Collective subspaces for large amplitude motion and the generator coordinate method

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The collective path $|\phi(q)\rangle$ to be used in a microscopic description of large amplitude collective motion is determined by means of the generator coordinate method. By varying the total energy with respect to $|\phi(q)\rangle$ and performing an adiabatic expansion a hierarchy of equations is obtained which determines uniquely a hierarchy of collective paths with increasing complexity. To zeroth order the $|\phi(q)\rangle$ are Slater determinants, to first order they include 2p-2h correlations. In both cases simple noniterative prescriptions for an explicit construction of the path are derived. For a correlated path their solutions agree at the Hartree-Fock minimum with random phase approximation eigenmodes. The resulting equations for the path are compared with the outcome of related theories, particularly of semiclassical nature. It is remarkable that both sorts of approaches, on one hand the generator coordinate method with correlated states and on the other the quantized adiabatic time dependent Hartree-Fock theory, are virtually identical in the results, although they are of different conceptual origin and use different techniques. It is shown that the use of a correlated path does not cause numerical complications.

[NUCLEAR STRUCTURE Collective path derived by GCM, inclusion of RPA correlations, relation to adiabatic TDHF.]

I. INTRODUCTION

In recent years there has been renewed interest in theories suitable for the microscopic description of large amplitude collective motion. Although those phenomena occur in all many fermion systems, particularly nuclear processes such as fission, heavy ion reactions and anharmonic multipole vibrations are a sensitive testing ground. The aim is to reduce the many body problem to a simpler one in terms of one (or few) collective degrees of freedom. One promising way to achieve this is provided by the concept of a collective path $|\phi(q)\rangle$. This is a set of suitably chosen A-body wave functions, which depends on a parameter q in such a way as to reflect properly the various stages of distortions of the system during the collective motion, like snapshots. The set $\{|\phi(q)\rangle\}$ spans a certain collective subspace of the full Hilbert space. In choosing $|\phi(q)\rangle$, one is guided by the objective that the Hilbert space splits as far as possible into a direct product of the collective subspace with the corresponding subspace of the noncollective degrees of freedom or, in other words, that the Hamiltonian of the system splits into a sum of a collective Hamiltonian and a noncollective one. If this is fulfilled, collective and noncollective motions are decoupled, and one can treat them separately. In general the splitting will only be fulfilled approximately, giving rise to phenomena such as friction, dissipation, damping, etc. However, it is hoped that a proper choice of the collective path allows us to minimize the residual coupling and treat it in low order perturbation theory.

There are two conceptually different ways to treat collective motion by means of a collective path $|\phi(q)\rangle$. One is provided by the generator coordinate method[1,2] (GCM). There, one diagonalized the total Hamiltonian H of the system in the subspace spanned by the $|\phi(q)\rangle$, using the ansatz

$$|\psi\rangle = \int dq f(q) |\phi(q)\rangle . \tag{1.1}$$

The superposition function $f(q)$ is to be evaluated by solving the well known Griffin-Hill-Wheeler equation[1]

$$\int dq' \langle\phi(q)|H-E|\phi(q')\rangle f(q') = 0 . \tag{1.2}$$

The GCM, employing the superposition principle (1.1), is a thoroughly quantum mechanical theory. The other group of theories is more classically minded, extracting the collective dynamics by studying the explicit time evolution of the system along the given path $|\phi(q(t),p(t))\rangle$. These theories are all embedded in the framework of time dependent Hartree-Fock (TDHF) theory. We will call

them hereafter mean field theories. They are widely used in their various stages of refinement as, e.g., the deformed shell model, or the constrained Hartree-Fock (HF) model together with various cranking approaches, and finally the adiabatic TDHF approach (ATDHF).[3-7]

Furthermore, there are essentially two basic questions to be solved in a microscopic description of collective motion by means of a path $|\phi(q)\rangle$: First, one has to determine the path $|\phi(q)\rangle$. A good choice of $|\phi(q)\rangle$ is important for a proper description of the processes, since large amplitude phenomena are characterized by the fact that $|\phi(q)\rangle$ substantially changes its structure, and therefore, it is not satisfying to have just an educated guess of the path. One really should have an equation of path (EOP) which uniquely determines an optimal $|\phi(q)\rangle$. Second, for a given path one has to recover the proper collective Hamiltonian H_c for the motion within the collective subspace $\{|\phi(q)\rangle\}$. The second problem, the evaluation of H_c, has been solved and discussed extensively for both approaches, the GCM and the mean field theories, with the result[5,8,9] that both conceptually different ways finally yield the same unique H_c if they use the same dynamic collective path $|\phi(q,p)\rangle$ depending on a pair of conjugate collective parameters.

It is the aim of this paper to study the first problem, i.e., the derivation of EOP, by means of the GCM. The GCM seems to be very appropriate for such an approach, since it is a genuine quantal theory and there is a strict variational principle for it. The use of the GCM for the construction of $|\phi(q)\rangle$ has already been suggested by Holzwarth and Yukawa.[10] The present approach goes beyond this by a more general treatment and by considering also correlated states $|\phi(q)\rangle$.

The present derivation of an EOP using the GCM is the last step towards a complete and unified view of the microscopic collective theories. The counterpart, the derivation of EOP using the mean field theories, has already been given by various authors[3-7] and leads eventually to the so-called ATDHF (adiabatic TDHF) equations for the path. The remarkable outcome of the present investigation will be that the ATDHF equations are virtually identical to those derived by means of the GCM if proper correlations are incorporated into the states $|\psi(q)\rangle$ of the path. Together with the known result that both ways yield the same quantized collective Hamiltonian,[8,9] this feature actually unifies two basic sorts of theories for large amplitude collective motion which are of entirely different conceptual background.

The contents of the paper are as follows: Section II describes the variational principle to be employed for the construction of the path. Section III displays a local algebra appropriate for the variation of the path. Section IV considers a path consisting of Slater determinants. In Sec. V it is shown that one can easily generalize the approach to states incorporating random phase approximation (RPA)-like correlations without complicating the numerical procedures. Section VI considers a dynamic generalization of the GCM which includes also the momentum p as a generator coordinate. The unification with other large amplitude approaches, particularly with the quantized form of ATDHF, is done in Sec. VII. Summary and conclusions are given in Sec. VIII. The present approach can easily be generalized to quasiparticles and to several coordinates. However, for the sake of simplicity this is not done here.

II. THE VARIATIONAL PRINCIPLE

Consider, e.g., the set of all A-body Slater determinants. It provides a complete basis for the Hilbert space of all A-body state vectors, which means that any A-body state $|\psi\rangle$ can be expressed as a linear superposition of Slater determinants. If the Hamiltonian of a system exhibits a well-developed collective degree of freedom, we can expect that the states of the collective spectrum are confined to a small subspace of states with nearly constant intrinsic (noncollective) excitation. One generally assumes that this collective subspace spanned by a set of Slater determinants $|\phi(q)\rangle$, depending on one generator coordinate q, i.e., all states within the subspace, can be superposed as

$$|\psi\rangle = \int dq f(q) |\phi(q)\rangle . \tag{2.1}$$

This ansatz is motivated by imagining that the $|\phi(q)\rangle$ represent a series of successive collective deformations, so to say, "snapshots" of the collective motion. The set $\{|\phi(q)\rangle\}$ constitutes the collective path. The $|\phi(q)\rangle$ need not to be restricted to Slater determinants, but can have a more general structure, see Sec. V.

Usually, in the generator coordinate method (GCM) one assumes the path $|\phi(q)\rangle$ to be given and derives an equation of motion (EOM) for $f(q)$ by variation

$$\delta_f \langle\psi|H-E|\psi\rangle = 0 \tag{2.2}$$

with respect to f. This yields the well known Griffin-Hill-Wheeler integral equation.[1]

$$\int dq \langle\phi(q')|H-E|\phi(q)\rangle f(q) = 0 , \tag{2.3}$$

which may be solved directly in the above form,

or which can often be transformed into a collective Schrödinger equation.[9,11,12]

In this paper, we aim at obtaining the equations of path (EOP) for the $|\phi(q)\rangle$, i.e., we want to determine the best possible path to be inserted in the ansatz (2.1). The EOP are found by variation

$$\delta_\phi \langle\psi|H-E|\psi\rangle=0 \tag{2.4}$$

with respect to ϕ. This yields

$$\delta_\phi \int dq\, dq' f^*(q')\langle\phi(q')|H-E|\phi(q)\rangle f(q)=0, \tag{2.5}$$

which determines the path $|\phi(q)\rangle$ for a given $f(q)$. This equation has already been discussed by Holzwarth and Yukawa.[10] Both Eqs. (2.3) and (2.5) form a coupled set which generates, in general, a spectrum of superposition functions $f_n(q)$ together with (f_n-dependent) paths $|\phi_n(q)\rangle$. Nothing guarantees yet that the resulting $|\phi_n(q)\rangle$ span a collective subspace distinguished by its decoupling properties.[7] In order to achieve this, one has to remember that a collective Hamiltonian corresponding to a well-established collective motion should not describe just one collective state, but a spectrum of states with different eigenenergies. Hence the GCM, which corresponds to a true collective motion, should be distinguished by the fact that *one* path $|\phi(q)\rangle$ fulfills Eq. (2.5) for a *full* spectrum $f_n(q)$. This means that Eq. (2.5) reduces to

$$\delta_\phi \langle\phi(q)|H-E|\phi(q')\rangle=0 \tag{2.6}$$

for *all* combinations of q and q'. This is actually a very strong requirement which might only be exactly fulfilled in the ideal case of collective motion corresponding to a symmetry of H.

