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THE GENERATOR COORDINATE METHOD IN NUCLEAR PHYSICS

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ABSTRACT

The generator coordinate method is introduced as a physical description of a N-body system in a subspace of a reduced number of degrees of freedom. Special attention is placed on the identification of these special, "collective" degrees of freedom. It is shown in particular that the method has close links with the Born-Oppenheimer approximation and also that considerations of differential geometry are useful in the theory. A set of applications is discussed and in particular the case of nuclear collisions is considered.

I. INTRODUCTION. NUCLEAR COLLECTIVITY

A major, and somewhat surprising property of nuclear dynamics is that the low-lying spectrum of a nucleus is often dominated by collective states and transitions. The observation of collectivity results from experimental data and more recently, from time-dependent-Hartree-Fock (TDHF) calculations. Indeed, one often finds bands of nuclear levels, or a path of nuclear states, strongly connected by specific transitions, and the point is that in such cases the nuclear dynamics is expressed in terms of a small number of simple modes (translations, rotations, quadrupole vibrations, octupole vibrations, and so on).

Such a reduction of the number of degrees of freedom of a nucleus can be described by phenomenological models of course. It would be more satisfactory to understand why it occurs. A first, and qualitative answer, is available. A certain amount of correlation between the single-nucleon coordinate degrees of freedom $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$ (or the associate momenta $\underset{\sim}{p}_1 \ldots \underset{\sim}{p}_A$) is obviously the result of the binding of nucleus, into a quantal liquid drop, with its surface tension and its surface and volume waves. The Pauli principle, furthermore, obviously correlate $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$. It is therefore not surprising that some combinations $Q(\underset{\sim}{x}_1 \underset{\sim}{p}_1 \ldots \underset{\sim}{x}_A \underset{\sim}{p}_A)$ emerge finally as normal, dominant degrees of freedom rather than $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$.

The exact nature of the new variables Q as well as an explicit change of variables from x_i's to Q's represent, however, a formidable mathematical and physical problem. The purpose of these lectures is to show that a few steps to solve this problem

have been undertaken, in particular with the help of the generator coordinate method.

The central concept in these lectures is that of the collective subspace. This subspace must be, up to a good accuracy, an eigensubspace of the many-body Hamiltonian $\mathcal{H}$. For a significant amount of decoupling is necessary to isolate a degree of freedom.

It must also likely contain, up to a good accuracy, the orbit of a Lie group, generated by the algebra of the collective degrees of freedom Q and their associate momenta P. For a time-dependent description of the dynamics will replace the evolution operator $\exp(-i\mathcal{H}t)$ by an approximation $\exp[-i\,\mathcal{H}_c(Q,P,t)]$ where $\mathcal{H}_c$, a time-dependent function of the collective variables, will often be linear like in the case of translations, rotations and small amplitude vibrations.

As a third property of the subspace, its collective states Φ have to show a large amount of coherence with respect to Q, best expressed by the limit case of factorization between Q's and complementary (spectator) degrees of freedom ξ,

$$\Phi_\nu(\underset{\sim}{x}_1 \cdots \underset{\sim}{x}_A) = \Phi_\nu(Q,\xi) \simeq \varphi_\nu(Q)\ \chi(\xi) \quad , \tag{I.1}$$

where the "spectator" wave function χ weakly depends on the collective quantum numbers ν in the subspace. This ensures that transition matrix elements inside the subspace

$$\langle\Phi_{\nu'}|Q|\Phi_\nu\rangle \simeq \langle\varphi_{\nu'}|Q|\varphi_\nu\rangle\,\langle\chi|\chi\rangle \quad , \tag{I.2}$$

are large, with $\langle\chi|\chi\rangle = 1$.

Last but not least, the collective operators Q, P are expected to be essentially one-body operators. For an exponential $\exp(-i\mathcal{H}_c)$, with $\mathcal{H}_c$ linear in Q, P, can then be interpreted as an evolution operator for which all nucleons move alike, since the one-body nature of Q, for instance, reads

$$Q = \sum_{i=1}^{A} Q_i \quad . \tag{I.3}$$

Another advantage of one-body operators is that their commutators remain one-body operators, a useful condition for the closure of a Lie algebra. Furthermore it is known that exponentials of one-body operators convert Slater determinants into Slater determinants, a result of interest for the connection of the theory with the time-dependent Hartee-Fock (TDHF) approximation. One thus expects to span the collective subspace by means of a path of Slater determinants. It may also be noticed that well-known collective operators, such as the centre-of-mass position and momentum, the total angular momentum, the quadrupole, octupole...(etc) momenta and various RPA operators are one-body operators. Finally it may be conjectured that there is less ergodicity to be expected from the exponential of a one-body operator than from the true evolution operator $(-i\mathcal{H}t)$, the latter being known to induce ergodicity in many general cases. Prevention of ergodicity is essential for the isolation of the degrees of freedom under study.

The main emphasis in these lectures will be laid upon the fulfilment of these four criteria, in an attempt to derive collectiveness from $\mathcal{H}$ rather than guess it. This is the subject of subsections III A to III D. As a preliminary subject, the formal aspects of the generator coordinate method will be described briefly in section II. Finally a set of applications is displayed in sections IV and V.

II. ELEMENTARY TECHNOLOGY OF GENERATOR COORDINATES

The one-channel, one-generator-coordinate ansatz

$$\Psi(\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A) = \int dq\ f(q)\ \Phi_q(\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A)\ , \tag{II.1}$$

can be generalized into a multi-channel, multi-generator-coordinate form

$$\Psi(\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A) = \sum_n \int dq_1 \ldots dq_N\ f_n(q_1 \ldots q_N)\ \Phi^n_{q_1 \ldots q_N}(\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A), \tag{II.2}$$

which is of interest in a coupled-wave theory of nuclear collisions with polarization phenomena. We shall mainly be concerned in the following with the simpler form, eq.(II.1).

The continuous label (generator coordinate) q acquires a physical meaning if it is the expectation value of the collective coordinate Q in the generator function Φ_q

$$q = \langle \Phi_q | Q | \Phi_q \rangle\ . \tag{II.3}$$

It will be assumed in this section that $Q(\underset{\sim}{x}_1 \underset{\sim}{p}_1 \ldots \underset{\sim}{x}_A \underset{\sim}{p}_A)$ is known in advance and that the set $\{\Phi_q\}$, usually a path of Slater determinants, is also known.

The physical meaning of q becomes even more transparent if it turns out that the fluctuation

$$\Delta_q^2 \equiv \langle \Phi_q | Q^2 | \Phi_q \rangle - q^2 \tag{II.4}$$

remains small when compared to a typical order of magnitude q_o^2 of the range of q in the problem under study. It is then clear that Φ_q represents a wave packet narrow with respect to Q,

$$\Phi_q(Q,\xi) \simeq \Gamma\left(\frac{Q-q}{\Delta q}\right) \chi_q(\xi)\ , \tag{II.5}$$

where the wave packet Γ has a width Δq and one recognizes from eq.(I.1) the "spectator" wave function χ_q and spectator degrees of freedom ξ. It must be checked separately whether χ depends strongly on q or not. A weak dependence will be assumed in the following.

When χ is fixed the ansatz, eq.(II.1), induces

$$\Psi = g(Q)\ \chi(\xi)\ , \tag{II.6}$$

with

$$g(Q) = \int dq\ \Gamma\left(\frac{Q-q}{\Delta q}\right) f(q) \quad . \tag{II.7}$$

It must be stressed here, and this is maybe the main property of the generator coordinate formalism, that eq.(II.6) achieves in practice a change of coordinate from the microscopic coordinates $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$ to the collective and spectator coordinates Q, ξ. This change of coordinates was impossible in an explicit, direct way. It is remarquable that the ansatz, eq.(II.1), has solved this problem in an indirect way, while all calculations remain explicitly in the representation $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$, a most practical feature.

It is interesting at this stage to introduce the "sharp basis", where the change of variables becomes even more obvious. The diagonalization of Q in the generator subspace proceeds via the equation

$$\int dq' \ \langle \Phi_q | (Q-k) | \Phi_{q'} \rangle \ j_k(q') = 0 \ , \tag{II.8}$$

to generate "sharp states"

$$|k\rangle = \int dq' \ j_k(q') \ |\Phi_{q'}\rangle \ . \tag{II.9}$$

Under suitable conditions of normalization, spectrum density and so on, the sharp states obey the conditions

$$\langle k | k' \rangle = \delta(k-k') \ , \tag{II.10}$$

$$\langle k | Q | k' \rangle = k \ \delta(k-k') \ . \tag{II.11}$$

The sharp states, as approximations to eigenstates of Q, yield the interpretation

$$\langle Q \ \xi | k \rangle = \delta(Q-k) \ \chi_k(\xi) \ . \tag{II.12}$$

They still make a basis of the generator (collective) subspace, but this basis identifies the label k with the coordinate itself. The change of variables from $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$ to Q, ξ is thus very explicit.

In this sharp representation the collective Hamiltonian is now trivial. Its matrix element reads

$$h_{coll}(k,k') = \langle k | \mathcal{H} | k' \rangle \ , \tag{II.13}$$

where again all calculations remain in the $\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A$ representation. A collective Schrödinger equation may result from an expansion of the non locality of h_{coll} up to second order

$$h_{coll}(k,k') = v_{coll}\left(\frac{k+k'}{2}\right)\delta(k-k') - \left[\frac{1}{2m_{coll}\left(\frac{k+k'}{2}\right)}\delta''(k-k')\right]_{sym} \qquad (II.14)$$

provided of course m_{coll} remains positive.

