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A FEW METHODS FOR THE THEORY OF COLLECTIVE MOTIONS AND COLLISIONS

by

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1. Introduction and foreword

The title originally planned for this series of lectures was "Time-dependent Hartree Fock Theory of Nuclear Motions and Collisions". In fact, in what follows, the TDHF method will be considered for collective motion only. This is because a new, more practical theory of collisions has recently emerged. These lectures thus contain two main and distinct chapters, the first dedicated to this new theory of collisions and the second to collective motion. As a distraction to the reader, a last and small chapter recalls elementary ideas about some conjectured mechanisms for the dynamics of a very special system with collective motions, namely a living organ in the nervous system. This Summer School being dedicated to the subject of order and chaos, it is hoped that the considerations which follow never go too far from that fascinating subject indeed.

2. The Boosted Shell Model Theory of Collisions

2.1 Jacobi coordinates versus individual coordinates

Consider, for the sake of simplicity, 5 particules with coordinates $\vec{x}_1 \ldots \vec{x}_5$, and a 3-body final channel where, for instance, particles 1 and 2 are bound in a first cluster and particules 3 and 4 are bound in a second cluster. An intuitive representation which is adjusted to this situation deals with the Jacobi degrees of freedom

$$\vec{r}' = \vec{x}_2 - \vec{x}_1, \quad \vec{r}'' = \vec{x}_4 - \vec{x}_3, \quad \vec{c}' = \frac{\vec{x}_3+\vec{x}_4}{2} - \frac{\vec{x}_1+\vec{x}_2}{2}, \quad \vec{c}'' = \vec{x}_5 - \frac{\vec{x}_1+\vec{x}_2+\vec{x}_3+\vec{x}_4}{4}$$

and

$$\vec{R} = \frac{\vec{x}_1+\vec{x}_2+\vec{x}_3+\vec{x}_4+\vec{x}_5}{5}. \qquad (2.1.1)$$

Whenever long range forces do not complicate the theory the channel

wave function is

$$\chi'_{ex} = \psi'_{int}(\vec{\xi}')\ \psi''_{int}(\vec{\xi}'')\ \exp[i(\vec{k}'.\vec{\rho}'+\vec{k}''.\vec{\rho}'')]\ \Gamma(\vec{R}), \qquad (2.1.2)$$

where ψ'_{int} and ψ''_{int} are the internal wave functions for the clusters, and Γ is any state for the physically irrelevant total center of mass.

The difference in boundary conditions for $\vec{\xi}'$, $\vec{\xi}''$ on one hand and $\vec{\rho}'$, $\vec{\rho}''$ on the other hand is striking, since the former involve square integrable, decaying tail states while the latter occur in plane waves extending to infinity. Such a difference is a fundamental feature of the theory of collisions and seems to enforce the use of Jacobi coordinates. It is clear, however, that the use of such coordinates becomes a nightmare when the particle number reaches more than a few units. If only because of antisymmetrization problems, a $^{19}F + {}^{56}Fe$ channel description in Jacobi coordinates is utterly beyond any practicability.

It is necessary to return to individual coordinates $\vec{x}_i$. Let $\psi'_{sm}(\vec{x}_1,\vec{x}_2)$ and $\psi''_{sm}(\vec{x}_3,\vec{x}_4)$ be shell model descriptions of the two clusters, namely ψ'_{sm} is a product of two orbitals $\varphi_1(\vec{x}_1)\ \varphi_2(\vec{x}_2)$, with antisymmetrization if necessary, and ψ''_{sm} is also a product $\varphi_3\varphi_4$. As a matter of fact ψ'_{sm} is often a sum of such products $\varphi_1\varphi_2$, in order to improve the cluster wave function by configuration mixing, and ψ''_{sm} can also be enlarged to a similar configuration mixing. The point of interest is that

$$\psi'_{sm}(\vec{x}_1,\vec{x}_2) \simeq \psi'_{int}(\vec{\xi})\ \gamma'\left(\frac{\vec{x}_1+\vec{x}_2}{2}\right), \qquad (2.1.3)$$

where the approximate equality sign $\simeq$ means that the factorization for a center-of-mass were packet γ' is excellent (it is even exact in Gaussian models). In the same way $\psi''_{sm} \simeq \psi''_{int}\ \gamma''$ and we further stress that the average momenta carried by γ' and γ'' vanish.