In general cases, however, collectivity is mostly exhibited for adiabatic motion. Hence we first write the kernel of Eq. (2.5) in an expansion which is suited to the adiabatic limit, i.e., which counts orders of the collective momentum $\hat{p}$. For large systems, the overlaps $\langle\phi(q)|\phi(q')\rangle$ and $\langle\phi(q)|H|\phi(q')\rangle$ are peaked at $q=q'$, and for slow motion a differential expansion in orders $(q'-q)$ is appropriate, yielding

$$\langle\phi(q)|H|\phi(q')\rangle = I(q,q')\{\mathcal{H}_0-\tfrac{1}{2}i(q'-q)\mathcal{H}_1-\tfrac{1}{8}(q'-q)^2\mathcal{H}_2\pm\cdots\}, \tag{2.7}$$

where the overlap

$$\langle\phi(q)|\phi(q')\rangle=1-i(q'-q)\langle P_0\rangle-\tfrac{1}{2}(q'-q)^2\langle P_0^2\rangle\pm\cdots \tag{2.8}$$

is approximated by

$$I(q,q')=\exp\{-i(q'-q)\langle P_0\rangle-\tfrac{1}{2}(q'-q)^2\langle P_0^2\rangle\}. \tag{2.9}$$

The operator P_0 is defined by

$$P_0|\phi(q)\rangle=i\frac{\partial}{\partial q}|\phi(q)\rangle \tag{2.10}$$

and the coefficients $\mathcal{H}_n$ of $(q'-q)^n$ are given by

$$\mathcal{H}_0(\bar{q})=\langle\phi(\bar{q})|H|\phi(\bar{q})\rangle, \tag{2.11a}$$

$$\mathcal{H}_1(\bar{q})=\langle\phi(\bar{q})|\{\bar{H},P_0\}|\phi(\bar{q})\rangle, \tag{2.11b}$$

$$\mathcal{H}_2(\bar{q})=\left\langle\phi(\bar{q})\middle|\{P_0,\{\bar{H},P_0\}\}-i\left\{\bar{H},\frac{\partial P_0}{\partial q}\right\}\middle|\phi(\bar{q})\right\rangle. \tag{2.11c}$$

The $\bar{H}=H-\langle H\rangle$ and all expectation values in Eqs. (2.8)–(2.11) are to be evaluated at $\bar{q}=\frac{1}{2}(q+q')$. In contrast to the usual treatment,[11,12] we have to retain terms that are linear in $q'-q$ for the later variation. These formulas allow us to transform the integral Eq. (2.5) to a differential equation in terms of the collective momentum operator $\hat{p}=-id/dq$. The derivation is given in Appendix A in detail and yields the result

$$\delta_\phi \int dq\, g^*(q)(H_c(q,\hat{p})-E)g(q)dq=0, \tag{2.12}$$

with

$$H_c(q,\hat{p})=H_0+:\hat{p}H_1:+:\hat{p}^2H_2:+\cdots, \tag{2.13}$$

with

$$:\hat{p}^nA:=2^{-n}\sum_{m=0}^{n}\binom{n}{m}\hat{p}^mA\hat{p}^{n-m}.$$

The various terms are given by

$$H_0(q)=\mathcal{H}_0(q)-\frac{\langle P_0\rangle}{2\langle P_0^2\rangle}\mathcal{H}_1(q)+\left(\frac{\langle P_0\rangle^2}{16\langle P_0^2\rangle^2}-\frac{1}{8\langle P_0^2\rangle}\right)\mathcal{H}_2(q)\pm\cdots, \tag{2.14a}$$

$$H_1(q)=-\frac{1}{\langle P_0^2\rangle}\mathcal{H}_1(q)+\frac{\langle P_0\rangle}{4\langle P_0^2\rangle^2}\mathcal{H}_2(q)\pm\cdots, \tag{2.14b}$$

$$H_2(q)=\frac{1}{4\langle P_0^2\rangle}\mathcal{H}_2(q)\pm\cdots. \tag{2.14c}$$

The $g(q)$ is related to $f(q)$ by

$$g(q)=\int I^{1/2}(q,q')f(q')dq'.$$

The expectation values in Eq. (2.14) are to be evaluated at $|\phi(q)\rangle$.

If one requires the path $|\phi(q)\rangle$ to be the same for a full spectrum $g_n(q)$, then the group of Eqs. (2.11) is equivalent to postulating separately $\delta_\phi H_0=\delta_\phi H_1=\delta_\phi H_2=\cdots=0$, which is exactly as strong a condition as Eq. (2.6). However, for an adiabatic mo-

tion, the terms in Eq. (2.12) with increasing powers in $\hat{p}$ are of decreasing importance for the description of the motion. This defines in a natural way an order counting such that to zeroth order the path is determined by the terms proportional to $\mathcal{H}_0$, which originate from $(q'-q)^0$, to first order by the terms proportional to $\mathcal{H}_0$ and proportional to $\mathcal{H}_1$, which originate from $(q'-q)^0$ *and* $(q'-q)^1$, etc. To zeroth order one obtains explicitly

$$\delta_\phi \langle H \rangle = 0 \tag{2.15}$$

and to first order in addition

$$\delta_\phi \langle \{\overline{H}, P_0\} \rangle = 0 . \tag{2.16}$$

Actually, the term proportional to $\mathcal{H}_1$ in the first-order expansion of H_0 has been neglected, since its variation is automatically zero with $\delta_\phi \mathcal{H}_1 = 0$, i.e., with Eq. (2.16). This is a general feature of Eqs. (2.14) persisting to all orders with the consequence that only the leading terms on the right hand side, i.e., $\mathcal{H}_0$, $\mathcal{H}_1$, $\mathcal{H}_2, \ldots$ have to be varied. [The expectations in Eqs. (2.14) are to be evaluated at $|\phi(q)\rangle$. To require $\delta_\phi H_n = 0, \ldots, \delta_\phi H_0 = 0$ up to a given order n is equivalent to require $\delta_\phi \mathcal{H}_n = 0$, $\delta_\phi \mathcal{H}_0 = 0$, since the subtraction terms in $\delta_\phi H_i = 0$, $i < n$ are just $\delta_\phi H_{i+k}$, which are already solved in $\delta_\phi H_{i+k} = 0$ up to the given order, $i+k \leq n$.] This shows that an order counting in terms of $(q'-q)^n$ is equivalent to an order counting in terms of $\hat{p}^n$. Apparently, to second and higher orders one obtains more and more complicated expressions. As will be shown in the next sections, the dominating term in the zero-order variation can be met by a pure Slater determinant, in the first-order variation by an RPA-type correlated state, in the second-order variation by second-order RPA, etc. In the present paper we will consider in detail the zeroth and first order.

III. THE VARIATION OF THE PATH

The collective path should belong to a family of simple wave functions. In the following, we will consider Slater determinants or RPA-correlated states. As in the case of Slater determinants, we can also assume for the RPA-correlated states that Thouless's theorem applies,[13] viz., that for a given state $|\phi(q)\rangle$ any infinitesimally neighbored state $|\tilde{\phi}(q)\rangle$ can be expressed by weakly excited 1p-1h excitations

$$|\tilde{\phi}(q)\rangle = \left(1 + \sum C_{ni} a_n^\dagger a_i\right) |\phi(q)\rangle , \tag{3.1}$$

where $a_n^\dagger$ creates a particle in state n and a_i a hole in state i. The grouping into empty states n and occupied states i depends on the reference point $|\phi(q)\rangle$ and so does the definition of a 1p-1h operator. The algebra of 1p-1h excitations can be handled in different ways. For the following, it is most convenient to couple them to a basis of Hermitian operators[7]

$$P_\alpha(q) = \sum_{n,i} \frac{i}{\sqrt{2}} (p_{ni}^{(\alpha)} a_n^\dagger a_i - p_{ni}^{(\alpha)*} a_i^\dagger a_n) , \tag{3.2}$$

$$Q_\alpha(q) = \sum_{n,i} \frac{i}{\sqrt{2}} (q_{ni}^{(\alpha)} a_n^\dagger a_i + q_{ni}^{(\alpha)*} a_i^\dagger a_n) . \tag{3.3}$$