The diagonalization of $\mathcal{H}$ in the sharp basis has thus more physical interpretation than the usual Griffin -Hill-Wheeler derivation of the energy basis

$$\Psi_E = \int dq'\ f_E(q')\ \Phi_{q'}\ , \qquad (II.15)$$

where $f_E(q')$ is given by the integral equation

$$\int dq'\ \langle\Phi_q|(\mathcal{H}-E)|\Phi_{q'}\rangle\ f_E(q') = 0\ . \qquad (II.16)$$

With the usual energy and overlap kernels

$$H(q,q') = \langle\Phi_q|\mathcal{H}|\Phi_{q'}\rangle\ , \qquad (II.17)$$

$$I(q,q') = \langle\Phi_q|\Phi_{q'}\rangle\ , \qquad (II.18)$$

the matrix notation (H-EI) f = 0 of eq.(II.16) can be reduced into a diagonalization form more general than the usual transform via the square root $I^{1/2}$. Any kernel J, possibly non Hermitian, which fulfills the equation $I = J^+J$, may provide a reduced Hamiltonian kernel h under the condition $H = J^+hJ$. The final equation to solve is thus

$$J^+(h-E)\ Jf = 0\ , \qquad (II.19)$$

where J^+ may be erased and (Jf) is the new unknown.

In particular, if one uses a matrix notation $\{|k\rangle\} = j\{|q'\rangle\}$ for eq.(II.9), then eq.(II.13) reads $h_{coll} = j^+\ H\ j$. Although j may be nearer to a rectangular than a square matrix (because of null states in the subspace), it is obvious that the sharp basis corresponds formally to the special case $J = j^{-1}$. All these considerations can be made more rigorous, the details being omitted in the present lectures.

There is another technical point with generator coordinates which is not connected with diagonalization, however. It has rather to do with inversion and is of special interest for the theory of nuclear collisions since this theory makes great use of the resolvent $(E-\mathcal{H})^{-1}$.

Consider the functional

$$F = \langle\Psi_f|\Psi\rangle + \langle\Psi'|\Psi_i\rangle - \langle\Psi'|(E-\mathcal{H})|\Psi\rangle\ , \qquad (II.20)$$

where $\Psi_{i,f}$ are given, square integrable vectors (usually the product of an optical wave and a residual potential). A variational principle with respect to Ψ gives

$$0 = \frac{\delta F}{\delta \Psi} = \langle \Psi_f | - \langle \Psi' | (E - \mathcal{H}) = 0 \ . \qquad \text{(II.21)}$$

With respect to Ψ' one obtains

$$|\Psi_i\rangle = (E - \mathcal{H}) |\Psi\rangle \ . \qquad \text{(II.22)}$$

As a consequence of eqs.(II.21) and (II.22) the stationnary value of F is

$$\bar{F} = \langle \Psi_f | (E - \mathcal{H})^{-1} | \Psi_i \rangle \ . \qquad \text{(II.23)}$$

There is no need to stress that such a resolvent matrix element is exactly what is needed in a theory of nuclear collisions.

In the generator coordinate method, with a trial function Ψ defined by eq.(II.1), the form taken by eq.(II.22) reads

$$\int dq' \langle \Phi_q | (\mathcal{H} - E) | \Phi_{q'} \rangle f(q') + \langle \Phi_q | \Psi_i \rangle = 0 \ , \qquad \text{(II.24)}$$

which is an inhomogeneous generalization of the Griffin-Hill-Wheeler equation. The same holds, of course, for eq.(II.21), with a source term given by Ψ_f instead of Ψ_i.

III. SEARCH FOR COLLECTIVE PATHS

A. Curvature as a necessary condition

As mentionned ealier the generator coordinate description of an eigenstate (time independent) is provided by the ansatz, eq.(II.1). Collective motion can rather be expressed by time dependent states

$$\Psi(t) = \int dq \ f(q,t) \ \Phi_q \ , \qquad \text{(III.1)}$$

and, if furthermore the generator states are sufficiently coherent to be long-lived, it then occurs that f may be a sharply peaked wave-packet around a classical position in phase space, $q_o(t)$

$$f(q,t) \simeq \Gamma [q - q_o(t)] \ . \qquad \text{(III.2)}$$

The path $\{\Phi_{q_o(t)}\}$, and actually $\{\Phi_q\}$ itself if one takes q rather than t as current parameter, is therefore more than an abstract basis of a subspace. It can actually be understood like the physical trajectory of the system in its Hilbert space when the collective motion occurs.

As mentioned also in section I, it is felt that this trajectory is (at least part of) an orbit of a Lie group, generated by an algebra of collective operators Q. All these geometrical intuitions lead to the need for the definition of a metric, for instance the following

$$\left(\frac{ds}{dq}\right)^2 = \left\langle \frac{d\Phi_q}{dq} \mid \frac{d\Phi_q}{dq} \right\rangle , \qquad \text{(III.3)}$$

in order to define various characterizations of the trajectory, such as curvatures.

The choice, eq.(III.3), of the metric may not be unique. It appears at first, however, like that which naturally uses the length in Hilbert space and applies it to the tangent $\frac{d\Phi_q}{dq}$ of the trajectory. The unit tangent vector is then

$$|T\rangle = \left| \frac{d\Phi_q}{ds} \right\rangle , \qquad \text{(III.4)}$$

and the unit normal vector comes with the next derivative. A curvature C is then defined by

$$C^2 = \left\langle \frac{dT}{ds} \mid \frac{dT}{ds} \right\rangle . \qquad \text{(III.5)}$$

In the special case, of wide interest, where Φ_q is a Slater determinant or a correlated RPA state and where the time dependent evolution is approximated by

$$\Phi_{q_o}(t) = \exp\left[-ikt\mathcal{Q}\right] \Phi_{q_o}(o) , \qquad \text{(III.6)}$$

with $\mathcal{Q}$ a quasi-boson operator, it can be checked that the curvature resulting from eqs.(III.6) and (III.5) reaches a critical value, $C^2 = 3$, when $\mathcal{Q}$ is a traditional collective quasi-boson operator. The basic step of the proof of this result is to consider the spreading of the particle-hole matrix elements $\mathcal{Q}_{ph}$. One finds that the curvature reaches a maximum when all $\mathcal{Q}_{ph}$ have the same order of magnitude.

It is empirically well known that the particle-hole matrix elements of those RPA boson operators which correspond to maximum collectivity are evenly spread. The same magic value $C^2 = 3$ can also be found in the orbits of various groups such as SU(3), SP(1,R), SP(3,R)... which are known to be of interest in the theory of collective motion.

It can be concluded that a curvature close to $\sqrt{3}$ is likely necessary (but certainly not sufficient) for a path $\{\Phi_q\}$ to be a good candidate for collectivity.

B. Born-Oppenheimer approach

Let us assume that $\mathcal{Q}$ is known in advance. Such a collective degree of freedom must likely have a large inertia, since all nucleons move alike when governed by this mode $\mathcal{Q}$. The other degrees of freedom ξ must therefore have a smaller inertia.

If these degrees of freedom ξ are light enough when compared to $\mathcal{Q}$, the Born-Oppenheimer approximation becomes valid. Indeed, like in eq.(II.12), a spectator wave function $\chi_k(\xi)$ develops with a minimal energy locked to the sharp value k taken by $\mathcal{Q}$. The sharp basis of the generator coordinate formalism thus proves the

equivalence between this formalism and the Born-Oppenheimer approximation.

To find χ_k one may think of a minimization of the total energy (involving both Q and ξ) under the constraint $\delta(Q-k)$. Such a δ-function constraint, however, is obviously too sharp for practical purposes, for it restricts all moments $\langle k|Q^n|k\rangle$ at the same time, whatever the value of the exponent n. A milder constraint, clearly a more practical one, takes care of the first moment $\langle\Phi_q|Q|\Phi_q\rangle$ only. This is nothing but the form shown by eq.(II.5). When Φ_q is a Slater determinant, it is thus obtained by a constrained Hartree-Fock calculation.

There are cases, however, where precautions are necessary in a constrained variational principle. This occurs when $\langle Q\rangle$ may diverge while $\langle\mathcal{H}\rangle$ remains finite. Let for instance Q be the quadrupole moment operator and consider a fixed wave-function Φ_o, with a finite energy $e_o = \langle\Phi_o|\mathcal{H}|\Phi_o\rangle$ and a finite quadrupole moment $q_o = \langle\Phi_o|Q|\Phi_o\rangle$. Consider now an auxiliary wave function Φ_1 lying around Φ_o like the "Saturn ring" around the planet Saturn. This function Φ_1 is designed to have an enormous quadrupole moment q_1, through its extension and ellipsoidal deformation in space. Simultaneously, the nuclear matter density shown by Φ_1 is designed to be very thin. Because of this thin spreading, Φ_1 carries no kinetic or potential energy. Because of Φ_1 lying around Φ_o, and far enough, there is no coupling matrix element between Φ_o and Φ_1. Therefore any small admixture of Φ_1 into Φ_o, of the form $\Psi = \Phi_o + \varepsilon\Phi_1$, keeps for Ψ the energy e_o. It is clear, however, that the quadrupole moment shown by Ψ will be $q_o + \varepsilon^2 q_1$, which can differ arbitrarily from q_o. This arbitrary value of the constraint $\langle\Psi|Q|\Psi\rangle$ for a fixed value of the energy $\langle\Psi|\mathcal{H}|\Psi\rangle$ makes the constrained variational principle inefficient.

