this level of approximation, all the parametrizations considered in Sec. II E, with proper inclusion of the constraints when necessary, yield the same result, Eq. (5.14). Now the functional integral (5.13) is identical to that of a system of coupled harmonic oscillators; more precisely it can be written

$$\int_{\substack{Z^*(\beta)=0 \\ Z(0)=0}} \mathscr{D}(Z^*,Z) \exp\left\{ - \int_0^\beta [Z^* \dot{Z} + H_2(Z^*,Z)] dt \right\}$$

$$= {}_B\langle 0 \mid \exp -\beta (C^\dagger \cdot A \cdot C + \tfrac{1}{2} C^\dagger \cdot B \cdot C^\dagger + \tfrac{1}{2} C \cdot B \cdot C) \mid 0 \rangle_B , \tag{5.15}$$

where we have used the matrix notation

$$C^\dagger \cdot A \cdot C = \sum_{\substack{ph \\ p'h'}} C_{ph}^\dagger A_{ph,p'h'} C_{p'h'} .$$

$C_{ph}^\dagger$ and C_{ph} denote boson creation and annihilation operators and $\mid 0 \rangle_B$ is the boson vacuum. By using the canonical form which diagonalizes the quadratic form in (5.15) one easily obtains:

$${}_B\langle 0 \mid \exp(C^\dagger A C + \tfrac{1}{2} C^\dagger B C^\dagger + \tfrac{1}{2} C B^\dagger C) \mid 0 \rangle_B = e^{\Delta E_0} , \tag{5.16}$$

where ΔE_0 is the correlation energy associated with the random phase approximation (RPA) vibrations, that is,

$$\Delta E_0 = \tfrac{1}{2} \sum_N \omega_N - \tfrac{1}{2} \mathrm{Tr} A . \tag{5.17}$$

This expression is easily shown to be equal to the sum of all the ring diagrams calculated with antisymmetrized matrix element and including the well known double counting of the second order term.

The boson degrees of freedom which appear naturally in the calculation of the integral (5.15) are the usual RPA phonons. The successive corrections to the expression (5.15) represent the various couplings between these RPA phonons. A systematic expansion can be derived in the following way. We first expand $H(Z^*,Z)$ to all order in Z^* and Z. Since we have treated explicitly the terms of order 2, this expansion starts at third order. These higher order terms can be treated in perturbation, which leads to the expression

$$\langle\phi_0|e^{-\beta H}|\phi_0\rangle = e^{-\beta E_{\rm HF}}\exp\left[-\int_0^\beta dt\sum_{n>3}H_n\left[\frac{\delta}{\delta j},\frac{\delta}{\delta j^*}\right]\right]$$
$$\times\int_{\substack{Z^*(\beta)=0\\Z(0)=0}}\mathscr{D}(Z^*,Z)\exp\left\{-\int_0^\beta[Z^*\dot{Z}+H_2(Z^*,Z)+j^*\cdot Z+Z^*\cdot j]\right\}\Big|_{\substack{j=0\\j^*=0}}. \quad (5.18)$$

The expression (5.18) is very reminiscent of the familiar perturbative boson expansion. The unperturbed propagator for the bosons is the RPA propagator and the term H_n describes a coupling between n RPA bosons. The occurrence of n-body interactions between the RPA bosons arises from the Pauli principle, or in other words from the constraints necessary to project onto the physical subspace. It must be kept in mind that we are not making here an exact connection between our formalism and a perturbative boson expansion. Indeed, when going beyond the quadratic approximation, technical problems arise with the treatment of the constraints, the integration measure or the domain of integration, depending upon whether one chooses, respectively, the parametrization (2.53), (2.45), or (2.50) for the Slater determinant. In the absence of a careful treatment of these points, we consider the expression (5.18) as approximate. It is clear, however, that the physical content of (5.18) will not be very much altered by a more rigorous derivation. This physical content is indeed quite transparent. The functional integral "quantizes" as bosons the coordinates which were introduced to parametrize the states of the overcomplete set. Inversely, the classical limit obtained in the saddle-point approximation is achieved by replacing the boson operators by c numbers (see Ref. 18).

