OPTIMAL COLLECTIVE PATHS*

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I. INTRODUCTION

In this work we consider microscopic theories appropriate for describing large amplitude nuclear collective motion such as fission or oscillations of transitional nuclei. Since an exact solution of the nuclear many-body problem is impossible, the approach is to isolate a subspace of the many-body Hilbert space maximally decoupled such that the time evolution of the states within the subspace is equivalent to the motion of a few collective degrees of freedom. In the ideal case this subspace, which we call the collective subspace, is an invariant subspace of the many-body Hilbert space.

One theory which can be used to construct the collective subspace is the generator coordinate method (GCM)[1,9-11]. In this method we consider the many-particle states which can be written as a linear superposition of the generator states $|\psi(\underset{\sim}{\alpha})\rangle$,

(1) $$|f\rangle = \int d\alpha \; f(\underset{\sim}{\alpha}) \; |\psi(\underset{\sim}{\alpha})\rangle$$

The generator states are chosen ã priori usually based on educated guesses as to the nature of the collective motion in consideration. Energy levels and wave functions are determined by the variational principle which leads to the GHW equation for $f(\underset{\sim}{\alpha})$

(2) $$\int d\underset{\sim}{\alpha}' \; (\langle\underset{\sim}{\alpha}|\hat{H}|\underset{\sim}{\alpha}'\rangle - E\langle\underset{\sim}{\alpha}|\underset{\sim}{\alpha}'\rangle) \; f(\underset{\sim}{\alpha}') = 0$$

The states which can be written as in eq. (1) span a subspace of the many-body Hilbert space which we identify with the collective subspace. The collective hamiltonian is defined by the restriction of the many-body hamiltonian to the collective subspace and the collective operators as any complete set of commuting observables where these observables are defined in the collective subspace[1,9-11].

If the generator states $|\psi(\underset{\sim}{\alpha})\rangle$ span the manifold of Slater determinants, the many-particle states given by the "ansatz" eq. (1) span the many-body Hilbert space. However the aim of the microscopic theories of large amplitude nuclear collective motion is to select an optimal submanifold of the manifold of Slater determinants on the bases of dynamical considerations as stated by Rowe and Bassermann[1-3], Villars[4], Goeke and Reinhard [5] and by Villars and Moya de Guerra[6] (see also references 7 and 8). This optimal submanifold of Slater deteminants is called the optimal collective path (O.C.P.). To construct the collective subspace we use the determinants of the O.C.P. as generator states in the "ansatz" of GHW, eq. (1). Even though it is possible to use the GCM and the variational principle to find not only the weight function but the generator states $|\psi(\underset{\sim}{\alpha})>$[2] the theories considered here uses a time-dependent approach based on the TDHF equations. They also restrict the determinants to the manifold of time-even Slater determinants (TED) since they are interested in a static optimal collective path (except references 1-3). For easier of presentation, we will suppose that it is sufficient to consider only one collective degree of freedom, the generalization to more than one being in principle straightforward. In this case the O.C.P. is a curve $|\psi_0(q)>$ in the manifold of TED. In the following development, based on reference 12, we will discuss a clear and concise way of deriving the equations which determine the O.C.P. of R-B, V-G-R and V-M studying the decoupling properties of the TDHF equations in the neighbourhood of a given Slater determinant $|\psi_0>$. This approach was used in reference 1 to derive the Rowe-Bassermann O.C.P. and one of the advantages of this approach is that it exhibits the physical content of the differences of the three theories mentioned above. We also argue that the aim of the theories of R-B, V-G-R and V-M is to construct the O.C.P. such that the generator of infinitesimal displacements along the path at each point $|\psi_0(q)>$ on the path and the force which acts on this determinant be always in the direction of a local normal mode and we investigate the conditions under which this is actually achieved.

II. TDHF EQUATIONS

The Thouless theorem says that any Slater determinant non-orthogonal to a given Slater determinant $|\psi_0>$ can be parametrised as

$$(3) \qquad |\psi(\underset{\sim}{\alpha},\underset{\sim}{\Pi})> = e^{i\,\hat{S}(\underset{\sim}{\alpha},\underset{\sim}{\Pi})}\,|\psi_0>$$

where

$$(4) \qquad \hat{S}(\alpha,\Pi) = \sum_j(\Pi_j\hat{q}_j - \alpha_j\hat{p}_j)$$

The one-body operators $\hat{q}_j$ and $\hat{p}_j$ have only particle-hole matrix elements with respect to $|\psi_o\rangle$ and they satisfy canonical commutation relations when the commutators act on $|\psi_o\rangle$[13],