Such a breakdown casts doubt on many theories of fission, for instance, if the fission barrier has been predicted by a constrained calculation. Indeed the life time is very sensitive to the barrier and it has just been seen that the barrier may be washed away by Saturn-ring-like admixtures.

To solve the paradox one may notice that the admixture of Φ_1 also increases enormously the fluctuation Δq as defined by eq.(II.4). Indeed the quadrupole moment is a local operator, whose eigenstates are localized while Φ_1 is thinly spread. If therefore one considers a doubly constrained variational principle including both moments $\langle Q\rangle$ and $\langle Q^2\rangle$, a reduction of Δq forces Φ_1 to shrink. The shrinking produces density (and phase) gradients, thus kinetic energies, and it also induces larger densities, thus potential energies. The energy will then differ from e_o and generate a significant energy surface.

To summarize these considerations, an equivalence between the Born-Oppenheimer and the generator coordinate approximations can be derived, provided one keeps under control the fluctuations of the collective coordinates Q.

C. Fiber bundle and adiabatic time-dependent Hartree-Fock approach

It is obviously desirable to have a theory which contains more dynamics than the considerations of subsection A, which are only geometrical, and those of subsection B, where one is prejudiced about the nature of Q. It is known that the random phase approximation provides a dynamical description for which the collective operators Q are by-products of the theory rather than prerequisite. Unfortunately the RPA is restricted to small amplitude nuclear motions. Large amplitude collective paths must therefore be identified by a more general theory. The adiabatic time-dependent Hartree-Fock (ATDHF) approximation has been suggested by Baranger and Veneroni for that purpose. It will now be considered.

Let Φ be a Slater determinant and ρ the corresponding one-body density matrix. Out of ρ and the many-body Hamiltonian $\mathcal{H} = \mathcal{T} + \mathcal{V}$, one makes the Hartree-Fock Hamiltonian

$$W = \mathcal{T} + \mathcal{U} \quad , \tag{III.7}$$

where the average, one-body potential $\mathcal{U}$ is given by the usual antisymmetrized trace

$$\mathcal{U} = \mathrm{Tr} \ \hat{\mathcal{V}} \rho \quad . \tag{III.7a}$$

The time-dependent Hartree-Fock (TDHF) approximation then specifies which determinant will occur at time dt on the path if one starts with Φ at time $t = 0$

$$\begin{aligned} \Phi(dt) &= [1 - i\ dt\ W]\ \Phi + 0(dt^2) \\ &= \exp[-i\ dt\ W]\ \Phi + 0(dt^2) \quad . \end{aligned} \tag{III.8}$$

The two forms of eq.(III.8) are equivalent up to order dt only, of course. It is clear, however, that they suggest that W is the generator of a Lie group, actually the generator of displacement along the TDHF trajectory. One expects a close connection between W and a collective operator Q.

Since W depends on Φ, see eq.(III.7a), the connection between W and Q will likely provide too many Q's if one follows an arbitrary TDHF trajectory. To reduce the variety of Q's we might follow the suggestion by several authors to consider only periodic TDHF solutions. This is clearly a global approach. Alternately, one may try to select Q's which <u>locally</u> correspond to <u>several</u> TDHF trajectories. This can be achieved in the framework of the adiabatic (ATDHF) trajectory.

It is useful at this point to realize that in the simplest and most frequent case a generator coordinate path $\{\Phi_q\}$ is made of <u>real</u> Slater determinants Φ_q. More precisely the single-particle orbitals which are filled in Φ_q can then be described by real wave-functions in coordinate representation and the density ρ is even under time reversal. An even density like that will be denoted ρ_o in the following and the

corresponding Hartree-Fock Hamiltonian by W_o. It is clear that W_o, given by

$$W_o = \mathcal{C} + \mathrm{Tr}\ \tilde{v}\ \rho_o \ , \tag{III.9}$$

is also real (even under time reversal).

On the other hand, a TDHF trajectory is complex most of the time. As shown by eq.(III.8), if one starts at time t = 0 with a real Φ, then $\Phi(dt)$ acquires at once an imaginary part. Also $W(dt)$ is complex

$$\begin{aligned} W(dt) &= \mathcal{C} + \mathrm{Tr}\ \tilde{v}\ \rho(dt) \\ &= \mathcal{C} + \mathrm{Tr}\ \tilde{v}(\rho_o - i\ dt[W_o,\rho_o]) \\ &= W_o - i\ dt\ W_1 \ , \end{aligned} \tag{III.10}$$

$$\text{with } W_1 = \mathrm{Tr}\ \tilde{v}\ [W_o,\rho_o] \tag{III.11}$$

The main feature of the ATDHF theory is that $\Phi(t)$ always remain almost real. Imaginary components in wave functions and operators are associated to velocities and kept small. The splitting of W into a real and imaginary component W_o and W_1 can thus be retained as of interest despite its validity limited to first order with respect to imaginary parts, see eq.(III.10). It can be stressed at this point that there are one and only one, well defined W_o and W_1 for each real determinant Φ_o. Indeed Φ_o defines ρ_o, then one finds W_o through eq.(III.9) and W_1 through eq.(III.11).

One then notices that W_o is a real, Hermitian operator and that $i\ W_1$ is a purely imaginary (odd under time reversal) and Hermitian operator. If one uses $i\ W_1$ as a Lie group generator

$$\begin{aligned} \Phi_o(d\theta) &= [\,1 + i\ d\theta\ i W_1\,]\ \Phi_o(0) \\ &= (1 - d\theta\ \mathrm{Tr}\ \tilde{v}\,[W_o,\rho_o])\ \Phi_o(0) \end{aligned} \tag{III.12}$$

it is a clear that $\Phi_o(dt)$ is real, like $\Phi_o(0)$. This induces a step along a real path and can be considered as the beginning of the making of a generator coordinate path.

This path equation can be written, from eq.(III.12)

$$\frac{d\Phi_q}{dq} = (\mathrm{Tr}\ \tilde{v}[\mathcal{C} + \mathrm{Tr}\ \tilde{v}\ \rho_q,\ \rho_q])\ \Phi_q \ , \tag{III.13}$$

where ρ_q is the real density defined by Φ_q and one writes Φ_q instead of $\Phi_o(0)$ in order to specify that one is running along the path, step by step. It generates a path as soon as one initial determinant Φ_o is given. The question, of course, is whether the path is acceptable as collective.

One first check is to measure the curvature along the path, as discussed in subsection A. A second check consists first in noticing that $i\ W_1$, the displacement

operator, behaves like a momentum since it is imaginary and Hermitian. One then notices that W_o, real and Hermitian, behaves like a position operator. Indeed, consider eq.(III.8) with $\Phi = \Phi_o$ real. It must here be remembered that real determinants, in the Baranger-Veneroni analysis, are interpreted as motionless. The imaginary component $-i\, dt\, W_o\, \Phi_o$ which then appears in $\Phi(dt)$ is thus associated to the creation of collective velocity, under the acceleration operator W_o. The acceleration being usually given by the coordinate operator, one may relate W_o to the collective coordinate. Because of the high coherence which has been assumed for the collective states in section I, the second check now consists in assuming that W_o (coordinate) and $i\, W_1$ (momentum) have proportional particle-hole matrix elements, like in RPA,

$$[\mathcal{C} + \mathrm{Tr}\, \tilde{U} \rho_q - \lambda\, \mathrm{Tr}\, \tilde{V}[T + \mathrm{Tr}\, \tilde{U} \rho_q, \rho_q],\ \rho_q] = 0 \ . \qquad \text{(III.14)}$$

It is interesting to point out that this path equation, eq.(III.14), is a constrained Hartree-Fock equation. Indeed W_o is nothing but the Hartree-Fock Hamiltonian for the real determinant Φ_q. Then the constraint is $\lambda\, W_1$, with λ as Lagrange multiplier and W_1 as a rather unusual, because anti-Hermitian, constraining operator.

A consequence of eq.(III.14) is the existence of a fiber bundle of ATDHF trajectories. Indeed, consider at time $t = 0$ the set of initial determinants

$$\Phi(0) = (1 - i\, d\tau\, W_o)\, \Phi_o(0) \ , \qquad \text{(III.15)}$$

with $\Phi_o(0)$ one of the real determinants Φ_q on the path. The path $\{\Phi_q\}$ will be the basis of the bundle. The functions $\Phi(0)$ parametrized by the real and small number $d\tau$ will be the first fiber of the bundle. The point is that, at time dt, one obtains

$$\Phi(dt) = [1 - i\, dt(W_o - i\, d\tau\, W_1)]\, \Phi(0)$$

$$= (1 - i\, d\tau'\, W_o)\, \Phi_o(0) \qquad \text{(III.16)}$$

with

$$d\tau' = dt + d\tau - i\, \frac{d\tau\, dt}{\lambda} \ , \qquad \text{(III.17)}$$

because the particle-hole matrix elements of W_o and W_1 are proportional. Except for the fact that $d\tau'$ is complex, the form of eq.(III.16) is exactly that of the fiber, eq.(III.15).