The technical difficulties mentioned above do not show up when one considers the expansion around a solution of the Hartree equation. In this case, the expansion can then be given easily a diagrammatic interpretation, using the standard technics of perturbation theory. We shall again restrict ourselves to a time-independent problem and consider the expression

$$\langle\phi_0|e^{\beta H_0}e^{-\beta H}|\phi_0\rangle = N\int\mathscr{D}W\exp\left[\tfrac{1}{2}\int_0^\beta W(t)\cdot V^{-1}\cdot W(t)dt\right]e^{\mathrm{Tr}\ln(1-WG_0)}, \quad (5.19)$$

which follows trivially from (4.11) and the identity

$$\langle\phi_0|T\exp\int_0^\beta W(u)a^\dagger(u)a(u)du\,|\phi_0\rangle = \exp\mathrm{Tr}\ln(1-WG_0), \quad (5.20)$$

where G_0 is the single particle Green's function:

$$G^0_{\alpha\beta}(u_1-u_2) = \langle\phi_0|Ta_\alpha(u_1)a^\dagger_\beta(u_2)|\phi_0\rangle. \quad (5.21)$$

Equation (5.19) can also be derived from (3.16) (see Ref. 18). Application of the saddle-point approximation on the integral over W leads to the equation

$$W\cdot V^{-1} = V^{-1}\cdot W = G_0(1-WG_0)^{-1} = G[W], \quad (5.22)$$

where $G[W]$ is the single particle Green's function in presence of the external field W:

$$G^{-1}[W] = G_0{}^{-1} - W. \quad (5.23)$$

The density matrix is related to G by

$$\rho(t) = \lim_{\tau\to 0_+}G\left[t-\frac{\tau}{2},t+\frac{\tau}{2}\right]. \quad (5.24)$$

It satisfies the equation of motion

$$\partial_t\rho + [H_0 - W,\rho] = 0, \quad (5.25)$$

which is the time-dependent Hartree equation written in imaginary time. The expansion around a static solution is obtained easily. Let W_0 a static field, solution of

$$[H_0 - W_0,\rho_0] = 0. \quad (5.26)$$

The expansion of (5.19) in powers of $W' = W - W_0$ reads

$$\langle\phi_0|e^{\beta H_0}e^{-\beta H}|\phi_0\rangle = Ne^{(\beta/2)\rho_0\cdot V\cdot\rho_0}\int\mathscr{D}W\exp\left[\int_0^\beta\tfrac{1}{2}W'\cdot V^{-1}\cdot W' - \tfrac{1}{2}\int_0^\beta\mathrm{Tr}W'\cdot G(W_0)\cdot W'\cdot G(W_0)\right]$$
$$\times\exp\left\{\int_0^\beta\mathrm{Tr}\sum_{n>2}-\frac{1}{n}[G(W_0)\cdot W']^n\right\}. \quad (5.27)$$

In order to calculate the remaining integral, we first regroup the two quadratic terms defining

$$\Gamma^{-1} = V^{-1} - Q \ , \tag{5.28}$$

where

$$Q_{\alpha\beta,\gamma\delta}(u_1 - u_2) = G_{\beta\gamma}[W_0;u_1 - u_2]G_{\gamma\alpha}[W_0;u_2 - u_1] \ . \tag{5.29}$$

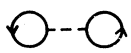
Using a standard procedure, one introduces a source term for the field W' and treats in perturbation the terms of order higher than 2 in W', in the exponent of (5.27). One then gets

$$\langle \phi_0 | e^{\beta H_0} e^{-\beta H} | \phi_0 \rangle = e^{-(\beta/2)\rho_0 \cdot V \cdot \rho_0} e^{-1/2 \operatorname{Tr} \ln(1 - VQ_0)} \times \exp\left\{ - \sum_{n>2} \int_0^\beta \operatorname{tr} \frac{1}{n} \left[G(W_0) \cdot \frac{\delta}{\delta j} \right]^n \right\} e^{-(1/2) j \cdot \Gamma \cdot j} \Big|_{j=0} \ , \tag{5.30}$$

where the factor $e^{-1/2 j \Gamma j}$ comes from the Gaussian integral over W'

$$e^{-(1/2) j \cdot \Gamma \cdot j} = \frac{\int \mathscr{D} W e^{(1/2) W \cdot \Gamma^{-1} \cdot W + j \cdot W}}{\int \mathscr{D} W e^{(1/2) W \cdot \Gamma^{-1} \cdot W}} \ . \tag{5.31}$$

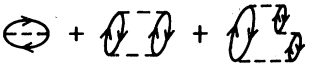
The diagrammatic interpretation of the formula (5.30) is very simple (we consider vacuum-vacuum diagrams corresponding to the ground state energy). The first term is the Hartree energy