Consider now

$$\begin{aligned}\chi' = &\exp\left[i\left(\vec{k}' - \frac{\vec{k}''}{2}\right).\frac{\vec{x}_3+\vec{x}_4}{2}\right]\psi'_{sm}(\vec{x}_3,\vec{x}_4)\\ &\exp\left[-i\left(\vec{k}' + \frac{\vec{k}''}{2}\right).\frac{\vec{x}_1+\vec{x}_2}{2}\right]\psi''_{sm}(\vec{x}_1,\vec{x}_2)\\ &\exp(i\,\vec{k}''.\vec{x}_5)\ \gamma(\vec{x}_5)\end{aligned} \qquad (2.1.4)$$

where γ is, like γ' and γ'', a wave packet centered at the origin of the coordinate frame and motionless on the average. It is obvious that the

orbits φ_3, φ_4 present in ψ'' are now boosted by $\vec{k}' - \frac{\vec{k}''}{2}$ and the orbits φ_1, φ_2 are boosted by $-\vec{k}' - \frac{\vec{k}''}{2}$, while the fifth particle is boosted by an amount $\vec{k}''$. The balance of momenta thus amounts to an *average* relative momentum $\vec{k}'$ between the two clusters and an *average* momentum $\vec{k}''$ between the fifth particle and the center of mass of the two clusters. In other words, upon taking advantage of Eq.(2.1.3) and its equivalent for ψ''_{sm}, we find

$$\chi' \simeq \psi'_{int}(\vec{\xi}')\ \psi''_{int}(\vec{\xi}'')\ \exp[i(\vec{k}'.\vec{\rho}' + \vec{k}''.\vec{\rho}'')]$$
$$\gamma'\left(\frac{\vec{x}_1+\vec{x}_2}{2}\right)\ \gamma''\left(\frac{\vec{x}_3+\vec{x}_4}{2}\right)\ \gamma(\vec{x}_5)\ . \qquad (2.1.5)$$

The last step is to recognize that the product $\gamma'\gamma''\gamma$ of wave packets also reads

$$\gamma'\left(\frac{\vec{x}_1+\vec{x}_2}{2}\right)\ \gamma''\left(\frac{\vec{x}_3+\vec{x}_4}{2}\right)\ \gamma(\vec{x}_5) \simeq \Gamma'(\vec{\rho}')\ \Gamma''(\vec{\rho}'')\ \Gamma(\vec{R})\ , \qquad (2.1.6)$$

where Γ', Γ'' and Γ are localized around the origin with vanishing average momenta. This occurs because, as shown by Eq.(2.1.1), $\vec{\rho}'$, $\vec{\rho}''$ and $\vec{R}$ are just rearrangements of $\frac{\vec{x}_1+\vec{x}_2}{2}$, $\frac{\vec{x}_3+\vec{x}_4}{2}$ and $\vec{x}_5$, and because the latter degrees of freedom are localized by $\gamma'\gamma''\gamma$ around the origin with vanishing average momenta. It is easy to check such properties in the case of Gaussian waves packets with suitable widths, for which all the factorizations shown in Eqs.(2.1.5) and (2.1.6) can be made exact.

We now insert Eq.(2.1.6) in Eq.(2.1.5) and compare with Eq.(2.1.2). It is seen that χ' differs from the exact χ'_{ex} by just the cut-off factors $\Gamma'(\vec{\rho}')\ \Gamma''(\vec{\rho}'')$. Such factors can be extremely useful in practical calculations of matrix elements involving that channel, for they prevent the integration domain to extend to infinity. Hence divergences are eliminated from the theory. An even greater advantage is that, according to Eq.(2.1.4), χ' is still a shell model-like state, namely a product of (boosted) orbitals or a sum of such products. Hence all calculations can be done in a representation of individual coordinates $\vec{x}_i$. In particular, the problem of antisymmetrization is not formidable any more.