Actually nothing prevents to write eq.(III.16) as

$$\Phi(dt) = (1 - i\, d\tau''\, W_o)\, \Phi_o(d\theta) \qquad \text{(III.18)}$$

with

$$\Phi_o(d\theta) = \left(1 - \frac{d\tau\, dt}{\Lambda}\ W_o\right) \Phi_o(0)$$

$$= (1 - d\tau\, dt\ W_1)\ \Phi_o(0) \qquad \text{(III.19)}$$

and

$$d\tau'' = dt + d\tau,\ d\theta = d\tau\, dt. \qquad \text{(III.20)}$$

It can be stressed that $\Phi_o(d\theta)$ is real, like $d\tau\, dt$, and that $d\tau''$ is again real. A new fiber, strictly analogous to that described by eq.(III.15), has been described by eq.(III.18).

The physical meaning of this fiber bundle approach is obvious. Under various initial velocities $d\tau$ as specified by eq.(III.15) the system follows always the same kind of steps on the basis of the bundle , the path generated by eq.(III.19) and acquires always the same kind of accelerations, described by the fiber, eq.(III.18). In other words the system is stable under changes of velocities. Although this conclusion is based on first order arguments in dt and $d\tau$ and should be checked up to second order at least, it corresponds to a decoupling of the mode, governed by W_o and W_1, from other modes perpendicular to the fiber bundle. Thus the number of degrees of freedom has been (approximately) reduced.

Last but not least a third check is necessary. For W_o (and W_1) may change strongly along the path, while one expects the collective algebra to be reasonably constant. Despite this last difficulty the two path equations, eqs.(III.13) and (III.14), seem to provide a self-contained (dynamical) derivation of a generator coordinate path of some interest for collective motion.

D. Time as a generator coordinate

Let $\Psi(t)$ be the solution of the time-dependent Schrödinger equation. Any eigenstate Ψ_E can be recovered by a Fourier transform

$$\Psi_E = \int dt\ e^{+iEt}\ \Psi(t)\ , \qquad \text{(III.21)}$$

which is actually nothing but a generator coordinate ansatz with respect to time where $f_E(t) = \exp(iEt)$. Of course one needs that the initial condition $\Psi(0)$ have a non-vanishing component on Ψ_E.

One may notice at this stage that any eigenstate can be obtained from eq.(III.21) if $\Psi(0)$ is "random" enough, namely, in the present context, if it has components on all eigenstates of $\mathcal{H}$. This may be understood as a kind of ergodicity, the trajectory $\Psi(t)$ winding around so much on the unit sphere that the ansatz,

eq.(III.21) allows one to pick up any unit vector.

In that sense, the opposite case of "non ergodicity" corresponds to $\Psi(t)$ having components upon the states of a collective band only. Incidentally, if the number of eigenstates in that band is finite, the trajectory $\{\Psi(t)\}$ is seen to coil around a kind of multidimensional torus.

This geometrical image reminds one of the fiber bundle discussed in the previous subsection. Since an exact time-dependent Schrödinger trajectory is not available in practice, one may rather consider the ansatz

$$\Psi_E = \int dt\ f_E(t)\ \Phi(t)\ , \qquad \text{(III.22)}$$

where $\Phi(t)$ is now a TDHF trajectory. Obviously there is now no reason for $f_E(t)$ to be equal to $\exp(iEt)$, so that one needs to solve explicitly a Griffin-Hill-Wheeler equation identical to that shown by eq.(II.16). Conversely, if it turns out that the solution $f_E(t)$ looks like $\exp(iEt)$ one may conclude that TDHF is an excellent dynamical approximation in that special case.

Of special interest of course would be the case where $\Phi(t)$, instead of showing a large amount of "ergodicity", would remain collective at "all" times (during at least a typical time for collective processes, namely a few 10^{-21}s). Although the curvature criterion of subsection 1 is neither necessary nor sufficient, it is clear that one may calculate the curvature as a function of time and that time intervals where the curvature remains of order $\sqrt{3}$ may provide an interesting first guess for $\Phi(t)$ in the ansatz, eq.(III.22).

An other advantage of this ansatz relates with the theory of nuclear collisions. It turns out that, as time goes to $+\infty$, a TDHF solution $\Phi(t)$ usually does not reach an asymptotic state. This difficulty prevents one to use in TDHF the standard concept of channels, and TDHF "cross sections" are thus often of a classical and statistical nature. On the contrary it can be shown that a suitable choice of boundary conditions for $f_E(t)$ allows to <u>reconstruct</u> a <u>quantal</u> scattering wave Ψ_E^+ from eq.(III.22). The details of the proof are too technical to be given in these lectures, but they have been published elsewhere. It can be stressed here that the TDHF theory is non linear, hence the difficulties for asymptoticity, while the generator coordinate ansatz is linear. It is the linearity which allows the various channels to evolve independently and provide cross-sections without spurious interferences.

A third advantage of the TDHF ansatz, eq.(III.22), is a stability property of the energy of Ψ_E with respect to a change of the trajectory $\{\Phi(t)\}$. Indeed, the energy is

$$E = \int dt\ dt'\ f_E^*(t)\ \langle \Phi(t) \mid \mathcal{H} \mid \Phi(t') \rangle\ f_E(t'), \qquad \text{(III.23)}$$

whose variation under a modification $\delta\,\Phi(t)$ is

$$\delta E = f_E^*(t) \int dt' \; < \delta\,\Phi(t) \; |\mathcal{H}| \; \Phi(t') > f_E(t'). \qquad \text{(III.24)}$$

It is reasonable to consider as dominant, in this integral, the neighbourhood of $t = t'$. Since $\delta\,\Phi(t)$ is then a set of particle-hole elements with respect to $\Phi(t)$, the full Hamiltonian can be replaced by the Hartree-Fock Hamiltonian. One thus obtains

$$< \delta\,\Phi(t) \; |\mathcal{H}| \; \Phi(t) > \; = \; < \delta\,\Phi(t) \; |W| \; \Phi(t) > \; , \qquad \text{(III.25)}$$

and, because of the TDHF equation of motion

$$< \delta\,\Phi(t) \; |W| \; \Phi(t) > \; = \; i \; < \delta\,\Phi(t) | \frac{d\Phi}{dt} > \; . \qquad \text{(III.26)}$$

A significant variation of the generator coordinate trajectory, however, must at least be orthogonal to the trajectory itself. For both $\Phi(t)$ and $\Phi(t+dt)$, thus $\frac{d\Phi}{dt}$, are already in the generator subspace. Therefore $< \delta\,\Phi(t) \mid d\Phi/dt >$ identically vanishes in eq.(III.26), which is the stability property considered earlier for E.

IV. APPLICATION TO NUCLEAR REACTIONS

A. Definitions

Typically one considers here an elastic scattering $a + A \rightarrow a + A$, with the projectile a and the target A, or a transfer reaction $a + A \rightarrow b + B$, where b is considered as the core of a, and A as the core of B. In other words $a = (b+\nu_i)$ and $B = (A+\nu_f)$, where ν_i and ν_f are the initial and final clouds of transferred nucleons.

One defines the creation operator $A^\dagger(\underset{\sim}{r})$ of nucleus A around the shell model center $\underset{\sim}{r}$

$$A^\dagger(\underset{\sim}{r}) = \sum \eta_1^\dagger(\underset{\sim}{r}) \; \ldots \; \eta_A^\dagger(\underset{\sim}{r}) \; , \qquad \text{(IV.1)}$$

where $\eta^\dagger(\underset{\sim}{r})$ is a single-nucleon creation operator in a shell model state $\varphi(\underset{\sim}{x}-\underset{\sim}{r})$ centered around $\underset{\sim}{r}$ and where the necessary configuration mixing is shown symbolically by $\sum$.

In coordinate representation one demands

$$<\underset{\sim}{x}_1 \ldots \underset{\sim}{x}_A | A^\dagger(\underset{\sim}{r}) | 0> \; = \; \Psi^A(\underset{\sim}{x}_1-\underset{\sim}{r}, \ldots, \underset{\sim}{x}_A-\underset{\sim}{r})$$

$$= \Gamma_A(\underset{\sim}{R}_A-\underset{\sim}{r}) \; \Psi^A_{int}(\underset{\sim}{\xi}_1 \ldots \underset{\sim}{\xi}_{A-1}). \qquad \text{(IV.2)}$$

Here $|0>$ is the vacuum, the variables $\underset{\sim}{x}_i$ are the single nucleon coordinates, Ψ^A is the total wave function of the nucleus, $\underset{\sim}{R}_A$ is the center of mass coordinate and one defines the usual (A-1) Jacobi coordinate (internal degrees of freedom) $\underset{\sim}{\xi}$. It is

important that Ψ^A factorize into a wave packet Γ_A for the center of mass and an internal wave-function Ψ^A_{int}. Otherwise the formalism would be plagued by center of mass spuriosity. For the sake of simplicity Γ_A will be assumed to be Gaussian in the following.

In the same way one defines creation operators $a^\dagger(\underset{\sim}{r}')$, $B^\dagger(\underset{\sim}{r}'')$, $b^\dagger(\underset{\sim}{r}''')$, $\nu_i^\dagger(\underset{\sim}{r}')$ and $\nu_b^\dagger(\underset{\sim}{r}'')$ for the other nuclei and clouds of nucleons around their respective shell model centers. One finds in particular that $a^\dagger = \nu_i^\dagger b^\dagger$ and $B^\dagger = \nu_f^\dagger A^\dagger$.