(5.32)

The second term is the sum of all ring diagrams (calculated here with direct matrix elements), plus actually the exchange counterpart of (5.32)

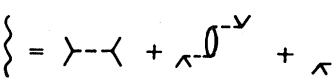
tr ln $(1 - VQ_0)$ =



(5.33)

To pursue the analysis we give the following representation of Γ

$\Gamma \equiv$



(5.34)

Thus (5.33) can be represented by

(5.35)

and

$$\sum_{n>2} \frac{1}{n} \operatorname{Tr} \left[G(W_0) \cdot \frac{\delta}{\delta j} \right]^n e^{-(1/2) j \cdot \Gamma \cdot j} \Big|_{j=0} \tag{5.36}$$

is the sum of all diagrams with one closed fermion loop and an arbitrary number of Γ lines:

(5.37)

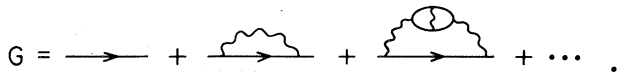
The single particle Green's function can be written as follows:

$$G_{\alpha\beta}(u_1 - u_2) = \frac{\int \mathscr{D} W \exp\left[\frac{1}{2} \int_0^\beta W \cdot V^{-1} \cdot W + \operatorname{Tr} \ln(1 - WG_0) \right] G_{\alpha\beta}[W;u_1 - u_2]}{\int \mathscr{D} W \exp\left[\frac{1}{2} \int_0^\beta W \cdot V^{-1} \cdot W + \operatorname{Tr} \ln(1 - WG_0) \right]} \ . \tag{5.38}$$

Following a derivation similar to the one which leads to (5.30), one obtains the following expression:

$$G_{\alpha\beta}(u_1-u_2)=\left[\exp\left\{-\int_0^\beta \mathrm{tr}\sum_{n>2}\frac{1}{n}\left[G(W_0)\cdot\frac{\delta}{\delta j}\right]^n\right\}G_{\alpha\beta}\left[W_0+\frac{\delta}{\delta j}\right]e^{-(1/2)j\cdot\Gamma\cdot j}\Big|_{j=0}\right]_L , \tag{5.39}$$

where the symbol $\{\ \}_L$ means that we have to consider only the linked diagrams. G has the following diagrammatic representation:



The first term may be veiwed as the classical propagator. It describes the motion of a particle in the field W_0. The other terms which describes the coupling of a particle to a vibration, *with propagation of the vibration,* are the quantum effects which are left out in the classical approximation.

VI. CONCLUSIONS

The functional integrals built on overcomplete sets of the Hilbert space provide a unifying understanding of different approaches to the nuclear many body problem. The role and the significance of the overcomplete set are best understood when calculating the functional integral using the saddle-point approximation, and its successive corrections. Then, it can be seen that the parameters which are used to label the states of the overcomplete set obey classical equations of motion. The state labels may then be viewed as classical coordinates in a generalized phase space. The classical equations of motion are identical to those obtained applying a time-dependent variational principle, using as trial states the states of the overcomplete set. But in contrast to the variational principle, the functional integral does provide a way of calculating corrections to the variational solution. A proper treatment of the fluctuations around the classical path introduces a quantization of the classical coordinates in terms of boson degrees of freedom.

As we have seen throughout this paper bosons play an important role in the functional integral formalism. In particular boson coherent states appear to be very useful because they are eigenstates of the destruction operators. This greatly facilitates the calculation of matrix elements. But more than that, it makes the structure of the functional integral simpler. Also we have seen that some changes of variables are allowed only if the overcomplete set is a set of coherent states. We have also shown that the functional integral transforms a fermion theory into a boson theory in very much the same way as the usual boson expansions do.

We have also obtained a clear physical interpretation of the classical features of the mean field approximations. In the language of boson representations, this approximation is obtained by replacing the boson propagators, e.g., the propagators corresponding to the RPA vibrations, by their classical approximation. This implies that only the static part of the particle-vibration interactions are taken into account in the mean field approximation. This point is further illustrated by diagrammatic expansion around the mean field. The processes involving a real propagation of a phonon between the time when it is emitted and the time when it is absorbed appear as quantum corrections to the mean field. Another equivalent statement, also suggested by the functional integral formalism, is that the mean field has at each time a given classical value. The functional integral allows for possible approximate schemes for calculating the "quantum" fluctuations around this value.