(5)
$$\left[\hat{q}_j,\hat{q}_k\right]|\psi_o\rangle = \left[\hat{p}_j,\hat{p}_k\right]|\psi_o\rangle = 0$$
$$\left[\hat{q}_j,\hat{p}_k\right]|\psi_o\rangle = i\ \delta_{jk}\ |\psi_o\rangle$$

Given any one-body operator its particle-hole component with respect to $|\psi_o\rangle$ can be written as

(6)
$$\hat{F}^A = \sum_j \langle\psi_o|\left[\hat{F},-i\hat{p}_j\right]|\psi_o\rangle\hat{q}_j + \sum_j \langle\psi_o|\left[\hat{F},i\hat{q}_j\right]|\psi_o\rangle\hat{p}_j$$

The equation which gives the time-evolution of the Slater determinants is the TDHF equation, and it can be derived by the TDVP[4,13]

(7)
$$\langle\delta\psi(t)|\ \hat{H} - i\vec{\partial}_t\ |\psi(t)\rangle = 0$$

If $|\psi_o\rangle$ is a time-even Slater determinant we can always choose the $\hat{q}_k$ and $\hat{p}_k$ as time-even and time-odd operators, respectively. Using this fact and the parametrization given by eqs. (3) and (4) it can be shown that the TDHF equations reduce, in the neighbourhood of $|\psi_o\rangle$, to

(8)
$$\dot{\alpha}_k = \sum_j B_{kj}\ \Pi_j \qquad\qquad -\dot{\Pi}_k = -F_k + \sum_j V_{kj}\ \alpha_j$$

where

(9)
$$F_k = -\langle\psi_o|\left[\hat{H},-i\ \hat{p}_k\right]|\psi_o\rangle$$
$$B_{kj} = B_{jk} = \langle\psi_o|\left[\hat{q}_k,\left[\hat{H},\hat{q}_j\right]\right]|\psi_o\rangle$$
$$V_{kj} = V_{jk} = \langle\psi_o|\left[\hat{p}_k,\left[\hat{H},\hat{p}_j\right]\right]|\psi_o\rangle$$

The eqs. (8) are analogous to classical canonical equations of motion whose hamiltonian is the expectation value of the many-body hamiltonian in the state $|\psi(\underset{\sim}{\alpha},\underset{\sim}{\Pi})\rangle$ expanded to second order in $\underset{\sim}{\alpha}$ and $\underset{\sim}{\Pi}$,

(10)
$$\hat{H}(\underset{\sim}{\alpha},\underset{\sim}{\Pi}) = \langle\psi_o|\hat{H}|\psi_o\rangle - \sum_k F_k\alpha_k + \frac{1}{2}\sum_{k,j}\left(B_{kj}\Pi_k\Pi_j + V_{kj}\alpha_k\alpha_j\right)$$

Thus we can interpret the parameters $\underset{\sim}{\alpha}$ and $\underset{\sim}{\Pi}$ as local canonical variables at the point $|\psi_o>$. These local canonical variables define the phase-space at $|\psi_o>$. Furthermore to each local canonical variable α_k ,Π_k we associate the pair of local canonical operators $\hat{q}_k$ and $\hat{p}_k$. The eqs.(8) show that F_k is the component in the k direction of the force which acts on $|\psi_o>$ and that B_{kj} and V_{kj} are the components of the inverse inertia tensor and of the elastic tensor. Also they show that in general $|\psi_o>$ is not in equlibrium and has null velocity.

If $|\psi_o>$ is any determinant the TDHF trajectory which goes through it does not have any special decoupling property, when this trajectory is examined in the neighbourhood of $|\psi_o>$. On the other hand an O.C.P. should be distinguished by the decoupling properties of the collective and non-collective degrees of freedom. In the next section we are going to show how we can derive the equations which determine the optimal collective paths of R-B, V-G-R and V-M by studying the decoupling properties of the TDHF trajectory, when this trajectory is examined in the neighbourhood of a determinant on the path.