The generator function for the channel $\alpha \equiv A + a$ is then

$$|\alpha\underset{\sim}{r}\rangle \equiv A^\dagger(N_a\ \underset{\sim}{r}/N)\ a^\dagger(-N_A\ \underset{\sim}{r}/N)\ |0\rangle\ , \qquad \text{(IV.3)}$$

where N_a, N_A and N are the mass numbers of a, A and the total mass number, respectively. In coordinate representation this means

$$\langle \underset{\sim}{x}_1 \cdots \underset{\sim}{x}_A\ \underset{\sim}{x}_{A+1} \cdots \underset{\sim}{x}_{A+a} | \alpha\underset{\sim}{r}\rangle = \mathcal{A}\,\Gamma_A(\underset{\sim}{R}_A - N_a\ \underset{\sim}{r}/N)\ \Gamma_a(\underset{\sim}{R}_a + N_A\ \underset{\sim}{r}/N)$$
$$\Psi_A^{int}(\underset{\sim}{\xi}_1 \cdots \underset{\sim}{\xi}_{A-1})\ \Psi_a^{int}(\underset{\sim}{\xi}'_1 \cdots \underset{\sim}{\xi}'_{a-1})\ , \qquad \text{(IV.4)}$$

where $\mathcal{A}$ is the antisymmetrization operator.

Let $\underset{\sim}{\rho}_\alpha = \underset{\sim}{R}_a - \underset{\sim}{R}_A$ be the channel degree of freedom and $\underset{\sim}{R}$ be the total center of mass coordinate. The Gaussians Γ_A and Γ_a have a product which is also Gaussian with respect to $\underset{\sim}{\rho}_\alpha$ and $\underset{\sim}{R}$

$$\Gamma_A(R_A - N_a\ \underset{\sim}{r}/N)\ \Gamma_a(\underset{\sim}{R}_a + N_A\ \underset{\sim}{r}/N) = \mathcal{G}_\alpha(\underset{\sim}{R}, \underset{\sim}{\rho}_\alpha - \underset{\sim}{r})\ . \qquad \text{(IV.5)}$$

It can happen that $\mathcal{G}_\alpha$ also factorizes

$$\mathcal{G}_\alpha(\underset{\sim}{R}, \underset{\sim}{\rho}_\alpha - \underset{\sim}{r}) = G(\underset{\sim}{R})\ \Gamma_\alpha(\underset{\sim}{\rho}_\alpha - \underset{\sim}{r})\ , \qquad \text{(IV.6)}$$

where Γ_α may be called the channel wave-packet. In such a case the generator function $|\alpha\underset{\sim}{r}\rangle$ is non spurious, because the total center of mass factorizes out. If furthermore a generator function $|\beta\underset{\sim}{r}'\rangle$ for any other channel β is designed like $|\alpha\underset{\sim}{r}\rangle$, in a way strictly analogous to eq.(IV.3),

$$|\beta\underset{\sim}{r}'\rangle = B^\dagger(N_b\ \underset{\sim}{r}'/N)\ b^\dagger(-N_B\ \underset{\sim}{r}'/N)\ |0\rangle\ , \qquad \text{(IV.7)}$$

one may demand that the corresponding product $\Gamma_B\ \Gamma_b$ factorizes into a product of Gaussians $G\ \Gamma_\beta$ with the <u>same</u> $G(\underset{\sim}{R})$ as that for channel α, eq.(IV.6).

The multichannel ansatz

$$|\Psi\rangle = \int d\underset{\sim}{r}\ f_\alpha(\underset{\sim}{r})\ |\alpha\underset{\sim}{r}\rangle + \int d\underset{\sim}{r}'\ f_\beta(\underset{\sim}{r}')\ |\beta\underset{\sim}{r}'\rangle$$
$$+ \ldots(\text{other channels } \gamma) \qquad \text{(IV.8)}$$

reads in such a case, after insertion of eqs.(IV.4) and (IV.6),

$$\Psi = G(\underset{\sim}{R})\ \mathcal{A}\left[\psi_A^{int}\ \psi_a^{int}\ g_\alpha + \psi_B^{int}\ \psi_b^{int}\ g_\beta + \ldots\right], \qquad (IV.9)$$

where the same $G(\underset{\sim}{R})$ factorizes out for all channels (and commutes with $\mathcal{A}$) and one defines channel wave-functions

$$g_{\alpha,\beta}(\underset{\sim}{\rho}_{\alpha,\beta}) = \int d\underset{\sim}{r}(\text{or } d\underset{\sim}{r}')\ \Gamma_{\alpha,\beta}(\underset{\sim}{\rho}_{\alpha,\beta}-\underset{\sim}{r} \text{ or } \underset{\sim}{r}')\ f_{\alpha,\beta}(\underset{\sim}{r} \text{ or } \underset{\sim}{r}')\ . \qquad (IV.10)$$

It is clear that the factorization, eq.(IV.6), prevents any center-of-mass spuriosity from creeping into the generator coordinate formalism. This property will be assumed until subsection D, where it will be seen how it can be relaxed without damage.

B. Connection with the resonating group formalism

It is trivial that

$$G(R)\ \mathcal{A}\ \Gamma(\underset{\sim}{\rho}_\alpha-\underset{\sim}{r})\ \psi_A^{int}\ \psi_a^{int} = G(\underset{\sim}{R}) \int d\underset{\sim}{s}\ \Gamma_\alpha(\underset{\sim}{r}-\underset{\sim}{s})\left[\mathcal{A}\ \delta(\underset{\sim}{\rho}_\alpha-\underset{\sim}{s})\ \psi_A^{int}\ \psi_a^{int}\right]. \qquad (IV.11)$$

The antisymmetrized function between brackets is nothing but the resonating group basis function $|\alpha\underset{\sim}{s}\rangle_{RGM}$. Indeed, in the resonating group theory, the channel degree of freedom $\underset{\sim}{\rho}_\alpha$ is strictly localized by the corresponding δ-function. (The total center-of-mass wave-packet can be integrated out and forgotten.) Alternately, one may interpret $|\alpha\underset{\sim}{s}\rangle_{RGM}$ as the sharp basis of the generator coordinate subspace, as defined by eq.(II.12), with $\underset{\sim}{\rho}_\alpha$ as the collective degree of freedom.

Let us compare a generator coordinate kernel and a resonating group kernel, for instance the following

$$H_{\alpha\beta}(\underset{\sim}{r},\underset{\sim}{r}') = \langle\alpha\underset{\sim}{r}|\ \mathcal{H}\ |\beta\underset{\sim}{r}'\rangle\ , \qquad (IV.12a)$$

$$h_{\alpha\beta}(\underset{\sim}{s},\underset{\sim}{s}') = {}_{RGM}\langle\alpha\underset{\sim}{s}|\ \mathcal{H}\ |\beta\underset{\sim}{s}'\rangle_{RGM}\ . \qquad (IV.12b)$$

As seen in eq.(IV.11), a state $|\alpha\underset{\sim}{r}\rangle$ is a linear supersposition of states $|\alpha\underset{\sim}{s}\rangle_{RGM}$ and an analogous result holds for any other channel. It is thus obvious that

$$H_{\alpha\beta}(\underset{\sim}{r},\underset{\sim}{r}') = \int d\underset{\sim}{s}\ d\underset{\sim}{s}'\ \Gamma_\alpha(\underset{\sim}{r}-\underset{\sim}{s})\ h_{\alpha\beta}(\underset{\sim}{s},\underset{\sim}{s}')\ \Gamma_\beta(\underset{\sim}{r}'-\underset{\sim}{s}')\ . \qquad (IV.13)$$

In a short notation this reads $H_{\alpha\beta} = \Gamma_\alpha * h_{\alpha\beta} * \Gamma_\beta$, in order to express the convolution product. In the same way eq.(IV.10) can be shortened into $g_{\alpha,\beta} = \Gamma_{\alpha,\beta} * f_{\alpha,\beta}$. This convolution correspondence between the resonating group and the generator coordinate formalism is then general, and can trivially be extended to any Hamiltonian, overlap or transition kernel such $H_{\alpha\alpha}$, $I_{\alpha\beta}$ and so on.

C. The high frequency catastrophe. Various methods of solution

Except for unessential coefficients, the Fourier transform of eq.(IV.10) reads

$$\tilde{g}(\underset{\sim}{\pi}) = \exp(-\pi^2)\ \tilde{f}(\underset{\sim}{\pi}) \ , \tag{IV.14}$$

where $\underset{\sim}{\pi}$ is the momentum conjugate to $\underset{\sim}{\rho}$ (or $\underset{\sim}{r}$) and $\tilde{f}$, $\tilde{g}$ are the Fourier transforms of f, g respectively. As it is known from the resonating group theory that g behaves like a wave-function, the singularities of $\tilde{g}$ in the continuum are thus of a mild nature (principal parts, etc). It is then clear, however, that $\tilde{f}$ diverges strongly, like $\exp(+\pi^2)$, when $\pi \to +\infty$. Thus a Fourier transform of $\tilde{f}(\underset{\sim}{\pi})$ back to a coordinate space $f(\underset{\sim}{r})$ will diverge.