ACKNOWLEDGMENTS

One of the authors (J.P.B.) gratefully acknowledges the warm hospitality of the Physics Department of the University of Illinois at Urbana-Champaign where this work was completed.

APPENDIX

We construct explicitly the measures which have been used in Sec. II E to construct closure relations. The general idea underlying the method is to associate the parameters Z with some group operation and to construct the invariant measure over the group. In the case of the Slater determinants the group to be considered is the group of unitary transformations in the space of single particle states. A general element of the group is represented by the matrix

$$U=\begin{bmatrix}A & B\\ C & D\end{bmatrix},\quad UU^\dagger=U^\dagger U=1 , \tag{A1}$$

where A, B, C, and D are $n_h \times n_h$, $n_h \times n_p$, $n_p \times n_h$, and $n_p \times n_p$ matrices, respectively. These matrices satisfy:

$$\begin{aligned} &AA^\dagger + BB^\dagger = 1, \quad CA^\dagger + DB^\dagger = 0 \ , \\ &AC^\dagger + BD^\dagger = 0, \quad CC^\dagger + DD^\dagger = 1 \ , \\ &A^\dagger A + C^\dagger C = 1, \quad A^\dagger B + C^\dagger D = 0 \ , \\ &B^\dagger A + D^\dagger C = 0, \quad B^\dagger B + D^\dagger D = 1 \ . \end{aligned} \tag{A2}$$

Let us now consider the states (2.43), normalized:

$$|\tilde{Z}\rangle = N e^{Z_{ph} a_p^\dagger a_h} |\phi_0\rangle \ , \tag{A3}$$

where N is a normalization constant. Let S be the unitary transformation which carries $|\tilde{Z}\rangle$ into $|\tilde{Z}'\rangle$:

$$|\tilde{Z}'\rangle = S\,|\tilde{Z}\rangle \ . \tag{A4}$$

We look for an invariant measure $\mu(Z)$ such that

$$\begin{aligned} \mu(Z) &= \mu(Z')\,|J(Z',Z)| \\ &= \mu(0)\,|J(0,Z)| \ , \end{aligned} \tag{A5}$$

where $J(Z',Z)$ is the Jacobian of the transformation which transforms Z into Z'.

The law of transformation of the coordinates Z the transformation (A4) is easily derived. Indeed $|\tilde{Z}\rangle$ can be written

$$|\tilde{Z}\rangle = N \prod_h (a_h^\dagger + Z_{ph} a_p^\dagger)\,|0\rangle \ . \tag{A6}$$

Under the unitary transformation (A4), this becomes

$$|\tilde{Z}\rangle = N \prod_h (a_h^\dagger + Z_{ph} a_p^\dagger)\,|0\rangle \ . \tag{A7}$$

where

$$b_h^\dagger = S a_h^\dagger S^\dagger, \quad b_p^\dagger = S a_p^\dagger S^\dagger, \quad S\,|0\rangle = |0\rangle \ . \tag{A8}$$

To the operator S is associated a matrix U of the form (A1) which realizes the linear transformation of the creation operators

$$(b_h^\dagger b_p^\dagger) = (a_h^\dagger a_p^\dagger) \begin{pmatrix} A & B \\ C & D \end{pmatrix} \ . \tag{A9}$$

Replacing $b_h^\dagger$ and $b_p^\dagger$ in the equation (A7) by their expression in terms of $a_h^\dagger$ and $a_p^\dagger$ given above, one gets:

$$\begin{aligned} |\tilde{Z}'\rangle &= N \prod_h [a_{h'}^\dagger (A + BZ)_{h'h} \\ &\qquad + b_{p'}^\dagger (C + DZ)_{p'h}]\,|0\rangle \\ &= N' \prod_h (a_h^\dagger + Z'_{ph} a_p^\dagger)\,|0\rangle \ , \end{aligned} \tag{A10}$$

where

$$Z' = (C + DZ)(A + BZ)^{-1} \ . \tag{A11}$$

This is the desired transformation law. From this it is easy to evaluate the Jacobian which appears in (A5). First we write

$$Z'(A + BZ) = C + DZ$$

then differentiate,

$$dZ'(A + BZ) + Z'BdZ = DdZ \ .$$

We replace Z by its expression in terms of Z' by inverting the equation (A11) and finally put $Z' = 0$. We then get