III. OPTIMAL COLLECTIVE PATHS FOR LARGE AMPLITUDE COLLECTIVE MOTION

III.A. O.C.P. of Rowe and Bassermann

To derive the O.C.P. of R-B we introduce the local normal modes which are defined as local canonical operators which makes the quadratic term of the hamiltonian (10) diagonal. As in our case a determinant along the O.C.P. is time-even, there is no coupling between coordinate and momentum and the quadratic term of the hamiltonian (10) can be diagonalized by a linear point transformation

$$\hat{Q}_i^L = \sum_j \hat{q}_j (a^{-1})_{ij}$$

(11)

$$\hat{P}_i^L = \sum_j \hat{p}_j \, a_{ji}$$

This point transformation is such that the normal modes satisfy the equations

$$<\psi_o|\left[\hat{P}_i^L,\left[\hat{H},\hat{P}_j^L\right]\right]|\psi_o> = C_i \, \delta_{ij}$$

(12)

$$<\psi_o|\left[\hat{Q}_i^L,\left[\hat{H},\hat{Q}_j^L\right]\right]|\psi_o> = B_i \, \delta_{ij}$$

We suppose that among the local normal modes there is one which near the minimum (solution of the HF eq.) is the lowest frequency mode which transforms into the only one unstable mode far from equilibrium. At each point this mode will be denoted by $\hat{Q}_o^L$, $\hat{P}_o^L$. The determinants of the O.C.P. of Rowe-Bassermann are selected by imposing that the force which acts on these determinants is in the direction of the local normal mode $\hat{Q}_o^L$, $\hat{P}_o^L$. This condition leads to

(13) $$<\psi_o| \left[\hat{H}, -i\, \hat{P}_j^L\right] |\psi_o> = 0 \quad , \quad j \neq 0$$

Parametrizing the curve described by the determinants which have the above property by a label q, where q is the expectation value of a measured operator $\hat{D}$

(14) $$q = <\psi_o(q)|\hat{D}|\psi_o(q)> \quad ,$$

eq. (13) can be written as a constrained equation where the operators $\hat{Q}_k(q)$ and $\hat{P}_k(q)$ are the local normal modes[1,13]

$$<\delta\psi_o(q)|\hat{H} + F_o^L(q)\hat{Q}_o^L(q)|\psi_o(q)> = 0 \qquad (I)$$

(15) $$<\delta\psi_o(q)|\left[\hat{H},\hat{P}_k^L(q)\right] - i\, C_k(q)\hat{Q}_k^L(q)|\psi_o(q)> = 0 \qquad (II)$$

$$<\delta\psi_o(q)|\left[\hat{H},\hat{Q}_k^L(q)\right] + i\, B_k(q)\hat{P}_k^L(q)|\psi_o(q)> = 0 \qquad (III)$$

If, for some q, $F_o^L(q)$ is equal to zero, $|\psi_o(q)>$ is in equilibrium and the eqs. (15) reduce to the R.P.A. Furthermore in equations (15)(II) and (15)(III) we can replace $\hat{H}$ by $H_{const}(q)$,

$$\hat{H}_{const}(q) = \hat{H} + F_o^L(q)\hat{Q}_o^L(q)$$

This shows that the R-B equations are a generalization of the R.P.A. to determinants outside an equilibrium point where the force of constraint which we should apply to the system in order for it be in equilibrium is along a local normal mode.

III.B. O.C.P. of Villars, Goeke and Reinhard

Identifying a determinant along the O.C.P. of V-G-R by a label q which is the expectation value of a measured operator $\hat{D}$,

$$q = <\psi_o(q)|\hat{D}|\psi_o(q)>$$

the particle-hole component of the generator of infinitesimal displacements along the path at the point q is defined by the equation

$$(16) \qquad (|\psi_0(q+\Delta q) - |\psi_0(q)>)_{ph} = -i\Delta q \; \hat{P}_0^V(q)\,|\psi_0(q)>$$

and an operator canonically conjugate to $\hat{P}_0^V(q)$ by

$$(17) \qquad \left[\hat{Q}_0^V(q),\hat{P}_0^V(q)\right]|\psi_0(q)> = i\,|\psi_0(q)>$$

The determinants $|\psi_0(q)>$ on the O.C.P. of V-G-R satisfy the properties that, given a complete set of local canonical operators which includes $\hat{Q}_0^V(q)$, $\hat{P}_0^V(q)$:

i) The force which acts on $|\psi_0(q)>$ is in the direction of the degree of freedom associated to $\hat{Q}_0^V(q)$, $\hat{P}_0^V(q)$

ii) The inertia tensor is diagonal and the elastic tensor is diagonal for i, j $\neq 0$.