How sensitive is the theory with respect to the widths of the wave packets γ', γ'', γ or Γ', Γ'', Γ? As regards the total center of mass, the physics is *a priori* completely insensitive to Γ, provided that wave packet is the same in all the channel functions χ which appear in the theory. If Γ depends on χ, special precautions can be taken, but these

technicalities will not be discussed in these lectures. More important is the rôle of Γ', Γ''. As long as the ranges of the nucleus-nucleus interactions which prevail in the channels under study are *smaller* than the ranges b of those wave packets, little is changed to the physics. This is because anyhow these interactions would have provided a cut-off. If the ranges of the interactions are larger than the ranges b of Γ', Γ'', then the spreads $\Delta k'$, $\Delta k''$ induced by Γ', Γ'' around the physical, central momenta $\vec{k}'$, $\vec{k}''$ cannot be neglected. In other words, the physical amplitudes, which should be calculated at sharp values of the momenta, are smeared by the wave packets. This is however a well documented problem, for there exists standard techniques for unfolding and recovery of an averaged signal. This technical question will not be discussed here but the considerations which follow will show how the representation of χ' in terms of individual coordinates $\vec{x}_i$ is a decisive advantage for practical calculations.

2.2 Variational estimates of amplitudes

We now consider an initial and a final channel, with wave functions χ_{ex} and χ'_{ex} respectively. In any realistic case, the initial channel will be a two-body channel, for ternary reactions are exceptional. Thus χ_{ex} contains only one label $\vec{k}$. On the other hand any fragmentation can occur in the final channel and thus χ'_{ex} can contain any number of relative momenta $\vec{k}'$, $\vec{k}''$,...$\vec{k}^{(N-1)}$, where N is the number of elementary particles involved. As described in paragraph 2.1, χ_{ex} and χ'_{ex} will now be replaced by boosted shell model wave packets χ and χ'.

The traditional T-matrix theory of collisions derives the transition amplitude from the matrix element

$$T_{ex} = \langle \chi'_{ex} | \Psi_{ex} \rangle + \langle \Psi'_{ex} | (E + i\varepsilon - H)^{-1} | \Psi_{ex} \rangle \ , \qquad (2.2.1)$$

where E is the total physical energy carried by χ_{ex} and χ'_{ex} (relative kinetic energies minus binding energies), ε is an infinitesimal, H is the N-particle Hamiltonian with subtraction of the center of mass kinetic energy,

$$H = \sum_{i=1}^{N} t_i - T_{cm} + \sum_{i>j=1}^{N} v_{ij} \qquad (2.2.2)$$

and Ψ_{ex}, Ψ'_{ex} are defined by

$$|\Psi_{ex}\rangle = (H-E)\,|\chi_{ex}\rangle, \quad |\Psi'_{ex}\rangle = (H-E)\,|\chi'_{ex}\rangle \ . \qquad (2.2.3)$$

The Born term, $\langle\chi'_{ex}|\Psi_{ex}\rangle$ is not very difficult to calculate in a practical case, at least up to an excellent approximation. The only difficult part of a theory of collisions, and thus the only interesting problem, is the multistep amplitude ΔT_{ex} as defined by the second term in the right-hand side of Eq.(2.2.1).

There are many reasons why it is impossible to calculate ΔT_{ex} exactly. The first is that $|\chi_{ex}\rangle$ and $|\chi'_{ex}\rangle$ are not perfectly well known, since one does not know how to solve accurately the asymptotic Schrödinger equations

$$(H_o-E)|\chi_{ex}\rangle = (H'_o-E)|\chi'_{ex}\rangle = 0 \quad ,$$

where H_o and H'_o are the channel Hamiltonians. More important, one does not know how to invert exactly the many-body operator $(E+i\Gamma-H)$, even where Γ is a finite imaginary part. Last but not least the limit where Γ becomes an infinitesimal ε is not trivial.