In order that the P_α and Q_α provide a basis for the 1p-1h operators, they should form an orthogonal

$$\langle \phi(q) | [Q_\alpha(q), P_\beta(q)] | \phi(q) \rangle = i \delta_{\alpha\beta} , \tag{3.4a}$$

$$\langle \phi(q) | [Q_\alpha(q), Q_\beta(q)] | \phi(q) \rangle = 0 , \tag{3.4b}$$

$$\langle \phi(q) | [P_\alpha(q), P_\beta(q)] | \phi(q) \rangle = 0 \tag{3.4c}$$

and complete set,

$$A_{\text{ph}} = \sum_\alpha \{ i Q_\alpha(q) \langle \phi(q) | [P_\alpha(q), A] | \phi(q) \rangle - i P_\alpha(q) \langle \phi(q) | [Q_\alpha(q), A] | \phi(q) \rangle \} , \tag{3.5}$$

where A may be any operator and A_{ph} is its 1p-1h part with respect to $|\phi(q)\rangle$. With respect to all possible 1p-1h operators, the Q_α, P_α are a complete set. The set of state vectors $Q_\alpha|\phi(q)\rangle$ and $P_\alpha|\phi(q)\rangle$, however, is overcomplete. Each $Q_\alpha|\phi(q)\rangle$ can be represented as a linear superposition

$$Q_\alpha |\phi(q)\rangle = \sum_\beta \gamma_\beta i P_\beta |\phi(q)\rangle$$

and vice versa. It is thus possible to assume a coupling (3.2) and (3.3) for which

$$P_\alpha(q) |\phi(q)\rangle = i Q_\alpha(q) |\phi(q)\rangle . \tag{3.6}$$

This assumption establishes a relation between the $q_{ni}^{(\alpha)}$ and $p_{ni}^{(\alpha)}$, depending on the state $|\phi(q)\rangle$. With Eq. (3.4a) one sees that this corresponds to the orthogonality relations

$$\langle \phi(q) | \{P_\alpha, P_\beta\} | \phi(q) \rangle = \langle \phi(q) | \{Q_\alpha, Q_\beta\} | \phi(q) \rangle = \delta_{\alpha\beta} .$$

In the Q_α, P_α representation, the neighborhood of $|\phi(q)\rangle$ can be represented as

$$|\tilde{\phi}(q)\rangle = \left(1 - i \sum_\alpha \delta q_\alpha P_\alpha(q) + i \sum_\alpha \delta p_\alpha Q_\alpha(q)\right) |\phi(q)\rangle , \tag{3.7}$$

where δq_α and δq_α can be restricted to real values, since $i\,\delta q_\alpha$ is equivalent to δp_α and vice versa, owing to Eq. (3.6). We now assume a labeling α so that $P_0(q)$ is the generator of the neighbor state *within* the path

$$|\phi(q+\delta q)\rangle=(1-i\,\delta q P_0(q))|\phi(q)\rangle\,. \tag{3.8}$$

The variations of the path $\delta_\phi|\phi(q)\rangle$ consist then in all states *not* proportional to (3.8). These are indicated by the superscript $\perp$ and are

$$|\phi(q)+\delta^\perp_\phi(q)\rangle=\Big(1-i\sum_{\alpha\neq 0}\epsilon_\alpha(q)P_\alpha(q) +i\sum_{\beta=\text{all}}\epsilon'_\beta(q)Q_\beta(q)\Big)|\phi(q)\rangle \tag{3.9}$$

for all possible choices of real $\epsilon_\alpha(q)$ and $\epsilon'_\beta(q)$. [In fact one has in mind thereby localized variations, i.e., $\epsilon(q)\propto\delta(q-q_0)$.]

It should be remarked that without changing the structure of the 1p-1h space, one could assume a more general form of Eq.(3.6) containing a proportionality factor λ_α, i.e., $P_\alpha|\phi\rangle=i\lambda_\alpha Q_\alpha|\phi\rangle$, with $\lambda_\alpha=2\langle P_\alpha{}^2\rangle$. This would merely change the scale in Eq. (3.8). Thus we are free to choose a scale which is most convenient, i.e., $\lambda_\alpha=1$ for all q which lead to Eq. (3.6).

IV. THE EOP FOR A DETERMINANTAL PATH

In this section, we are going to derive the EOP for a one parameter path $|\phi_0(q)\rangle$, which consists strictly of Slater determinants. In that case, the neighborhood is given by all 1p1h excitations, and the developments of the previous section can be applied. For pure Slater determinants we have

$$a_i^\dagger a_n|\phi_0(q)\rangle=0 \tag{4.1}$$

and thus obtain from the condition (3.6) the relation

$$q_{ni}^{(\alpha)}=p_{ni}^{(\alpha)}\,, \tag{4.2}$$

which links Q_α and P_α. If one knows Q_α, one immediately knows P_α, and vice versa.

From the hierarchy of conditions (2.14) we consider now only the first, i.e., (2.15) and look how far this does determine the path. The variations in (3.9) yield

$$\langle\phi_0(q)|\,[P_\alpha(q),H]\,|\phi_0(q)\rangle=0\,,\quad\text{for }\alpha\neq 0 \tag{4.3}$$

$$\langle\phi_0(q)|\,[Q_\beta(q),H]\,|\phi_0(q)\rangle=0\quad\text{for all }\beta\,. \tag{4.4}$$

These zero-order equations already determine the path: Suppose that one point $|\phi_0(q)\rangle$ on the path is known. There the total Hamiltonian can be expanded in 1pp, 1hh, 1ph, 2pp, ... operators. The above equations are only sensitive to the 1p-1h part of H which can be written, using the completeness (3.5)

$$H_{\text{ph}}=\sum_\beta iQ_\beta(q)\langle\phi_0(q)|\,[P_\beta(q),H]\,|\phi_0(q)\rangle - iP_\beta(q)\langle\phi_0(q)|\,[Q_\beta(q),H]\,|\phi_0(q)\rangle\,. \tag{4.5}$$

Due to Eqs. (4.3) and (4.4) only one term remains:

$$H_{\text{ph}}=iQ_0(q)\langle\phi_0(q)|\,[P_0(q),H]\,|\phi_0(q)\rangle\,. \tag{4.6}$$

We thus obtain the path generator P_0 as

$$P_0(q)=i\,cH_{\text{ph}}(q)\,, \tag{4.7}$$

with c being a real proportionality factor. Its choice is free and determines merely the scale of the collective path. It can be chosen such that $\langle P_0{}^2\rangle=\text{const}$, as suggested at the end of Sec. III. Another way of fixing the scale is, e.g., the use of a measuring operator $\mathcal{Q}$, such that

$$\langle\phi_0(q)|\,\mathcal{Q}\,|\phi_0(q)\rangle=q\,.$$

In this case we derive from

$$\langle\phi_0(q+\delta q)|\,\mathcal{Q}\,|\phi_0(q+\delta q)\rangle=q+\delta q$$

the c as

$$c^{-2}=\langle\phi_0(q)|\,\{H_{\text{ph}},\mathcal{Q}\}\,|\phi_0(q)\rangle\,.$$

No matter how c is chosen, Eqs. (4.7) with (3.8) show that if we know one point $|\phi_0(q)\rangle$ on the path, we know also its neighbor $|\phi_0(q+\delta q)\rangle$, and thus the total path can be constructed successively.

One point which should be on the path is the Hartree-Fock minimum $|\phi(0)\rangle$ determined by

$$\langle\phi_0(0)|\,[P_\beta(0),H]\,|\phi_0(0)\rangle=\langle\phi_0(0)|\,[Q_\beta(0),H]\,|\phi_0(0)\rangle \tag{4.8}$$

for all β. But there the propagator $P_0(q)$ is not determined uniquely because Eq. (4.7) contains an undefined limit, $H_{\text{ph}}\to 0$ and $c\to\infty$. We have to study a small neighborhood of the HF point in order to specify the first step (rule of l'Hôspital). Taking the ∂_{q_0} derivative of Eqs. (4.3) and (4.4), we obtain

$$\langle\phi_0(q)|\,[P_0(q),[H,P_\alpha(q)]] -i[H,(\partial_q P_\alpha(q))_{\text{ph}}]\,|\phi_0(q)\rangle=0\,, \tag{4.9}$$

$$\langle\phi_0(q)|\,[P_0(q),[H,Q_\beta(q)]] -i[H,(\partial_q Q_\beta(q))_{\text{ph}}]\,|\phi_0(q)\rangle=0\,, \tag{4.10}$$

where we have used

$$\partial_q|\phi_0(q)\rangle=-iP_0(q)\,|\phi_0(q)\rangle\,,$$

$$\partial_q P_\alpha(q)=-i[P_0(q),P_\alpha(q)]+(\partial_q P_\alpha(q))_{\text{ph}},$$

and similarly for $\partial_q Q_\beta(q)$. (For an extensive discussion of the latter relations see Ref. 7.) At the HF point $|\phi_0(0)\rangle$, the 1p-1h terms from $\partial_q P$ and $\partial_q Q$ do not contribute, and we obtain the equations determining the first step $P_0(0)$:

$$\langle\phi_0(0)|\,[P_0(0),[H,P_\alpha(0)]]\,|\phi_0(0)\rangle=0\,,\quad\text{for }\alpha\neq 0 \tag{4.11}$$

$$\langle\phi_0(0)|\,[P_0(0),[H,Q_\beta(0)]]\,|\phi_0(0)\rangle=0\quad\text{for all }\beta\,. \tag{4.12}$$

These equations bear some resemblance to the RPA equations [see Eq. (5.18)]. In fact, they are half of them, viz., the part which determines $P_0(0)$. [The $Q_0(0)$ follows from Eq. (4.2).] Its solution becomes explicitly a matrix equation for the expansion coefficients $p_{ni}^{(0)}$ in Eq. (3.2). It will yield a whole spectrum of eigenoperators $P_\alpha(0)$, all mutually decoupling in Eq. (4.11), and all of them can formally be used as propagators to the first off-equilibrium point on the path,

$$|\phi_0(\delta q)\rangle = (1 - i\,\delta q P_0(0))\,|\phi_0(0)\rangle\,.$$

In practice, however, one has in mind a certain collective motion such as, e.g., fission or a multipole vibration. This preconceived knowledge of the motion can be used to select from the spectrum of Eqs. (4.11) and (4.12) that mode which is expected to be the small amplitude limit of the large amplitude motion under consideration. For initiating a fission path, e.g., one will use the lowest collective quadrupole mode.