This serious difficulty has been analyzed by many authors and brings many numerical technicities in the solution of the Griffin-Hill-Wheller equation. As an example, consider the two-channel equations, which read, with obvious notations

$$\begin{aligned} (H_{\alpha\alpha}-E\ I_{\alpha\alpha})\ f_\alpha + (H_{\alpha\beta}-E\ I_{\alpha\beta})\ f_\beta = 0 \\ (H_{\beta\alpha}-E\ I_{\beta\alpha})\ f_\alpha + (H_{\beta\beta}-E\ I_{\beta\beta})\ f_\beta = 0 \ . \end{aligned} \tag{IV.15}$$

Because of eq.(IV.13) and all necessary analogous relations for the kernels involved here, one finds as equivalent to eqs.(IV.15) the forms

$$\begin{aligned} \Gamma_\alpha(h_{\alpha\alpha}-E\ i_{\alpha\alpha})\ \Gamma_\alpha\ f_\alpha + \Gamma_\alpha(h_{\alpha\beta}-E\ i_{\alpha\beta})\ \Gamma_\beta\ f_\beta = 0 \\ \Gamma_\beta(h_{\beta\alpha}-E\ i_{\beta\alpha})\ \Gamma_\alpha\ f_\alpha + \Gamma_\beta(h_{\beta\beta}-E\ i_{\beta\beta})\ \Gamma_\beta\ f_\beta = 0 \end{aligned} \tag{IV.15a}$$

or

$$\begin{aligned} \Gamma_\alpha\left[(h_{\alpha\alpha}-E\ i_{\alpha\alpha})\ g_\alpha + (h_{\alpha\beta}-E\ i_{\alpha\beta})\ g_\beta\right] = 0 \\ \Gamma_\beta\left[(h_{\beta\alpha}-E\ i_{\beta\alpha})\ g_\alpha + (h_{\beta\beta}-E\ i_{\beta\beta})\ g_\beta\right] = 0 \ . \end{aligned} \tag{IV.16}$$

In coordinate space, there is difficulty in defining an inverse operator $\Gamma^{-1}_{\alpha,\beta}$. For, as shown by eq.(IV.14), the matrix element of $\Gamma_{\alpha,\beta}$ in momentum representation reads (unnecessary coefficients omitted)

$$\langle \underset{\sim}{\pi} | \Gamma | \underset{\sim}{\pi}' \rangle = \exp(-\pi^2)\ \delta(\underset{\sim}{\pi}-\underset{\sim}{\pi}') \ , \tag{IV.17}$$

and thus one obtains

$$\langle \underset{\sim}{\pi} | \Gamma^{-1} | \underset{\sim}{\pi}' \rangle = \exp(+\pi^2)\ \delta(\underset{\sim}{\pi}-\underset{\sim}{\pi}') \ , \tag{IV.18}$$

the Fourier transform of which to coordinate representation is obviously singular. Nothing prevents, however, to consider eqs.(IV.16) in momentum representation and

multiply the upper (lower) equation by $\Gamma_\alpha^{-1}(\Gamma_\beta^{-1})$ from the left. One then obtains

$$\begin{aligned}(h_{\alpha\alpha}-E\, i_{\alpha\alpha})\; g_\alpha + (h_{\alpha\beta}-E\, i_{\alpha\beta})\; g_\beta = 0 \\ (h_{\beta\alpha}-E\, i_{\beta\alpha})\; g_\alpha + (h_{\beta\beta}-E\, i_{\beta\beta})\; g_\beta = 0\ ,\end{aligned} \tag{IV.19}$$

which is nothing but the resonating group, coupled channel formulation. This is known to be a regular problem.

The transition from eqs.(IV.15) to eqs.(IV.19), which can be made without singularities in the momentum representation, is a first method to obviate the high frequency catastrophe. There is a second method, however, which has the advantage of avoiding the detour through the momentum representation. Indeed, as found by the Takacsy, a special case of eq.(IV.10) reads, after projection onto a channel partial wave

$$\sin(k\rho+\eta) = \int dr\, \exp\left[+k^2 - (\rho-r)^2\right] \sin(kr+\eta) + g_{s.r.}(\rho)\ , \tag{IV.20}$$

where η is the phase shift and $g_{s.r.}$ is a square integrable (short range) contribution to the resonating group wave-function. In other words, the asymptotic parts of g and f are proportional. It is easy to show that the same result is also valid for Coulomb waves

$$\sin(k\rho-\gamma\ \log 2k\rho+\eta) = \int dr\, \exp\left[+k^2 - (\rho-r)^2\right] \sin(kr-\gamma\ \log 2kr+\eta) + g_{s.r.}(\rho)\ . \tag{IV.21}$$

The phase shifts in the generator coordinate theory can thus be deduced from the short range properties of f, like in the usual theory of collisions.

Practically the second method may go as follows. One defines the short range part of f (in each channel) by the condition

$$\Gamma\, f_{s.r.} = g - \Gamma\, f_{as}\ , \tag{IV.22}$$

where f_{as} is known from eqs.(IV.20) and / or eq.(IV.2'), except for the phase shift η, to be determined later. Then the right hand side of eq.(IV.22) is the short range part $g_{s.r.}$ of g is that channel. It can be expanded, with strong convergence properties, in a suitable basis of square integrable functions, $\{u_n\}$,

$$g_{s.r.} = \sum_n c_n\, u_n \tag{IV.23}$$

and thus one obtains

$$f_{sr} = \sum_n c_n\, \Gamma^{-1}\, u_n\ , \tag{IV.24}$$

where the unknown coefficients c_n, and later the phase shifts, can be obtained by an insertion of eq.(IV.24) into eq.(IV.15). This makes eq.(IV.15) inhomogeneous, since a source term is brought by the identity $f = f_{s.r.} + f_{as}$. The phase shifts, which

are unknown parameters in the source term, must be determined by any usual variational principle of the theory of collisions or any standard matching procedure of f_{as} and $f_{s.r.}$, or g_{as} and $g_{s.r.}$.

In practice one truncates the expansion, eq.(IV.23), at a finite order of components u_n. It is easy to show that one may always choose this basis $\{u_n\}$ in such a way that, although Γ^{-1} is singular in coordinate representation, the product $\Gamma^{-1}u_n$ is still a regular wave function. Finite order expansions, eq.(IV.24), of the singular function $f_{s.r.}$ are thus regular and retain the convergence properties of eq.(IV.23) as regards the fact that the coefficients c_n make a square integrable series.

D. The biased density matrix

Among the various methods proposed by many authors we now discuss that of the "biased" case, namely that which is still available when eq.(IV.5) does not simplify into eq.(IV.6). When this factorization does not occur, the generator coordinate ansatz, eq.(IV.8), breaks down completely since the total center of mass and the relative degree of freedom, $\underset{\sim}{R}$ and $\underset{\sim}{\rho}$, are spuriously correlated.

An analogue of eq.(IV.11) is available, however. Indeed, one obtains from eq.(IV.4) and (IV.5) the trivial result

$$\mathcal{A}\,\mathcal{G}_\alpha(\underset{\sim}{R},\underset{\sim}{\rho}_\alpha-\underset{\sim}{r})\;\Psi_A^{int}(\underset{\sim}{\xi}\ldots)\;\Psi_a^{int}(\underset{\sim}{\xi}'\ldots) = \int d\,\bar{\underset{\sim}{R}}\,d\underset{\sim}{s}\;\mathcal{G}'_\alpha(\bar{\underset{\sim}{R}},\underset{\sim}{r}-\underset{\sim}{s})$$

$$\delta(\underset{\sim}{R}-\bar{\underset{\sim}{R}})\left[\mathcal{A}\;\delta(\underset{\sim}{\rho}_\alpha-\underset{\sim}{s})\;\Psi_A^{int}\;\Psi_a^{int}\right], \qquad \text{(IV.25)}$$

where again there appears the bracket $|\alpha\underset{\sim}{s}\rangle_{RGM}$. Here however, the total center of mass is frozen at position $\bar{R}$, while it could be integrated out in the case of eq.(IV.11).

According to eq.(IV.25) and any identical equation for another channel, a kernel $H_{\alpha\beta}$ now reads

$$\langle\alpha\underset{\sim}{r}|\,\mathcal{H}\,|\beta\underset{\sim}{r}'\rangle = \int d\,\bar{\underset{\sim}{R}}\,d\underset{\sim}{s}\,d\underset{\sim}{s}'\;\mathcal{G}_\alpha(\bar{\underset{\sim}{R}},\underset{\sim}{r}-\underset{\sim}{s})\;\mathcal{G}_\beta(\bar{\underset{\sim}{R}},\underset{\sim}{r}'-\underset{\sim}{s}')\;\;{}_{RGM}\langle\alpha\underset{\sim}{s}|\,\mathcal{H}\,|\beta\underset{\sim}{s}'\rangle_{RGM}\,, \qquad \text{(IV.26)}$$

where one has taken into account that the total center of mass must be frozen at the same location $\bar{R}$ in the bra and the ket provided by eq.(IV.25). If now one defines

$$\mathcal{G}_{\alpha\beta}(\underset{\sim}{r}-\underset{\sim}{s},\underset{\sim}{r}'-\underset{\sim}{s}') = \int d\bar{R}\;\mathcal{G}_\alpha(\bar{\underset{\sim}{R}},\underset{\sim}{r}-\underset{\sim}{s})\;\mathcal{G}_\beta(\bar{\underset{\sim}{R}},\underset{\sim}{r}'-\underset{\sim}{s}')\,,$$

one obtains from eq.(IV.26)

$$H_{\alpha\beta}(\underset{\sim}{r},\underset{\sim}{r}') = \int d\underset{\sim}{s}\,d\underset{\sim}{s}'\;\mathcal{G}_{\alpha\beta}(\underset{\sim}{r}-\underset{\sim}{s},\underset{\sim}{r}'-\underset{\sim}{s}')\;h_{\alpha\beta}(\underset{\sim}{s},\underset{\sim}{s}'). \qquad \text{(IV.27)}$$

In other words, the information carried by the resonating group kernel is still embedded inside the generator coordinate kernel $H_{\alpha\beta}$, although the ansatz, eq.(IV.8), is meaningless . If $h_{\alpha\beta}$ can be recovered from $H_{\alpha\beta}$, one may still solve eqs.(IV.16). This is of great physical interest for the frequent case where the generator functions $|\alpha\underset{\sim}{r}>$ are derived from Gaussians of unequal parameters, corresponding to the collision of ions of unequal masses.