These conditions are expressed by the equations

$$<\delta\psi_0(q)|\hat{H} - \frac{dV^{VGR}(q)}{dq}\,\hat{Q}_0^V(q)|\psi_0(q)> = 0 \qquad (I)$$

$$(18) \qquad <\delta\psi_0(q)|\left[\hat{H},\hat{Q}_0^V(q)\right] + iB_0(q)\;\hat{P}_0^V(q)|\psi_0(q)> = 0 \qquad (II)$$

$$(|\psi_0(q+\Delta q)> - |\psi_0(q)>)_{ph} = -i\;\Delta q\,\hat{P}_0^V(q)|\psi_0(q)> \qquad (III)$$

with

$$V^{VGR}(q) = <\psi_0(q)|\hat{H}|\psi_0(q)>$$

Eq. (18)(I) is an equation of constraint and the constraint is determined by equation (18)(II). The two properties i) and ii) allow us the following interpretation: If the system is placed at rest somewhere on the O.C.P. of V-G-R it starts to move first along the path[13].

III.C. The O.C.P. of Villars and Moya de Guerra

In this case we impose that the particle-hole component of the generator of infinitesimal displacements along the O.C.P. of V-M at a point $|\psi_0(q)>$ on the path is in the direction of a local normal mode. This condition gives

$$(19) \qquad (|\psi_0(q+\Delta q)> - |\psi_0(q)>)_{ph} = -i\;\Delta q\,\hat{P}_0^L(q)|\psi_0(q)>$$

As in the two previous cases we can write the equation for the O.C.P. as a constrained equation where the $\hat{Q}^L_j(q)$ and $\hat{P}^L_j(q)$ are the local normal modes

$$\langle\delta\psi_0(q)|\hat{H} + \sum_k F^L_k(q)\ \hat{Q}^L_k(q)|\psi_0(q)\rangle = 0 \qquad \text{(I)}$$

$$\langle\delta\psi_0(q)|\left[\hat{H},\hat{P}^L_k(q)\right] - i\,C_k(q)\hat{Q}^L_k(q)|\psi_0(q)\rangle = 0 \qquad \text{(II)}$$

(20)

$$\langle\delta\psi_0(q)|\left[\hat{H},\hat{Q}^L_k(q)\right] + i\,B_k(q)\hat{P}^L_k(q)|\psi_0(q)\rangle = 0 \qquad \text{(III)}$$

$$(|\psi_0(q+\Delta q)\rangle - |\psi_0(q)\rangle)_{ph} = -\,i\Delta q\ \hat{P}^L_0(q)|\psi_0(q)\rangle \qquad \text{(IV)}$$

IV. PROPERTIES OF THE OPTIMAL COLLECTIVE PATHS

Given a path in the space of Slater determinants we can find at each point on this path the force, the local normal modes and the generator of infinitesimal displacements along the path. If $|\psi_0\rangle$ is a stationary state there is no force acting on this determinant and we can always impose that the direction of the path at this point coincides with a local normal mode. When we are outside a stationary state, we can consider this determinant as instantaneously in equilibrium, as in the D'Alembert principle. As before we find the local normal modes at this point and impose that the direction of the path coincides with one of these normal modes. However the system placed at this point starts to move in the direction of the path only if the force which acts on this determinant is also along this normal mode. The O.C.P. considered here do not have this property. Using the developments of section III it can be easily seen that at each point on the O.C.P. of R-B the force is in the direction of a normal mode but the generator of infinitesimal displacements is not in this direction. At each point in the path of V-G-R the force and the generator of infinitesimal displacements are in the direction of a locally canonical degree of freedom but this degree of freedom is not a normal mode. And on the path of V-M, at each point, the generator of infinitesimal displacements is in the direction of a local normal mode but the force is not in this direction. This discussion suggests that the ultimate aim of the theories of O.C.P. considered here is to derive a path with the property that at each point the direction of the path is along a locally decoupled degree of freedom and that when the system is placed on the path it starts to move first in the direction of the path. When the above condition is satisfied the three O.C.P. coincide. To further clarify the physical meaning of the above condition it can be easily shown(2,14) that the path of R-B coincides at any point with a local valley of the local potential energy surface

$$V(\underset{\sim}{\alpha}) = - \sum_k F_k \alpha_k + \frac{1}{2} \sum_{k,j} V_{kj} \alpha_k \alpha_j \qquad (21)$$

in a space whose metric is the inverse inertia tensor at this point. The direction of the path of V-G-R coincides at any point with the direction of the local gradient line of the local energy surface eq.(21) in a space whose metric is the inertia tensor at this point(14). Finally the direction of the path of V-M coincides at any point with the direction of a local normal mode. When the paths are identical it coincides at any point with a local valley line and the direction of the path at this point is along a local gradient line.

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