An important feature of the path is its behavior under time reversal. Here Eqs. (4.11) and (4.12) come into play. Assume one given point on the path $|\phi(q)\rangle$ to be time even. Then $H_{\rm ph}$ will be time even and, according to Eq. (4.7), the $P_0(q)$ time odd. From step (3.8) we see finally that $|\phi_0(q+\delta q)\rangle$ again will be time even. Thus if one point on the path, off equilibrium, is time even, then the whole path is time even. The HF minimum itself is certainly time even and Eq. (4.12) is trivially fulfilled if we choose from the spectrum of Eq. (4.11) the solution $P_0(q)$ to be time even, which is a reasonable decision. Thus the whole path consists in time-even $|\phi(q)\rangle$, which represent statically deformed states. This means we have obtained the path in a zeroth-order adiabatic limit as a natural outcome of the expansion (2.14), which implies a counting in orders of the collective momentum.

Altogether we see that if we restrict the $|\phi_0(q)\rangle$ to be Slater determinants, being analytical in q, and to be determinants along real q, then the first of the conditions (2.9) alone is sufficient to determine uniquely the EOP [except for some freedom of choosing the mode at $|\phi_0(0)\rangle$]. Any further condition of (2.14) is met by chance or violated. If we want to take into account higher orders, we have to release some restriction on $|\phi_0(q)\rangle$.

V. THE COLLECTIVE PATH FOR CORRELATED STATES

As we have seen in the preceding section, the restriction of $|\phi(q)\rangle$ to Slater determinants allows only the lowest order condition (2.14a) to be met. The next possible generalization is to consider correlated states $|\phi_c(q)\rangle$ which contain weak 2p-2h excitations. (Owing to Thouless's theorem, the 1ph excitations cannot lead out of the determinantal space.) One could handle them explicitly as

$$|\phi_c(q)\rangle = \left(1 + \sum \gamma_{nmij}\, a_n^\dagger a_i\, a_m^\dagger a_j\right)|\phi(q)\rangle\,.$$

However, we prefer to determine the correlations by means of their 1p-1h properties; we require the $|\phi_c(q)\rangle$ to be a vacuum for a certain set of 1p-1h operators $B_\mu(q)$:

$$B_\mu(q)\,|\phi_c(q)\rangle = 0\,. \tag{5.1}$$

The B_μ can be represented in general by means of the operator algebra of Sec. III as $B_\mu = \sum_\alpha c_\alpha^{(\mu)} Q_\alpha + d_\alpha^{(\mu)} P_\alpha$. Their choice defines type and size of the correlations. This way of defining $|\phi_c\rangle$ is well known in RPA where the $B_\mu^\dagger$ are the boson operators $B_\mu^\dagger = (1/\sqrt{2})(Q_\mu + iP_\mu)$, with Q_μ, P_μ being the eigenmodes of RPA, and where Eq. (5.1) defines $|\phi_c\rangle$ as the so-called boson vacuum.[13,14] Thouless's theorem and the concept of the 1p-1h neiborhood still hold for this type of correlated states.

Since we are working in a state space more general than Slater determinants, we have to release condition (4.4) (which was $q_{ni}^{(\alpha)} = p_{ni}^{(\alpha)}$). This makes Q_α independent from P_α and we hope that, with this greater flexibility in the basis, we can also meet the first-order condition (2.16). We have to keep in mind, however, that the correlations are not completely arbitrary but are to be determined by condition (5.1). In the following, we will take into account only the least amount of correlations necessary to fulfill the first-order condition (2.16), i.e., we restrict the set B_μ just to the "path-boson" B_0 and remain with the condition

$$(Q_0(q) - iP_0(q))\,|\phi_c(q)\rangle = 0\,. \tag{5.2}$$

This condition links the correlation structure with the relation between Q_0 and P_0: If the correlations are given, then Q_0 and P_0 are no longer independent of each other. Or, in turn, the correlations can be determined by Eq. (5.2) if we evaluate P_0 independently from Q_0 by a further dynamical equation [further than Eqs. (4.3) and (4.4) alone], yet to be found by varying also the first-order condition (2.16).

Again we choose P_0 to be the path generator according to Eq. (3.8), i.e.,

$$|\phi_c(q+\delta q)\rangle = (1 - i\,\delta q P_0(q))\,|\phi_c(q)\rangle$$

and remain with the variations in (3.9). In contrast to the determinantal case, we have now to meet an additional condition, viz., Eq. (5.2). This is achieved by adding a constraining functional to the variational Eq. (2.15). We formulate it as

$$\Lambda=\int dq\,dq' f^*(q) \times\{\langle\phi_c(q)|P_0(q')-iQ_0(q')|\phi_c(q')\rangle\,\eta(q') + \eta^*(q)\langle\phi_c(q)|P_0(q)+iQ_0(q)|\phi_c(q')\rangle\}, \quad (5.3)$$

where $\eta(q)$ is a continuous set of Lagrange multipliers. Along the same lines as for $\langle\psi|H|\psi\rangle$, we perform a narrow overlap expansion for Λ (for details see Appendix B) yielding

$$\Lambda=\int dq\,dq' f^*(q)\langle\phi_c(q)|\phi_c(q')\rangle\{[\eta(\bar q)+\eta^*(\bar q)]\langle\phi_c(\bar q)|P_0|\phi_c(\bar q)\rangle - i[\eta(\bar q)-\eta^*(\bar q)]\langle\phi(\bar q)|Q_0|\phi_c(\bar q)\rangle - \tfrac{1}{2}i(q'-q)[(\partial_q[\eta(\bar q)+\eta^*(\bar q)])\langle\phi_0(\bar q)|Q_0|\phi_c(\bar q)\rangle + i(\partial_q[\eta(\bar q)-\eta^*(\bar q)])\langle\phi_c(\bar q)|P_0|\phi_c(\bar q)\rangle]\pm\cdots\}f(q'). \quad (5.4)$$

In zeroth order we then obtain

$$\langle\phi_c(q)|[P_\alpha(q),H]|\phi_c(q)\rangle=0, \quad \text{for } \alpha\neq 0 \quad (5.5)$$

$$\langle\phi_c(q)|[Q_\beta(q),H-\mathrm{Re}(\eta)P_0(q)]|\phi_c(q)\rangle=0 \quad \text{for all } \beta. \quad (5.6)$$

This seems to be a change compared to Eqs. (2.14) or (4.3) and (4.4). However, the Lagrangian multiplier $\mathrm{Re}(\eta)$ is not really in effect here. It can be chosen freely and we assume for convenience

$$\mathrm{Re}(\eta)=0. \quad (5.7)$$

[Any other choice would only introduce a recoupling within the operators Q_0 and P_0, being the eigensolutions of Eq. (5.7). If Q_0, P_0 is the set for $\mathrm{Re}(\eta)=0$, we can transform to $\tilde Q_0=\cos(\gamma)Q_0+\sin(\gamma)P_0$ and $\tilde P_0=\cos(\gamma)P_0-\sin(\gamma)Q_0$, which then fulfills Eqs. (5.5) and (5.6) for $\mathrm{Re}(\eta)=\sin(\gamma)(-i)\langle[P_0,H]\rangle$.] Thus we remain with the lowest order equations

$$\langle\phi_c(q)|[P_\alpha(q),H]|\phi_c(q)\rangle=0, \quad \text{for } \alpha\neq 0 \quad (5.8)$$

$$\langle\phi_c(q)|[Q_\beta(q),H]|\phi_c(q)\rangle=0, \quad \text{for all } \beta \quad (5.9)$$

which determine $Q_0(q)$, using the completeness (3.7) as

$$Q_0(q)=(\partial_0\mathcal{V})^{-1}H_{\mathrm{ph}}(q). \quad (5.10)$$

There the

$$\partial_q\mathcal{V}=-i\langle\phi_c(q)|[H,P_0(q)]|\phi_c(q)\rangle$$

can be interpreted as the slope of the collective potential $\mathcal{V}(q)=\langle\phi_c(q)|H|\phi_c(q)\rangle$. The slope, of course, depends on the scale of q and thus the $\partial_q\mathcal{V}$ plays a role similar to the proportionality factor c in Eq. (4.7). Equation (5.10) determines only $Q_0(q)$. We find the equation for $P_0(q)$ by performing the variation of the first-order condition (2.16) together with the first-order part of the constraint (5.6). Changing in addition $\langle\{H,P_0\}\rangle$ to $\langle[H,Q_0]\rangle$ by means of Eq. (5.2), we obtain

$$\langle\phi_c(q)|[P_\alpha(q),[H,Q_0(q)]]|\phi_c(q)\rangle=0, \quad \text{for } \alpha\neq 0 \quad (5.11)$$

$$\langle\phi_c(q)|[Q_\beta(q),[H,Q_0(q)]-i\,\mathrm{Im}(\partial_q\eta)P_0(q)]|\phi_c(q)\rangle=0 \quad \text{for all } \beta \quad (5.12)$$