In order to face these difficulties one first notices that

$$(H-E)|\chi_{ex}\rangle = V|\chi_{ex}\rangle \quad \text{and} \quad (H-E)|\chi'_{ex}\rangle = V'|\chi_{ex}\rangle \quad , \tag{2.2.4}$$

where V and V' are the prior and post interactions respectively,

$$V = H-H_o, \quad V' = H-H'_o \quad , \tag{2.2.5}$$

namely $V' = v_{31} + v_{32} + v_{41} + v_{42} + v_{51} + v_{52} + v_{53} + v_{54}$ if one considers for example a final channel with 5 particles, two-body interactions and the fragmentation scheme described by Eq.(2.1.2). Then rather that $|\Psi_{ex}\rangle$ and $|\Psi'_{ex}\rangle$, Eq.(2.2.3), we define, as an approximation to Eq.(2.2.4),

$$|\Psi\rangle = V|\chi\rangle \quad \text{and} \quad |\Psi'\rangle = V'|\chi'\rangle \quad , \tag{2.2.6}$$

where $|\chi\rangle$ and $|\chi'\rangle$ are now boosted shell model wave packets as discussed in the previous paragraph, see Eq.(2.1.4) for example. The quantity under study is now $\langle\Psi'|(E+i\varepsilon-H)^{-1}|\Psi\rangle$, which is still non trivial because the Green function is on shell.

We notice however that the wave packets $|\chi\rangle$, $|\chi'\rangle$ introduce a width for the momenta $\vec{k}$, $\vec{k}'$... hence a width for the energy E. It makes then sense to define

$$\Delta T = \langle\Psi'|(E+i\Gamma-H)^{-1}|\Psi\rangle \tag{2.2.7}$$

with a finite Γ. It will now be shown how ΔT is easy to evaluate, at least in an approximative and practical way, in order to obtain a preliminary but still physical information on the much more complicated quantity ΔT_{ex}.

The quantity ΔT is just the stationnary value of the functional [1]

$$F(\Phi',\Phi) = \langle\Phi'|\Psi\rangle + \langle\Psi'|\Phi\rangle - \langle\Phi'|(E+i\Gamma-H)|\Phi\rangle \quad , \tag{2.2.8}$$

with respect to variations of the trial functions Φ', Φ. Indeed, the coefficients of variations $\langle\delta\Phi'|$ and $|\delta\Phi\rangle$ are, respectively,

$$\delta F/\delta\langle\Phi'| = |\Psi\rangle - (E+i\Gamma-H)|\Phi\rangle \quad , \tag{2.2.9a}$$

$$\delta F/\delta|\Phi\rangle = \langle\Psi'| - \langle\Phi'|(E+i\Gamma-H) \quad . \tag{2.2.9b}$$

Hence stationarity is reached if

$$|\Phi\rangle = G|\Psi\rangle \text{ and } \langle\Phi'| = \langle\Psi'|G \quad , \tag{2.2.10a}$$

with

$$G = (E+i\Gamma-H)^{-1} \quad . \tag{2.2.10b}$$

It can be stressed here that G is a bounded operator since Γ is finite and H hermitian. Hence $|\Phi\rangle$ and $|\Phi'\rangle$ are in the Hilbert space, like $|\chi\rangle$, $|\chi'\rangle$, $|\Psi\rangle$ and $|\Psi'\rangle$. Inserting Eq.(2.2.10) in the functional, Eq.(2.2.8), provides the stationary value $F^{st} = \langle\Psi'|G|\Psi\rangle = \Delta T$.

It is remarkable that the calculation of F only demands straightforward matrix elements of H. Not even an unperturbed Green function G_0 is demanded as an inversion, like in the traditional Schwinger variational principle [2]. It is the stationarity, namely the cancellation of all derivatives with respect to the parameters which specify Φ and Φ' in a realistic calculation, which will generate an (approximate) inversion of $(E+i\Gamma-H)$. All calculations are made in the single particle coordinate representation $\{\vec{x}_i\}$, hence these calculations are only involving shell model techniques.

The method introduced in these two paragraphs 2.1 and 2.2 thus reduce the study of collisions to those techniques already familiar in the study of bound states. Several numerical applications [3-5] are already under way. The next paragraph will show how a mean field theory also emerges from this method.

2.3 Where physics starts : mean field approach

The two previous paragraphs show that calculations which were formerly unthinkable can now be undertaken. Two questions must now be raised, namely i) how fast can one have a reasonably convergent estimate of ΔT, and ii) what physical interpretation can one propose the result ?

The traditional approach to problem i) is to search for a mean field approximation. In other words, one first uses trial functions which are factorized, for example

$$|\Phi\rangle = \prod_{i=1}^{N} |\varphi_i(\vec{x}_i)\rangle \ , \qquad (2.3.1)$$

and one cancels the functional derivative of the functional F, Eq(2.2.8), with respect to these single particle orbitals φ_i. The same stationarity with respect to the orbitals φ_i' of Φ' is also implemented, and one obtains mean field equations for the φ_i, φ_i'.