$$|J(0,Z)| = |(\det D)^{2n_h} \det(A - BD^{-1}C)^{-2n_p}| \ . \tag{A12}$$

Using the relations (A2) one easily shows that

$$|\det(A - BD^{-1}C)| = |\det A|^{-1} = |\det D|^{-1} \ , \tag{A13}$$

so that the Jacobian takes the form

$$|J(0,Z)| = |\det A|^{2(n_p + n_h)} \ . \tag{A14}$$

It remains to relate the matrix A to the matrix Z. For that purpose one can use the following coset decomposition:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & -Z^\dagger \\ Z & 1 \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & U' \end{pmatrix} \begin{pmatrix} A_1 & 0 \\ 0 & D_1 \end{pmatrix} \ , \tag{A15}$$

where U and U' are, respectively, $n_h \times n_h$ and $n_p \times n_p$ arbitrary unitary matrices. A_1 and D_1 are, respectively, $n_h \times n_h$ and $n_p \times n_p$ matrices to be determined so that the matrix

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

satisfies the conditions (A2). One solution is

$$A_1 = (1 + Z^\dagger Z)^{-1/2}, \quad D_1 = (1 + Z^\dagger Z)^{-1/2} \ . \tag{A16}$$

These equations define the matrices A and D, with respect to an arbitrary transformation of the form

$$\begin{bmatrix} U & 0 \\ 0 & U' \end{bmatrix}$$

which does not change the state of the system and which can be ignored. It is easily checked that the transformation thus defined carries the state $|Z\rangle$ into $|\phi_0\rangle$. Therefore, the Jacobian (A14) can be written

$$|J(0,Z)| = [\det(1+Z^\dagger Z)]^{-(n_p+n_h)} = [\det(1+ZZ^\dagger)]^{-(n_p+n_h)} . \quad \text{(A17)}$$

The expression of the measure used in (2.24) follows trivially. This measure can also be obtained by identifying the set of Slater determinants with a complex Grassman manifold.[32] This method was used in Ref. 14. The method presented here is more elementary and similar to the methods used in Ref. 33 and Ref. 34. (See also Ref. 35.) We consider now the change of variables (2.27)

$$\beta_{ph} = \sum_{h'} Z_{ph'}[(1+Z^\dagger Z)^{-1/2}]_{h'h} . \quad \text{(A18)}$$

The expression of Z_{ph} in terms of β_{ph} is

$$Z_{ph} = \sum_{h'} \beta_{ph'}[(1-\beta^\dagger\beta)^{-1/2}]_{h'h} . \quad \text{(A19)}$$

In terms of these new variables, the matrix

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

of Eq. (A15) takes the form

$$\begin{bmatrix} (1-\beta^\dagger\beta)^{1/2} & -\beta^\dagger \\ \beta & (1-\beta\beta^\dagger)^{1/2} \end{bmatrix} . \quad \text{(A20)}$$

It is easily seen that the Jacobian of the transformation (A18) is precisely given by (A17). When the β are chosen as coordinates, the measure is, therefore, extremely simple. The domain of integration is complicated, however. The volume θ of this domain can be calculated. This fixes the arbitrary constant in the measure. One has[34]

$$\theta = \frac{1!2!\ldots(n_h-1)!1!2!\ldots(n_p-1)!}{1!2!\ldots(n_p+n_h-1)!}\ \pi^{n_p n_h} . \quad \text{(A21)}$$

Finally it is convenient to introduce new variables $\tilde{\alpha}$ and $\tilde{\beta}$ defined as follows:

$$\tilde{\alpha} = (1-\beta^\dagger\beta)^{1/2}U, \quad \tilde{\beta} = \beta U , \quad \text{(A22)}$$

where U is a $n_h \times n_h$ unitary matrix. It is easily seen that the integral over β transforms into

$$\int d\beta\, d\beta^* = \int d\tilde{\beta}\, d\tilde{\beta}^*\, d\tilde{\alpha}\, d\tilde{\alpha}^*\, \delta(\tilde{\alpha}^\dagger\tilde{\alpha} + \tilde{\beta}^\dagger\tilde{\beta} - 1) . \quad \text{(A.23)}$$

But $\tilde{\alpha}$ and $\tilde{\beta}$ are the expansion coefficients of a set of N single particle states on a fixed basis. Any basis may be used to write (A23). In particular, we can choose a wave function representation, in which case we shall write the integration measure (A23) as follows:

$$\int \prod_{k=1}^{N} \prod_{x} d\varphi_k^*(x) d\varphi_k(x) \prod_{l=1}^{N} \delta(\langle\varphi_k|\varphi_l\rangle - \delta_{kl}) . \quad \text{(A24)}$$

---

*On leave from Service de Physique Theorique, CEN Saclay, France.