[the

$$\partial_q\langle\phi_c|[Q_\beta,P_0]|\phi\rangle=\partial_q(i\delta_{\beta 0})$$

does not contribute in the variation]. Here the Lagrangian multiplier $\mathrm{Im}(\eta)$ is really necessary, it allows us to fulfill Eq. (5.12) for $\beta=0$. There one obtains

$$\mathrm{Im}(\partial_q\eta)=-\mathcal{C}_{00}, \quad (5.13)$$

where

$$\mathcal{C}_{00}(q)=\langle\phi_c(q)|[Q_0(q),[H,Q_0(q)]]|\phi_c(q)\rangle. \quad (5.14)$$

Thus Eq. (5.14) becomes explicitly

$$\langle\phi_c(q)|[Q_\beta(q),[H,Q_0(q)]+i\mathcal{C}_{00}(q)P_0(q)]|\phi_c(q)\rangle=0. \quad (5.15)$$

The two first-order Eqs. (5.13) with (5.17) allow us to determine $P_0(q)$ as

$$P_0(q)=\mathcal{C}_{00}^{-1}i[H,Q_0(q)]_{\mathrm{ph}} =\mathcal{C}_{00}^{-1}(\partial_q\mathcal{V})^{-1}[H,H_{\mathrm{ph}}]_{\mathrm{ph}}. \quad (5.16)$$

Thus if we know one point of the path $|\phi_c(q)\rangle$ and it is off equilibrium (since $\partial_q\neq 0$ is required), we know the path generator $P_0(q)$ and can construct the next point $|\phi_c(q+\delta q)\rangle$. From this one can proceed further and can successively construct the whole path.

There is a simplification, which makes use of a theorem proved by Thouless,[15] which states that commutators of the Hamiltonian between correlated states can equally well be evaluated between the corresponding uncorrelated single particle states. Hence the EOP for the uncorrelated $|\phi(q)\rangle$, associated with $|\phi_c(q)\rangle$, are given by

$$\langle\phi(q)|[P_\alpha(q),H]|\phi(q)\rangle=0, \quad \text{for } \alpha\neq 0$$
$$\langle\phi(q)|[Q_\beta(q),H]|\phi(q)\rangle=0, \quad \text{for all } \beta \quad (5.17)$$

with

$$\langle\phi(q)|[P_\alpha(q),[H,Q_0(q)]]|\phi(q)\rangle=0, \quad \text{for } \alpha\neq 0$$
$$\langle\phi(q)|[Q_\beta(q),[H,Q_0(q)]+i\mathcal{R}_{00}P_0(q)]|\phi(q)\rangle=0 \quad \text{for all } \beta. \quad (5.18)$$

For this uncorrelated $|\phi(q)\rangle$, the construction proceeds in a similar manner as outlined above for the correlated path, using successively the step $P_0\propto[H,H_{\rm ph}]_{\rm ph}$. In order to initiate the construction one must know one point of the path. Obviously the HF minimum belongs to $|\phi(q)\rangle$ and the corresponding RPA-correlated state to $|\phi_c(q)\rangle$. Unfortunately, there one has $\partial\mathcal{V}/\partial q=0$, with it $H_{\rm ph}=0$, and P_0 remains undetermined. Performing the ∂_q derivative of Eq. (4.11) one obtains

$$\langle\phi(q)|[P_\alpha(q),[H,P_0(q)]]|\phi(q)\rangle=0, \quad \text{for } \alpha\neq 0$$
$$\langle\phi(q)|[Q_\beta(q),[H,P_0(q)]]|\phi(q)\rangle=0, \quad \text{for all } \beta \quad (5.19)$$
$$\langle\phi(q)|[Q_\beta,[H,Q_0(q)]]|\phi(q)\rangle=\delta_{\beta 0}\mathcal{R}_{00}(q) \quad \text{for all } \beta.$$

These are the RPA equations at the HF minimum $q=0$. They can be solved in the standard way. As a solution, one obtains a spectrum of eigenmodes, each one characterized by a pair Q_α,P_α. Choosing one of them in particular as Q_0,P_0, we select the collective channel which we want to extend to large amplitudes [see the same discussion following Eqs. (4.11) and (4.12)]. We then can evaluate the first off-equilibrium point

$$|\phi(\delta q)\rangle=(1-i\delta q P_0(0)|\phi(0)\rangle$$

and, by means of the above step-by-step method, the full $|\phi(q)\rangle$ for all q. The correlated $|\phi_c(q)\rangle$ can then be constructed from $|\phi(q)\rangle$ according to Eq. (5.2).

For practical calculations it is important to note that in most of the cases it is not necessary to determine $|\phi_0(q)\rangle$ explicitly. It is sufficient to construct the uncorrelated path $|\phi(q)\rangle$ together with $P_0(q)$ and $Q_0(q)$ and to express the final quantities one is interested in by these three objects, thus handling the correlations implicitly. For example, if one consideres a GCM along $|\phi_c(q)\rangle$, a Schrödinger equation can be derived from it by means of techniques exposed in Appendix A, which finally can be expressed solely in terms of $|\phi(q)\rangle$, $|P_0(q)\rangle$, and $|Q_0(q)\rangle$. The inverse collective mass, e.g., is given by

$$M^{-1}=\langle\phi_c|\{P_0,\{H,P_0\}\}|\phi_c\rangle/4\langle P_0^2\rangle$$
$$=\langle\phi_c|[Q_0,[H,Q_0]]|\phi_c\rangle.$$

Since double anticommutators between correlated states agree with those between uncorrelated states,[15] the inverse mass equals $\langle\phi|[Q_0,[H,Q_0]]|\phi\rangle$. Details can be found in Refs. 8 and 9. If, nevertheless, an explicit construction of $|\phi_c(q)\rangle$ from $|\phi(q)\rangle$ is required, one can use Eq. (6.4) of the next section. It should be remarked that the uncorrelated path $|\phi(q)\rangle$ obtained by Eqs. (5.17) and (5.18) is different from the path $|\phi_0(q)\rangle$ determined by the zero-order Eqs. (4.3) and (4.4) of the previous section.

By comparing Secs. III and IV, one realizes that we have been studying the first two members of a systematic hierarchy of more and more complex collective paths. For purely Slater determinantal collective paths, already the zero-order Eq. (2.15) determined $|\phi_0(q)\rangle$ uniquely, using a sort of simplified RPA equation at the HF minimum as an initial condition. The next step consisted in allowing 2p-2h correlations in the path $|\phi_c(q)\rangle$ which was then determined by the zero- and first-order Eqs. (2.16). They lead to a $|\phi_c(q)\rangle$, which was the large amplitude extension of the full RPA at the HF minimum. Obviously one could implement higher and higher orders of correlations exhausting more and more terms in the $\hat{p}$ expansion (2.14) and leading to higher-order RPA solutions at $|\phi(0)\rangle$. It would correspond to approaching the exact solution in the framework of an np-nh expansion within the shell model description. This, however, is precisely what one wants to avoid by introducing the concept of a collective path in large amplitude theories. Hence from both a conceptual and practical point of view, it does not seem to make much sense to go to higher than the lowest orders in Eq. (2.14).

Equations (5.16) and (5.19) suggest the following procedure for the explicit construction of the collective path: (1) Find the stationary HF minimum. (2) Solve there the RPA Eqs. (5.19) and select the desired mode Q_0,P_0. (3) Step off the HF equilibrium

$$|\phi(\delta q)\rangle=(1-i\delta q P_0)|\phi_{\rm HF}\rangle.$$

(4) Use this off-equilibrium point as an initial condition for the differential Eq. (5.16) and construct successively the rest of the path going "uphill." However, since the fall lines of the potential valley are all infinitesimally close to each other and diverge with increasing distance from the HF point, this construction of the path is not stable. Hence it is preferred to find one off-equilibrium point in a finite distance from the HF point and proceed towards the HF minimum rather than away from it. Saddle points can be used for it or the off-equilibrium point can be constructed by simple iteration methods.