The derivation of $h_{\alpha\beta}$ from $H_{\alpha\beta}$ is simple when $H_{\alpha\beta}$ is a Gaussian. For, as seen earlier, the choice of Γ_A and Γ_a as Gaussians makes trivially $\mathcal{G}_{\alpha\beta}$ also a Gaussian. It is then easy to check that $h_{\alpha\beta}$ is also a Gaussian. More precisely, assume that, except for unessential coefficients,

$$H_{\alpha\beta} = \exp\left[-(\underset{\sim}{r},\underset{\sim}{r}')\ \mathcal{D}'\begin{pmatrix}\underset{\sim}{r}\\ \underset{\sim}{r}'\end{pmatrix}\right] , \tag{IV.28}$$

where $\mathcal{D}'$ is a (2×2) matrix, and denote the Gaussian form of $\mathcal{G}_{\alpha\beta}$ as

$$\mathcal{G}_{\alpha\beta} = \exp\left[-(\underset{\sim}{r}-\underset{\sim}{s},\underset{\sim}{r}'-\underset{\sim}{s}')\ \mathcal{C}\begin{pmatrix}\underset{\sim}{r}-\underset{\sim}{s}\\ \underset{\sim}{r}'-\underset{\sim}{s}'\end{pmatrix}\right] , \tag{IV.29}$$

where $\mathcal{C}$ is also a 2 × 2 matrix. Then eq.(IV.7) provides

$$h_{\alpha\beta} = \exp\left[-(\underset{\sim}{s},\underset{\sim}{s}')\ \mathcal{D}\begin{pmatrix}\underset{\sim}{s}\\ \underset{\sim}{s}'\end{pmatrix}\right] , \tag{IV.30}$$

with

$$\mathcal{D} = \left[\mathcal{D}'^{-1} - \mathcal{C}^{-1}\right]^{-1} \tag{IV.31}$$

except for special cases, where $h_{\alpha\beta}$ is a local kernel, and which can be handled explicitly.

In the more general case of Gaussian wave functions for clusters where $H_{\alpha\beta}$ (and all the other kernels under consideration) is slightly more complicated, namely contains products of polynomials and Gaussians, the result, eqs.(IV.30) and (IV.31), can be extended. One also finds polynomials and Gaussians. Incidentally this method induced by eq.(IV.31) can also be applied in the special case where eq.(IV.6) is valid. In this special case $\mathcal{C}$ is just diagonal.

It is now possible to define the "biased density matrix" which, analogously to eq.(IV.27), takes into account the conservation of the information about a state although some spuriosity is introduced by a spectator degree of freedom (the center of mass). Let $d(\underset{\sim}{\rho},\underset{\sim}{\rho}')$ be a density matrix in RGM representation. Assume that the RGM kernel $k(\underset{\sim}{\rho},\underset{\sim}{\rho}')$ and GCM kernel $K(\underset{\sim}{r},\underset{\sim}{r}')$ derive from each other through an equation analogous to eq.(IV.27)

$$K(\underset{\sim}{r},\underset{\sim}{r}') = \int d\underset{\sim}{\rho}\ d\underset{\sim}{\rho}'\ \mathcal{G}\ (\underset{\sim}{r}-\underset{\sim}{\rho},\underset{\sim}{r}'-\underset{\sim}{\rho}')\ k(\underset{\sim}{\rho},\underset{\sim}{\rho}') . \tag{IV.32}$$

Define the "biased" (GCM) density $D(\underset{\sim}{r},\underset{\sim}{r}')$ by the relation (notice the interchange of variables)

$$d(\underset{\sim}{\rho}',\underset{\sim}{\rho}) = \int d\underset{\sim}{r}\, d\underset{\sim}{r}'\, \mathcal{G}(\underset{\sim}{r}-\underset{\sim}{\rho},\underset{\sim}{r}'-\underset{\sim}{\rho}')\, D(\underset{\sim}{r}',\underset{\sim}{r}) \ . \tag{IV.33}$$

Then the RGM and GCM expectation values are equal,

$$\begin{aligned} \mathrm{Tr}\ k\, d &= \int d\underset{\sim}{\rho}\, d\underset{\sim}{\rho}'\, k(\underset{\sim}{\rho},\underset{\sim}{\rho}')\, d(\underset{\sim}{\rho}',\underset{\sim}{\rho}) \\ &= \int d\underset{\sim}{\rho}\, d\underset{\sim}{\rho}'\, d\underset{\sim}{r}\, d\underset{\sim}{r}'\, k(\underset{\sim}{\rho},\underset{\sim}{\rho}')\, \mathcal{G}(\underset{\sim}{r}-\underset{\sim}{\rho},\underset{\sim}{r}'-\underset{\sim}{\rho}')\, D(\underset{\sim}{r}',\underset{\sim}{r}) \\ &= \int d\underset{\sim}{r}\, d\underset{\sim}{r}'\, K(\underset{\sim}{r},\underset{\sim}{r}')\, D(\underset{\sim}{r}',\underset{\sim}{r}) \\ &= \mathrm{Tr}\ K\, D \ . \end{aligned} \tag{IV.34}$$

E. Distorted wave Born approximation

Rather than the methods described in subsections C and D, which are attempts towards a full solution of the dynamical problem of collision, one may look for a DWBA approximation.

The DWBA form factor for the transition from channel α to channel β has then obviously to do with the generator coordinate kernel

$$K_{\alpha\beta}(\underset{\sim}{r}',\underset{\sim}{r}) = \langle \beta \underset{\sim}{r}' | \mathcal{V}_T | \alpha \underset{\sim}{r} \rangle \ , \tag{IV.35}$$

where $\mathcal{V}$ is the two body potential operator present in $\mathcal{H}$ and the subscript T means that $\mathcal{V}$ has been truncated into a residual potential such as the post potential for instance.

More precisely, one may define a specific set of Wick's theorem contractions

$$\begin{aligned} K_{\beta\alpha}(\underset{\sim}{r}',\underset{\sim}{r}) = \langle 0 | & b(N_B \underset{\sim}{r}'/N) \left[A(N_b \underset{\sim}{r}'/N)\ \nu_f(N_b \underset{\sim}{r}'/N) \right] \mathcal{V}_T \\ & A^\dagger(N_A \underset{\sim}{r}/N) \left[\nu_i^\dagger(-N_A \underset{\sim}{r}/N)\ b^\dagger(-N_A \underset{\sim}{r}/N) \right] | 0 \rangle \end{aligned} \tag{IV.36}$$

where $A\nu_f$ corresponds to the decomposition of B into core and cloud and, similarly $\nu_i^\dagger b^\dagger$ corresponds to the decomposition of $a^\dagger$ into core and cloud. The rules for contractions are the following,

i) one pair of creation-annihilation operators of $\mathcal{V}$ contracts from ν_f to ν_i,

ii) the other pair contracts from b to $b^\dagger$,

iii) what is left inside $A\nu_f$ contracts with what is left inside $A^\dagger \nu_i^\dagger$, for instance A contracts with $A^\dagger$ and what is left in ν_f contracts with what is left in $\nu_i^\dagger$,

iv) what is left inside b contracts with $b^{\dagger}$.

The first two rules, i) and ii), correspond to a truncation of $\mathcal{V}$ into the residual interaction between core b and the cloud of transferred nucleons. The last two rules, iii) and iv), correspond to an inert core overlap approximation relating A to the core of B (and the core of a to b) when connecting the ket to the bra.

Once $K_{\alpha\beta}$ is obtained, nothing prevents to define a resonating group kernel $k_{\beta\alpha}(\underset{\sim}{\rho}',\underset{\sim}{\rho})$ by a formula analogous to eq.(IV.27) or eq.(IV.32). Let now $g_{\alpha}(\underset{\sim}{\rho})$ and $g_{\beta}(\underset{\sim}{\rho}')$ be optical waves for the initial and final channel, respectively. The DWBA amplitude is then

$$T_{DWBA} = \int d\underset{\sim}{\rho}\, d\underset{\sim}{\rho}'\; k_{\beta\alpha}(\underset{\sim}{\rho}',\underset{\sim}{\rho})\; g_{\alpha}(\underset{\sim}{\rho})\; g^{*}_{\beta}(\underset{\sim}{\rho}') \; . \tag{IV.37}$$

Alternately one may consider $g_{\alpha}(\underset{\sim}{\rho})\; g^{*}_{\beta}(\underset{\sim}{\rho}')$ as a density operator $d(\underset{\sim}{\rho},\underset{\sim}{\rho}')$ and define a density $D(\underset{\sim}{r},\underset{\sim}{r}')$ by a formula analogous to eq.(IV.33). One then obtains

$$T_{DWBA} = \int d\underset{\sim}{r}\, d\underset{\sim}{r}'\; K_{\beta\alpha}(\underset{\sim}{r}',\underset{\sim}{r})\; D(\underset{\sim}{r},\underset{\sim}{r}') \; . \tag{IV.38}$$

V. OTHER EXAMPLES OF APPLICATION

A. Axial rotations

This may be the oldest case of a generator coordinate model and it is well known since the paper of Peierls and Yoccoz. Let Φ_K be an eigenstate of J_z, with eigenvalue K, usually a deformed Slater determinant. A rotation band is derived from the angular momentum projected states

$$\Psi_{JK} = \int d(\cos\beta)\; d^{J}_{KK}(\beta)\; \exp(-i\beta\, J_y)\; \Phi_K \; . \tag{V.1}$$

The generating function is here, obviously, that obtained from Φ_K by a rotation of angle β around the y-axis. One then uses the reduced rotation matrix element d^{J}_{KK} as Griffin-Hill-Wheeler amplitude.