[1] A. K. Kerman and S. E. Koonin, Ann. Phys. (N.Y.) 100, 332 (1976).
[2] F. Villars, Nucl. Phys. A285, 269 (1977).
[3] K. Goeke and P. G. Reinhard, Ann. Phys. (N.Y.) 112, 328 (1978).
[4] M. Baranger and M. Veneroni, Ann. Phys. (N.Y.) 114, 123 (1978).
[5] E. R. Marshalek and J. Weneser, Phys. Rev. C 2, 1682 (1970).
[6] D. Janssen, F. Dönau, S. Frauendorf, and R. V. Jolos, Nucl. Phys. A172, 145 (1971).
[7] J. P. Blaizot and E. R. Marshalek, Nucl. Phys. A309, 422 (1978); A309, 453 (1978).
[8] J. R. Klauder, Ann. Phys. (N.Y.) 11, 123 (1960); J. Math. Phys. 4, 1055 (1963); 4, 1058 (1963).
[9] J. R. Klauder, in *Path Integrals and their Application in Quantum, Statistical and Solid State Physics*, edited by G. Papadopoulos and J. Devrese (Plenum, New York, 1977).
[10] H. Kleinert, Phys. Lett. 69B, 9 (1977).
[11] H. Reinhardt, Nucl. Phys. A251, 317 (1975).
[12] S Levit, Phys. Rev. C 21, 1594 (1980); S. Levit, J. W. Negele, and Z. Paltiel, *ibid.* 21, 1603 (1980).
[13] H. Kleinert and H. Reinhardt, Nucl. Phys. A332, 331 (1979).
[14] H. Kuratsuji and T. Suzuki, Phys. Lett. 92B, 19 (1980).
[15] A. Kerman and T. Troudet (unpublished).

[16]J. P. Blaizot and H. Orland, J. Phys. Lett. 41, 53 (1980); 41, 401 (1980).
[17]J. P. Blaizot and H. Orland, J. Phys. Lett. 41, 523 (1980).
[18]J. P. Blaizot and H. Orland, Phys. Lett. 100B, 195 (1981).
[19]H. Orland, in *Méthodes Mathématiques de la Physique Nucléaire,* edited by B. Giraud and P. Quentin (Collége de France, Paris, 1980).
[20]V. Bargman, Commun. Pure Appl. Math. 14, 187 (1961).
[21]Y. Ohnuki and T. Kashiwa, Prog. Theor. Phys. 60, 548 (1978).
[22]D. J. Thouless, Nucl. Phys. 21, 225 (1960).
[23]L. D. Faddeev, in *Les Houches 1975,* Proceedings of the Methods in Field Theory, edited by R. Balian and J. Zinn-Justin (North-Holland, Amsterdam, 1970), p. 1.
[24]E. R. Marshalek and G. Holzwarth, Nucl. Phys. A191, 438 (1972).
[25]H. Trotter, Proc. Amer. Math. Soc. 10, 541 (1959).
[26]J. Hubbard, Phys. Rev. Lett. 3, 77 (1959).
[27]B. A. Lippman and J. Schwinger, Phys. Rev. 79, 469 (1950).
[28]R. F. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. 12D, 2443 (1975).
[29]R. Shankar, Phys. Rev. Lett. 45, 1088 (1980).
[30]K. K. Kan, J. J. Griffin, P. C. Lichtner, and M. Dworzecka, Nucl. Phys. A332, 109 (1979).
[31]H. Reinhardt, Nucl. Phys. A346, 1 (1980).
[32]S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience, New York, 1969), Vol. II.
[33]M. I. Monastyrsky and A. M. Perelomov, Rep. Math. Phys. 6, 1 (1974).
[34]L. K. Hua, *Harmonic Analysis of Functions of Several Complex Variables in Classical Domains,* translation of Mathematical Monographs (American Mathematical Society, Providence, 1963), Vol. 6, p.46.
[35]The parametrization (A3) of Slater determinants and the derivation of the corresponding invariant measure has been extensively studied by H. Kuratsuji and T. Suzuki. These authors have also derived the invariant measure following arguments similar to those used in the first part of this appendix (private communication of T. Suzuki to one of us).