VI. THE EOP FOR A DYNAMIC PATH

An alternative way of extending a determinantal path $|\phi(q)\rangle$ consists in allowing a dependence on collective dynamics. This is achieved by introduc-

ing the collective momentum p as a second parameter, thus working with a two parameter, but still determinantal path $|\phi(q,p)\rangle$. (In fact, this sort of collective path is the natural starting point in the mean field theories, such as ATDHF.) We now ought to consider the twofold superposition

$$|\psi\rangle = \int dq\, dp f(q,p) |\phi(q,p)\rangle . \tag{6.1}$$

This defines the dynamic GCM which has been discussed extensively in Refs. 8 and 9. Unfortunately, two parameters within a GCM are too much for describing only one mode. This gives rise to difficulties in a direct numerical treatment and it forbids a straightforward derivation of a collective Schrödinger equation from the Griffin-Hill-Wheeler equation. In Refs. 8 and 9 a solution to these problems has been proposed, which relies on an expansion of the Griffin-Hill-Wheeler (GHW) equation for small fluctuations in p. Therefore, for slow collective motion, an adiabatic expansion is appropriate where $|\phi(q,p)\rangle$ is expanded in orders p^n about $p=0$. The first step is

$$|\phi(q,p)\rangle \cong (1+ip Q_0)|\phi(q,0)\rangle . \tag{6.2}$$

In that limit, the GHW equation for p can be solved analytically with Gaussian superpositions. This eventually leads to the reduction of the GCM with a pair of conjugate parameters to an equivalent one parameter GCM, i.e.,

$$|\psi\rangle = \int dq\, f(q) |\phi_c(q)\rangle , \tag{6.3}$$

using an improved path $|\phi_c(q)\rangle$, which is given by

$$|\phi_c(q)\rangle = \int dq'\, dp'\, F(q;q',p') |\phi(q',p')\rangle . \tag{6.4}$$

The folding function $F(q;q',p')$ is Gaussian in $(q-q')$ and p'; an explicit expression for it can be found in Eq. (7) of Ref. 8.

This path is an improved one in the sense that it decouples in order p^2 the collective velocities from the noncollective ones. As a result of this, we have, e.g., proportionality between collective current and progression:

$$Q_0|\phi_c(q)\rangle = iP_0|\phi_c(q)\rangle .$$

Obviously, the $|\phi_c(q)\rangle$ is no longer a Slater determinant and shows correlations. In fact, concerning the description of the collective channel, the $|\phi_c(q)\rangle$ is fully equivalent to the RPA-correlated path introduced in the previous section. The further evaluation of the variational equations can proceed as given there, and the resulting EOP will be identical. We thus end up with the interesting result that both above attempts to generalize a one parameter determinantal path finally prove to be identical.

Although transformation from $|\phi(q,p)\rangle$ to the improved static path $|\phi_c(q)\rangle$ and referring then to Sec. IV comprise a strict treatment for the dynamic path, it is interesting to note that a very naive approach to the problem also gives the right EOP, Eqs. (4.7) and (4.10). As we have seen in Sec. II, for a determinantal path the lowest order in an expansion of the Hamiltonian overlap will be sufficient to determine the EOP. In the case of the dynamic path $|\phi(q,p)\rangle$ this yields

$$\delta_\phi \langle \phi(q,p)|H|\phi(q,p)\rangle = 0$$

to be believed up to order p^1, i.e.,

$$\delta_\phi \langle \phi(q,0)|H|\phi(q,0)\rangle - ip\delta_\phi \langle \phi(q,0)|[H,Q_0]|\phi(q,0)\rangle = 0 ,$$

where the variations (3.10) and (3.11) now exclude also Q_0. Assuming that $|\phi(q,0)\rangle$ is time even, we immediately obtain Eq. (4.5) from the P_α variation, Eq. (4.9) from the Q_α variation, and (4.6) and (4.8) for time parity reasons.

VII. COMPARISON WITH OTHER THEORIES

There is a conceptually different way to determine the EOP, which is guided by the idea of an explicit time evolution of a determinantal wave packet. The emphasis is on studying operator averages whose time evolution obeys classical equations of motion and reveals the underlying classical collective Hamiltonian. These approaches can be subsumed[16,17] under the heading mean field theories (MFT). The optimal MFT for the static case is the HF theory. Its natural extension to dynamic motion is TDHF. Villars[4] and Goeke and Reinhard[5] derived a set of EOP for a determinantal $|\phi(q)\rangle$ by performing an adiabatic expansion of the TDHF equations assuming the system at all times to be close to a local equilibrium. They require the path to be independent of the actual velocity or energy, respectively, which allows one to overcome the difficulty of choosing the proper initial conditions in TDHF and yields the EOP

$$\left\langle \phi(q) \middle| \left[S_{\rm ph}, H - \frac{\partial \mathcal{U}}{\partial q} Q_0 \right] \middle| \phi(q) \right\rangle = 0 , \tag{7.1}$$

$$\langle \phi(q)| [S_{\rm ph}, [H,Q_0] + i\mathcal{R}_{00} P_0] |\phi(q)\rangle = 0 , \tag{7.2}$$

which uniquely determine the path $|\phi(q)\rangle$ and the operators $P_0(q)$, $Q_0(q)$ along it. [The $S_{\rm ph}$ in Eqs. (7.1) and (7.2) stands for all possible 1p-1h operators with respect to $|\phi(q)\rangle$.] These are the so-called ATDHF equations. With determining

$Q_0(q)$ in the dynamic equation (7.2) (in fact this is a generalized cranking formula), they implicitly determine also the dynamical extension of the path up to order p^1, i.e.,

$$|\phi(q,p)\rangle=(1+ipQ_0(q))|\phi(q)\rangle\,.$$

This dynamic path $|\phi(q,p)\rangle$ can then be used to determine the classical collective Hamiltonian as

$$\mathcal{H}(q,p)=\langle\phi(q,p)|H|\phi(q,p)\rangle=\frac{p^2}{2\mathfrak{M}(q)}+v(q)$$

from which a quantized collective Hamiltonian can be derived[5] by subtracting certain quantum fluctuations of the wave packets $|\phi(q)\rangle$ in (q,p). As discussed in Refs. 5 and 7, the ATDHF theory reduces to the RPA in the small amplitude limit, or in turn, ATDHF can be understood as the extension of the RPA to large amplitude collective motion.

We now have two conceptually different starting positions, the more classically minded MFT, such as ATDHF, and the thoroughly quantum mechanical GCM. Both have in common the concept of a collective path $|\phi(q)\rangle$, spanning a subspace in which the collective motion is assumed to take place. But they treat it differently, first with respect to determining the optimal path, and second with respect to deriving a collective Hamiltonian $H_c(q,\vartheta_q)$ for a path $|\phi(q)\rangle$. Concerning the H_c, both theories give identical results as has been shown extensively in Refs. 8 and 9. The outcome of the present paper is now that also the EOP are identical: Equations (5.17) and (5.18) obtained from a GCM variation of a correlated (see Sec. V) or dynamic (see Sec. VI) path are just the ATDHF Eqs. (7.1) and (7.2). Thus both theories give the same EOP for the uncorrelated portion of the path $|\phi(q)\rangle$, which serves as the single particle basis for the fully correlated path $|\phi_c(q)\rangle$, to be determined by Eq. (5.2), i.e., $(Q_0(q)+iP_0(q))|\phi_c(q)\rangle=0$.

At this point we find a subtle difference between both aspects: In ATDHF we are not forced to realize that we have a theory for correlated paths, whereas in GCM the assumption of a correlated path is necessary to obtain Eqs. (5.8)–(5.15), which then reduce to Eqs. (5.17) and (5.18) or (7.1) and (7.2) using the quasiboson approach. The reason is simply that GCM is a quantized theory from the beginning, which means that to get the path, quantized expressions are varied [see Eq. (2.12)], whereas in ATDHF the path is obtained from a classical equation of motion and the quantization, which introduces the correlations, is performed afterwards and independently. Following Sec. VI, one also realizes that both theories consider a collective path to order $\hat{p}$, the ATDHF explicitly and the GCM implicitly by using the correlated $|\phi_c(q)\rangle$. These features have some analog in the limit of small vibration, i.e., the RPA. Using the HF state as $|\phi(0)\rangle$, Eqs. (7.1) and (7.2) or (5.18) determine the excitation operators $Q_0(0)$ and $P_0(0)$. Usually in RPA their frequencies are interpreted as the excitation energies, tacitly assuming a correlated ground state without explicitly constructing it.

Actually in the above discussion the term "GCM variation" has to be used with a bit of care. In fact, we do not strictly minimize an energy functional in $f(q)$ and $|\phi(q)\rangle$. This would have led to coupled equations for $f_n(q)$ and $|\phi_n(q)\rangle$ determining *one* actual state system. We do, instead, employ the GCM variation as a means to derive the EOP for $|\phi(q)\rangle$ by requiring $|\phi(q)\rangle$ to be the same for a spectrum of $f_n(q)$ (see Sec. II). That is quite the analog to the case of ATDHF, where one employs the EOM of TDHF to derive the EOP by requiring the path to be independent of the collective momentum or energy.