B. Triaxial rotations

The deformed (intrinsic) Slater determinant Φ is no more an eigenstate of J_z. The generating function is obtained by the most general rotation, depending upon three Euler angles $\alpha\ \beta\ \gamma$

$$\Phi_{\alpha\beta\gamma} = \exp(-i\,\alpha\, J_z)\; \exp(-i\,\beta\, J_y)\; \exp(-i\,\gamma\, J_z)\; \Phi \; . \tag{V.2}$$

The Griffin-Hill-Wheeler equation can be solved in two steps. The first one is a quasi-band and angular momentum projection,

$$\Psi_{JMK} = \int d\alpha\; d(\cos\beta)\, d\gamma\; \mathcal{D}^{J}_{MK}(\alpha\beta\gamma)\; \Phi_{\alpha\beta\gamma}, \tag{V.3}$$

with the rotation matrix element $\mathcal{D}^{J}_{MK}$ as amplitude. The second step is a residual diagonalization between quasi-bands,

$$\sum_{K} \langle \Psi_{JMK'} | (\mathcal{H} - E^{\kappa}) | \Psi_{JMK} \rangle \; f^{J\kappa}_{K} = 0. \qquad (V.4)$$

The index K disappears, to be replaced by an index κ carried by the eigenvalue E^{κ} and the amplitude vector $f^{J\kappa}$. Full degeneracy with respect to M is obviously found.

C. Three-body problem

An exact, and technically available solution to the non-relativistic three-body problem is the set of Faddeev equations. When discrete degrees of freedom (spin, isospin, etc) are involved, however, the number of coupled channels in these equations may become unwieldy. As an example, if three quarks are heavy enough to be treated non relativistically and if the effective quark-quark interaction depends strongly on spin, flavor and color, it may be useful to look for an approximation such as the Hartree-Fock approximation.

For the sake of simplicity let the discrete degrees of freedom be discarded and the 3 quarks be considered as distinguishable. Assume, furthermore, that the quark bagamounts to a harmonic oscillator. The oscillator can be deformed, with three different constants α, β, γ along the three axes x, y, z. With Γ a Gaussian, a generating function reads, in an obvious notation

$$\begin{aligned} \Phi_{\alpha\beta\gamma}(\underset{\sim}{r}_1\ \underset{\sim}{r}_2\ \underset{\sim}{r}_3) = {} & \Gamma(x_1/\alpha)\ \Gamma(x_2/\alpha)\ \Gamma(x_3/\alpha) \\ & \Gamma(y_1/\beta)\ \Gamma(y_2/\beta)\ \Gamma(y_3/\beta) \\ & \Gamma(z_1/\gamma)\ \Gamma(z_2/\gamma)\ \Gamma(z_3/\gamma)\ . \end{aligned} \qquad (V.5)$$

It is easy to check that it has no center of mass spuriosity, namely that it factorizes

$$\Phi_{\alpha\beta\gamma} = \chi_{\alpha\beta\gamma}(\underset{\sim}{R})\ \psi^{int}_{\alpha\beta\gamma}(\underset{\sim}{\xi},\underset{\sim}{\xi}')\ . \qquad (V.6)$$

Here χ is a deformed Gaussian for the center of mass $\underset{\sim}{R}$ and Ψ^{int} is also a deformed Gaussian for the two Jacobi coordinates $\underset{\sim}{\xi}$, $\underset{\sim}{\xi}'$.

Since χ depends on α, β, γ, the GCM ansatz

$$\Psi = \int d\alpha\ d\beta\ d\gamma\ f(\alpha\beta\gamma)\ \Phi_{\alpha\beta\gamma} \qquad (V.7)$$

introduces center of mass spuriosity. It is clear however that the overlap kernel

$$I = \frac{\langle \Phi_{\alpha'\beta'\gamma'} | \Phi_{\alpha\beta\gamma} \rangle}{\langle \chi_{\alpha'\beta'\gamma'} | \chi_{\alpha\beta\gamma} \rangle} = \langle \psi^{int}_{\alpha'\beta'\gamma'} | \psi^{int}_{\alpha\beta\gamma} \rangle \qquad (V.8)$$

makes sense. Also, if $\mathcal{H}$ depends only on the Jacobi coordinates, the energy kernel

$$H = \frac{\langle \Phi_{\alpha'\beta'\gamma'} | \mathcal{H} | \Phi_{\alpha\beta\gamma} \rangle}{\langle \chi_{\alpha'\beta'\gamma'} | \chi_{\alpha\beta\gamma} \rangle} = \langle \psi^{int}_{\alpha'\beta'\gamma'} | \mathcal{H} | \psi^{int}_{\alpha\beta\gamma} \rangle, \qquad (V.9)$$

also makes sense. Although $\mathcal{H}$ depends only on $\underset{\sim}{\xi}$, $\underset{\sim}{\xi}'$ it can still be written in terms of $\underset{\sim}{r}_1$, $\underset{\sim}{r}_2$, $\underset{\sim}{r}_3$ and the numerator of the left hand side of eq.(V.9) can easily be calculated in second quantization. As regards denominators $\langle \chi_{\alpha'\beta'\gamma'} | \chi_{\alpha\beta\gamma} \rangle$, they can be easily derived analytically and/or tabulated.

The equation

$$(H-EI)\ f = 0 \qquad (V.10)$$

is then equivalent to the ansatz

$$\psi^{int}(\underset{\sim}{\xi},\underset{\sim}{\xi}') = \int d\alpha\ d\beta\ d\gamma\ f(\alpha\beta\gamma)\ \psi^{int}_{\alpha\beta\gamma}(\underset{\sim}{\xi},\underset{\sim}{\xi}')\ , \qquad (V.11)$$

a theory of bag vibrations. We insist, however, that all calculations can be made in the single quark coordinate representation.

D. Hard cores

It is usually assumed that a single nucleon orbital is concentrated in a certain domain, but that its tail extends everywhere. Nothing prevents, however, to restrict a single nucleon orbital φ_i to a finite, compact domain $\mathcal{D}_i$. This is only a more restricted class of wave functions.

Assume now that, for $i \neq j$, $\mathcal{D}_i$ and $\mathcal{D}_j$ have no point at a distance smaller than a certain radius r_c. If the nucleon-nucleon interaction has a strong short range repulsion (hard core) of radius smaller or equal to r_c, that repulsion cannot act between $\mathcal{D}_i$ and $\mathcal{D}_j$. A Slater determinant built out of such orbitals with disconnected domains is then compatible with the hard core. In other words, the Hartree-Fock theory applies to hard cores as well.

The parameters of such determinants are then the shapes of the domains $\mathcal{D}_i$ themselves. The radius r_c is also a parameter, for one may always take a larger separation than needed. In any case, the ansatz

$$\Psi = \int \prod_i [D\mathcal{D}_i]\ f(\mathcal{D}_1 \ldots \mathcal{D}_N)\ \Phi_{\mathcal{D}_1 \ldots \mathcal{D}_N} \qquad (V.12)$$

may be understood as a geometrical, or functional integral, generalization of the GCM ansatz. Here $\mathcal{D}_1 \ldots \mathcal{D}_N$ is a set of shapes for the domains allowed for N nucleons, $\Phi_{\mathcal{D}_1 \ldots \mathcal{D}_N}$ is the result of a Hartree calculation for that set of frozen shapes, and the symbol $\pi_i [D \mathcal{D}_i]$ means superposition of all allowed shapes. In a restricted approximation the amplitude f may be understood as a function of a more or less finite set of parameters for the shapes of $\mathcal{D}_1 \ldots \mathcal{D}_N$.

This opens the way to a theory of a new possible mode of nuclear vibrations, which can be understood as correlation vibrations.

VI CONCLUSION

There may be three ideas which can be retained from the above considerations. The first one is the amazing flexibility of the generator coordinate formalism. Any macroscopic degree of freedom can be forced into the generator function and the resulting dynamics studied. The second idea is the level of mathematical technology involved. A certain amount of caution is necessary in order to avoid unphysical singularities, but the situation is less complicated than it looks at first sight.

The third idea is probably the most important and corresponds actually to a major, and yet unsolved physical problem. Since the generator coordinate method finally amounts to diagonalization in a subspace and a reduction of the number of degrees of freedom, it is essential to understand why such subspace is of interest and why such degrees of freedom emerge from the many body dynamics. It is hoped that section III has brought a slight progress on this fundamental question.

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