Indeed, as an illustration, let us assume that Ψ and Ψ' are also product of single particle orbitals ψ_i, ψ_i' and that no antisymmetrization is needed in the theory. Let us further assume that $\Psi' = \Psi$, namely that we are only interested in a diagonal amplitude ΔT. An finally let us assume that Γ and H can simultaneously be written with just real numbers. All these restrictions are sometimes unrealistic, but the reader can find in Refs.[3-5] enough matter for generalization. The present, simplified case is the investigation of the functional

$$F_D = \langle\Phi'|\Psi\rangle + \langle\Psi|\Phi\rangle - \langle\Phi'|(W-H)|\Phi\rangle \ , \qquad (2.3.2)$$

where $W = E+i\Gamma$. It can be noticed at once that Eqs.(2.2.10) provide $|\Phi'\rangle = |\Phi^*\rangle$ in that special case. This is because only W goes to W^* when converting the stationarity solution $\langle\Phi'|$ into a ket $|\Phi'\rangle$. Thus F_D reduces to

$$F_E = 2\,(\Phi|\Psi) - (\Phi|(W-H)|\Phi\rangle \ , \qquad (2.3.3)$$

where we now use a round bracket $(\ |\ )$ and one only trial function in a Euclidian rather than Hermitian metric.

Let us now rewrite Eq.(2.3.3) as a function of $\lambda\Phi$ rather than Φ. In other words let us temporarily constrain the Euclidian norm $(\Phi|\Phi)$ to 1 and use λ as an explicit norm and phase variational parameter. Stationarity of F_E with respect to λ then provides the stationarity

condition

$$2(\Phi|\Psi) - 2\lambda\ (\Phi|(W-H)|\Phi\rangle = 0 \quad , \tag{2.3.4}$$

hence the functional F_E becomes

$$F_R = \frac{(\Phi|\Psi)^2}{(\Phi|(W-H)|\Phi)} \quad , \tag{2.3.5}$$

where in fact the norm condition on Φ could be relaxed again. But we shall retain this condition in the following way. For the definition of a mean field approximation the factorized ansatz, Eq.(2.3.1), provides that

$$(\Phi|\Phi) = \sum_{i=1}^{N} (\varphi_i|\varphi_i) \quad . \tag{2.3.6}$$

The variation of G, Eq.(2.3.5), will thus be made under the constraints

$$(\varphi_i|\varphi_i) = 1 \tag{2.3.7}$$

with corresponding Lagrange multipliers μ_i.

We thus consider the associated functional

$$F = f^{-1}(\Phi|\Psi)^2 - (\Phi|(W-H)|\Phi) + \sum_{i=1}^{N} \mu_i(\varphi_i|\varphi_i) \ , \tag{2.3.8}$$

where the Lagrange multiplier f^{-1} takes care of the ratio between the denominator and the numerator when stationarity is reached, namely

$$f = \langle\Phi|G|\Psi\rangle = (\Phi|\Phi) \tag{2.3.9}$$

when $|\Phi\rangle = G|\Psi\rangle$. The calculation of F and its derivative with respect to φ_i are straightforward, namely

$$\begin{aligned} F = f^{-1} \sum_{i=1}^{N} (\varphi_i|\varphi_i)^2 - W \sum_{i=1}^{N} (\varphi_i|\varphi_i) + \sum_{i=1}^{N} (\varphi_i|t|\varphi_i) \\ + \frac{1}{2} \sum_{i\neq j=1}^{N} (\varphi_i\varphi_j, v|\varphi_i\varphi_j) - \sum_{i=1}^{N} \mu_i(\varphi_i|\varphi_i) \quad , \end{aligned} \tag{2.3.10}$$

hence the stationarity conditions

$$\begin{aligned} 0 = \frac{1}{2}\,\delta F/\delta\varphi_i = f^{-1}\,(\Phi|\Psi)\,\frac{(\Phi|\varphi)}{(\varphi_i|\varphi_i)}\,|\varphi_i) - W|\varphi_i) + t|\varphi_i) \\ + U_i|\varphi_i) + \mu_i|\varphi_i) \quad , \end{aligned} \tag{2.3.11}$$

where the mean field U_i acting on orbital φ_i is defined as (notice the Euclidian density φ_j^2)

$$U_i(\vec{x}) = \int d\vec{x}' \; v(\vec{x}-\vec{x}') \sum_{j\neq i} \varphi_j^2(\vec{x}') \; . \tag{2.3.12}$$