Another approach in the framework of the mean field theories has been put forward by Rowe and Bassermann[3] and Marumori.[18] They suggest a nonadiabatic theory for the determination of the determinantal dynamic collective path $|\phi(q,p)\rangle$. The eventual outcome is a constrained HF equation

$$\langle\phi(q,p)|[S_{\rm ph},H-\lambda Q_0-\mu P_0]|\phi(q,p)\rangle=0\,,$$

where the constraining operators Q_0 and P_0 are determined by the local RPA equations

$$\langle\phi(q,p)|[S_{\rm ph},[H,Q_0]+iP_0\mathfrak{B}]|\phi(q,p)\rangle=0\,, \quad (7.3)$$

$$\langle\phi(q,p)|[S_{\rm ph},[H,P_0]-iP_0\mathfrak{C}]|\phi(q,p)\rangle=0\,, \quad (7.4)$$

where $\mathfrak{B}$ and $\mathfrak{C}$ are the local inverse mass parameters and spring constant, respectively. The derivation of this local harmonic approach (LHA) in the present framework provides some difficulties. In zeroth order one obtains the analog of Eqs. (4.3) and (4.4), i.e., $\langle[Q_\alpha,H]\rangle=\langle[P_\alpha,H]\rangle=0$ for $\alpha\neq 0$. From this if follows that

$$H=iQ_0\langle[P_0,H]\rangle-iP_0\langle[Q_0,H]\rangle\,,$$

which means that at a certain $|\phi(q,p)\rangle$ the Q_0 and P_0 are completely determined by the time even and time odd part of the p-h elements of H, respectively. However, this does not guarantee that $iQ_0|\phi(q,p)\rangle=P_0|\phi(q,p)\rangle$ persists in both directions, i.e., for $p+\delta p$ *and* for $q+\delta q$. In other words, the problem is that in general $\vartheta_q(H_{\rm ph,\,even})\neq\vartheta_p(H_{\rm ph,\,odd})$, and thus the P_0 and Q_0 cannot be simultaneously local RPA operators according to Eqs. (7.3) and (7.4) *and* path propagators, i.e.,

$$|\phi(q+\delta q,p+\delta p)\rangle=(1-i\,\delta q P_0+i\,\delta p Q_0)|\phi(q,p)\rangle\,.$$

The first attempt to employ the GCM for the derivation of an EOP has been made by Holzwarth and Yukawa.[10] They performed a local variation of the determinantal path and derived a set of equations for an explicit construction of $|\phi(q)\rangle$. Their result was that $|\phi(q)\rangle$ should be simultaneously the solution of a constrained HF equation and the local Tamm-Dancoff equation

$$\langle\phi(q)|[S_{\rm ph}, H-\lambda Q_0]|\phi(q)\rangle=0,$$

$$\langle\phi(q)|Q_0 H Q_\alpha|\phi(q)\rangle=0 \quad \text{for } \alpha\neq 0.$$

A comparison with Eqs. (4.9) and (4.10) shows that the present approach yields the same result, if one neglects in Sec. III terms such as $\langle HQ_\alpha Q_0\rangle$ (i.e., the backward going graphs in RPA) and the q dependence of P_0 and Q_0.

VIII. SUMMARY AND CONCLUSION

The present paper is concerned with a microscopic approach to large amplitude collective motion using the concept of a collective path $|\phi(q)\rangle$, i.e., a set of A-body wave functions labeled by a proper collective coordinate. The aim is to derive equations which determine the *optimal* collective path (EOP). This is important, since large amplitude collective phenomena are characterized by substantial changes of the wave function during the process. To this end, the variational principle of the generator coordinate method (GCM) is generalized to include also a variation of the path of integration, $|\phi(q)\rangle$. The resulting integral equation is transformed to a differential equation in terms of the collective momentum $\hat{p}=-id/dq$. For adiabatic motions this defines in a natural way a hierarchy of equations associated with increasing powers of $\hat{p}$. To fulfill these equations requires a corresponding hierarchy of collective paths of increasing complexity.

If the collective path is assumed to consist of Slater determinants $|\phi_0(q)\rangle$, the zeroth-order variational equation is already sufficient to determine $|\phi(q)\rangle$ unambiguously. It leads to a differential equation which determines the propagator $P_0(q)|\phi(q)\rangle=i\partial_q|\phi(q)\rangle$ for a given $|\phi(q)\rangle$ and allows one to construct the path successively by

$$|\phi(q+\delta q)\rangle=(1-i\delta q P_0(q))|\phi(q)\rangle.$$

For small amplitude vibrations around the Hartree-Fock minimum ($q=0$), the equations for P_0 ($q=0$) reduce to some sort of Tamm-Dancoff or RPA-like equations. They can be solved by standard methods, and yield a spectrum of eigensolutions $P_n(0)$ from which a $P_0(0)$ must be selected to start the collective path. Although already these zero-order equations uniquely determine a path, they seem to be unsatisfactory, since in the limit of small amplitudes they do not precisely reduce to the RPA equations.

The next reasonable generalization of the path consists in including 2p-2h correlations of the RPA type. They are defined by requiring that the correlated path $|\phi_c(q)\rangle$ is the vacuum of the local collective boson $B_0(q)=Q_0(q)+iP_0(q)$. This generalization requires to take into account also the first-order equation in the adiabatic heirarchy in order to determine $|\phi_c(q)\rangle$ uniquely. Nevertheless the equations deforming $P_0(q)$ and $Q_0(q)$ are rather simple: $Q_0(q)\propto H_{\rm ph}(q)$ and $P_0(q)\propto[H,Q_0(q)]_{\rm ph}$. They essentially involve the calculation of the 1p-1h part of the Hamiltonian H with respect to $|\phi_c(q)\rangle$. As expected for small vibrations around the HF minimum, the equations for $|\phi_c(q)\rangle$ reduce to the RPA equations. In order to start the path, one solution $Q_0(q), P_0(0)$ of the total RPA spectrum must be selected. This is the only point in the theory which requires physical intuition, i.e., some preconceived knowledge of the collective motion under consideration. It is important to note that in practical cases one needs not to evaluate the correlations in $|\phi_c(q)\rangle$ explicitly. It is possible to handle them implicitly by means of $Q_0(q), P_0(q)$ and the single particle basis $|\phi(q)\rangle$ corresponding to $|\phi_0(q)\rangle$. Thus in an explicit numerical calculation it is sufficient to construct $|\phi(q)\rangle$ rather than $|\phi_c(q)\rangle$.

An alternative generalization consists in assuming a path $\phi(q,p)$ still consisting of Slater determinants, but which are labeled now by a pair of conjugate parameters q and p. This leads to a dynamic GCM, where both q and p are integration variables. It is interesting that in the adiabatic limit, this procedure turns out to be identical to the one parameter GCM using a correlated path $|\phi_c(q)\rangle$. One gains thereby an explicit expression of $|\phi_c(q)\rangle$ in terms of $|\phi(q,p)\rangle$.

There are some very interesting relationships of the present approach to the adiabatic time dependent Hartree-Fock theory (ATDHF) of Villars[4] and of Goeke and Reinhard.[5] That theory optimizes an adiabatic determinantal collective path

$$|\phi(q,p)\rangle\cong(1+ip\,Q_0(q))|\phi(q)\rangle$$

employing the classical concept of an explicit time evoluation $q(t), p(t)$ and using the TDHF variational principle. The remarkable result is that the variation of the correlated path within GCM leads to an EOP for $|\phi(q)\rangle$, $Q_0(q)$, and $P_0(q)$ which is identical to the EOP obtained in ATDHF. Also, since the quantization process[5] in ATDHF has been shown to be identical to invoking a GCM with correlated states[8,9] (or equivalently a dynamic GCM), the present considerations are a final step in using

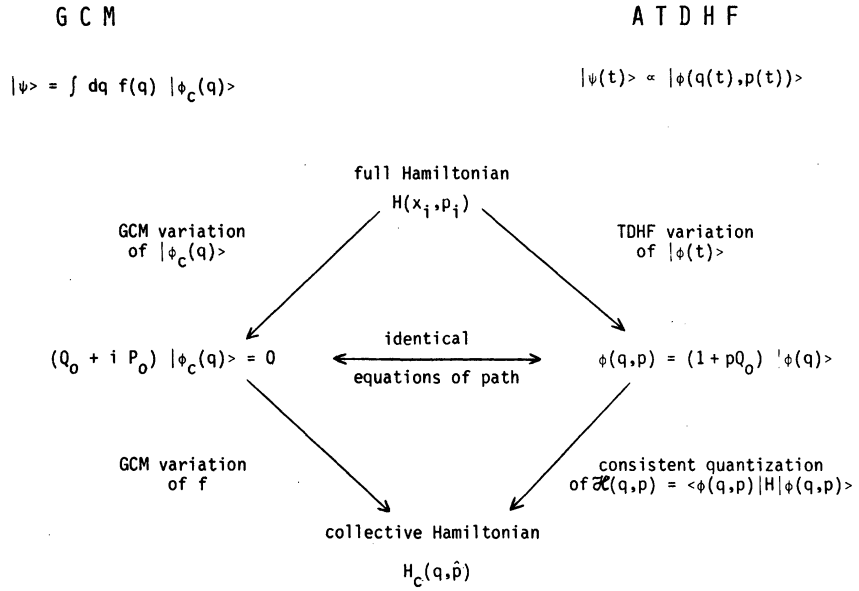

FIG. 1. The figure displays the basic two ways to derive a collective Hamiltonian $H_c(q, d/dq)$ from a full microscopic Hamiltonian $H(x_i, d/dx_i)$: On the left-hand side one finds the generator coordinate method (GCM) and on the right-hand side the quantized adiabatic time dependent Hartree-Fock approach (ATDHF). Both theories end up with the same expression for H_c and also closely related expressions for the collective path.

two concepts of treating microscopically large amplitude collective motion, viz., the more classically minded mean field theories, such as ATDHF including there *a posteriori* quantization, and the genuine quantum mechanical GCM. Both theories aim at extracting a collective Hamiltonian $H_c(q,\hat{p})$ from the full many body Hamiltonian $H(x_i, p_i)$ by means of a collective path $|\phi(q)\rangle$. Although they are of different conceptual origin, both theories derive identical equations for the optimized collective path, and both theories yield identical collective Hamiltonians H_c (to be used in a Schrödinger equation) and identical rules for evaluating collective transitions.

This remarkable correspondence can be visualized as in Fig. 1. Both theories are based on the concept of a collective path. They agree at the start by assuming a microscopic Hamiltonian $H(x_i, p_i)$ and the existence of an adiabatic collective mode. The very satisfying result is that both finally lead to the same quantized collective Hamiltonian $H_c(q,\hat{p})$, although they employ very different techniques underway.

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APPENDIX A: TRANSFORMATION OF THE INTEGRAL EQUATION TO A DIFFERENTIAL EQUATION

In terms of integral operators $\hat{I}$ and $\hat{H}$, Eq. (2.5) can be written as

$$\delta_\phi f^*(\hat{H} - E\hat{I})f = 0, \tag{A1}$$

which can be reordered to a Schrödinger-type equation as

$$\delta_\phi g^*(H_c - E)g = 0, \tag{A2}$$

with

$$H_c = \hat{I}^{-1/2}\hat{H}\hat{I}^{-1/2} \tag{A3}$$

and

$$g = I^{1/2} f. \tag{A4}$$

Assuming a rapid convergence of the expansion (2.6) one can approximate

$$\hat{I}(q,q') = \exp[-i(q'-q)\langle P_0\rangle - \tfrac{1}{2}(q'-q)^2\langle P_0^2\rangle], \tag{A5}$$

which can be represented as a Fourier integral as

$$\hat{I}(q,q') = (2\pi\langle P_0\rangle)^{-1/2}\int dk_2 \exp[ik_2(q-q') - 2p(k_2)], \tag{A6}$$

with

$$p(k) = \frac{1}{4\langle P_0^2\rangle}(k - \langle P_0\rangle)^2. \tag{A7}$$

From this expression one obtains easily

$$\hat{I}^{-1/2}(q,q') = (2\pi)^{-3/2}(2\pi\langle R_0^2\rangle)^{1/4} \times \int dk_1 \exp[-ik_1(q-q') + p(k_1)]. \tag{A8}$$

This can be proved by explicitly evaluating the expression

$$\int dq''\,dq'''\,\hat{I}^{-1/2}(q,q'')\,\hat{I}(q'',q''')\,\hat{I}^{-1/2}(q''',q') = \delta(q-q')\,. \tag{A9}$$

The integrals over q'' and q''' give $\delta(k_1-k_2)\,\delta(k_2-k_3)$, such that the $\delta(q-q')$ on the right hand side of Eq. (A9) results. In this and the following calculations we assume the coefficients of $(q-q')^n$ in Eqs. (2.7)–(2.11) to be so slowly varying that one can neglect their $\bar{q}=\frac{1}{2}(q+q')$ dependence in the integrations.

For the evaluation of $\hat{I}^{-1/2}\hat{H}I^{-1/2}$ one has to calculate terms of the sort

$$\int dq''\,dq'''\,\hat{I}^{-1/2}(q,q'')(q''-q''')^n\,\hat{I}(q'',q''')\,\hat{I}^{-1/2}(q''',q')\,. \tag{A10}$$

The term in the middle can be obtained by partial integration as

$$\begin{aligned}(q''-q''')^n\,\hat{I}(q'',q''') &= (-i)^n\int\left(\frac{\partial^n}{\partial k_2^n}e^{ik_2(q''-q''')}\right)e^{-2p(k_2)}\,dk_2\\ &= i^n\int e^{ik_2(q''-q''')}\left(\frac{\partial^n}{\partial k_2^n}e^{-2p(k_2)}\right)dk_2\,.\end{aligned} \tag{A11}$$

The integrals in (A10) over q'' and q''' yield again $\delta(k_1-k_2)\,\delta(k_2-k_3)$. Since $p(k)$ is a polynomial in k, one ends up with expressions such as

$$\int dk_2\,k_2^n\,e^{-ik_2(q-q')} = 2\pi i^n\,\frac{\partial^n}{\partial q^n}\delta(q-q')\,. \tag{A12}$$

Since the terms $\langle P_0\rangle$, $\langle\{P_0,\{H,P_0\}\}\rangle$, etc., of the expansion (2.6) are to be evaluated at $\bar{q}=\frac{1}{2}(q+q')$, one finally obtains from Eq. (2.5) terms such as

$$\delta_\phi\int dq\,dq'\,g^*(q)W_n(\bar{q})\left(\frac{\partial^n}{\partial q^n}\delta(q-q')\right)g(q')\,, \tag{A13}$$

with $W_n(\bar{q})$ containing expressions such as $\langle P_0\rangle$, $\langle\{\bar{H},P_0\}\rangle$, etc., which are to be evaluated at $\bar{q}=\frac{1}{2}(q+q')$. Changing the integration variables to $\bar{q}$ and $\Delta=q-q'$ gives

$$\delta_\phi\int d\bar{q}\,d\Delta\,g^*\left(\bar{q}+\frac{\Delta}{2}\right)W_n(\bar{q})\left(\frac{\partial^n}{\partial\Delta^n}\delta(\Delta)\right)g\left(\bar{q}-\frac{\Delta}{2}\right)=0 \tag{A14}$$

or

$$\delta_\phi\int d\bar{q}\,W_n(\bar{q})\left(\frac{\partial^n}{\partial\bar{q}^n}g^*(\bar{q})\,g(\bar{q})\right)d\bar{q}\,. \tag{A15}$$

Collecting all terms of the form (A15) up to $n=2$ yields directly Eq. (2.13).

APPENDIX B: NARROW OVERLAP EXPANSION OF THE CORRELATION CONSTRAINT

Outgoing from

$$= \int dq\,dq'\,f^*(q)\{\langle\phi_c(q)|P_0(q')-iQ_0(q')|\phi_c(q')\rangle\,\eta(q')+\eta^*(q)\langle\phi_c(q)|P_0(q)+iQ_0(q)|\phi_c(q')\rangle\}f(q')\,, \tag{5.5}$$

we want to expand in orders $(q'-q)$ about $\bar{q}=\frac{1}{2}(q+q')$. Thus we insert

$$q'=\bar{q}+\tfrac{1}{2}(q'-q)\,,\quad q=\bar{q}-\tfrac{1}{2}(q'-q) \tag{B1}$$

and employ

$$\partial_q|\phi_c(q)\rangle = -iP_0(q)\,|\phi_c(q)\rangle\,, \tag{B2}$$

$$\partial_q\big(A(q)\,|\phi_c(q)\rangle\big) = -iP_0(q)A(q)\,|\phi_c(q)\rangle+\big(\partial_q A(q)\big)_{\rm ph}|\phi_c(q)\rangle\,, \tag{B3}$$

where $A(q)$ replaces $Q_0(q)$ or $P_0(q)$. This yields

$$\begin{aligned}= \int dq\,dq'\,f^*(q)\{&(\eta+\eta^*)\langle P_0\rangle - i(\eta-\eta^*)\langle Q_0\rangle\\ &-\tfrac{1}{2}i(q'-q)\,[(\eta+\eta^*)\,2\langle P_0{}^2\rangle+(\eta+\eta^*)\langle Q_0\rangle+(\partial_q\eta+\partial_q\eta^*)\langle Q_0\rangle+i(\eta-\eta^*)\langle\partial_q P_0\rangle\\ &-i\eta 2\langle P_0Q_0\rangle+i\eta^*\,2\langle Q_0P_0\rangle+i(\partial_q\eta-\partial_q\eta^*)\langle P_0\rangle]\pm\cdots\}f(q)\,.\end{aligned} \tag{B4}$$

We now use relation (5.2) to evaluate

$$\begin{aligned}&2\langle P_0{}^2\rangle = -i\langle[P_0,Q_0]\rangle = -1\,,\\ &2\langle P_0Q_0\rangle = \langle\{P_0,Q_0\}\rangle+\langle[P_0,Q_0]\rangle = -i\,,\\ &\langle\partial_q P_0\rangle = \partial_q\langle P_0\rangle+i\langle[P_0,P_0]\rangle = \partial_q\langle P_0\rangle\,,\\ &\langle\partial_q Q_0\rangle = \partial_q\langle Q_0\rangle+i\langle[P_0,Q_0]\rangle = \partial_q\langle Q_0\rangle+1\,,\end{aligned} \tag{B5}$$

where all η are to be taken at $\bar{q}$ and all empty brackets at $|\phi_c(\bar{q})\rangle$.

With these relations we can compress the expression (B4) into the suggestive notation

$$= \int dq\, dq'\, f^*(q)\langle\phi_c(q)|\,\phi_c(q')\rangle\,\{(\eta+\eta^*)\langle P_0\rangle - i\,(\eta-\eta^*)\langle Q_0\rangle$$

$$-\tfrac{1}{2}i\,(q'-q)\,[\partial_q((\eta+\eta^*)\langle Q_0\rangle)+i\partial_q((\eta-\eta^*)\langle P_0\rangle)]\pm\cdots\}\,f(q)\,,$$

which finally is used in Eq. (5.6).

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