Several remarks are in order at this stage. First, the center of mass correction $-T_{cm}$ provided by Eq.(2.2.2) has been neglected here. This approximation has been voluntary, for the sake of simplicity, for otherwise the kinetic energy in Eqs.(2.3.10) and (2.3.11) would contain slightly tedious (but straightforward) two-body additional terms. Second, one notices a $\frac{1}{2}$ factor in front of $\delta F/\delta\varphi_i$, Eq.(2.3.11). This is because we have taken simultaneously the derivatives with respect to both bras and kets. Indeed the Euclidian metric provides analyticity with respect to φ_i, whether in a bra or a ket. Third, because of Eq.(2.3.9), the coefficient $f^{-1}(\;|\varphi)$ disappears in front of $|\chi_i\rangle$ in Eq.(2.3.11). Fourth, we have already taken advantage of the constraints, Eq.(2.3.7), in the derivation of Eqs.(2.3.10) and (2.3.11), although the presence of the Lagrange multipliers μ_i should actually let the scalar products $(\varphi_i|\varphi_i)$ be considered temporarily as variable quantities. It can be checked in Ref.[5], where a more general derivation of Eqs.(2.3.11) has been provided, that the final self consistency condition for the Lagrange multipliers μ_i actually reads

$$\mu_i = \sum_{j\neq i} (\varphi_j|t|\varphi_j) + \frac{1}{2} \sum_{\substack{j\neq i \\ k\neq i \\ j\neq k}} (\varphi_j\varphi_k|v|\varphi_j\varphi_k) . \tag{2.3.13}$$

Clearly, this Eq.(2.3.13) expresses the self energy of all the particles but particle i. It is now possible to summarize Eq.(2.3.11) as

$$(W-\mu_i-t-U_i)\;\varphi_i) = \;|\chi_i)\;\frac{(\;|\varphi)}{(\varphi_i|\varphi_i)} \quad , \tag{2.3.14}$$

where actually the coefficient $(\;|\varphi)/(\varphi_i|\varphi_i)$ can be temporarily discarded provided φ_i is immediately renormalized suitably to satisfy Eq.(2.3.7).

We do not know yet how to solve efficiently the N-coupled cubic equations (2.3.14). Preliminary results are described in Ref.[5], where one investigate a collision $p+{}^3H \to p+n+d$. In this Ref.[5] we have

attempted a brute force iteration. Namely one tries a first guess for the φ_i, which defines the U_i and μ_i, then one inverts the $(W-\mu_i-t-U_i)$ and this provides a second guess for the φ_i, which defines in turn a second guess for the U_i and μ_i and so on.

A certain amount of convergence is reached in some cases, but not all. In any case, the density patterns of the orbitals show reasonable tendancies. For instance the "spectator" particles, namely those which make the deuteron d, tend to be smooth. On the contrary the "participant" particles, namely the projectile p and the kicked out neutron n, do show more complicated density patterns for their orbitals. Density peaks, cleavage lines, vortices for the nucleon flow are possible interpretations, to be further confirmed or contradicted by a better analysis of the wave functions Φ and Φ'.

This brings us back to question ii) raised at the beginning of this paragraph, namely the physical significance of all this. It can be stressed that the main interest of present theory may be to suggest reaction mechanisms rather than calculate detailed cross sections. This can be seen in different ways, among which, of course, the participant vs spectator patterns which have just been discussed.

But what happens if Eqs.(2.3.14) turn out to have no solution ? Such a lack of solution is not impossible a priori, because the functional F also reads

$$F = -(\langle\Phi'| - \langle\Psi'|G)\ (E+i\Gamma-H)(|\Phi\rangle - G|\Psi\rangle) + \langle\Psi'|G|\Psi\rangle\ , \qquad (2.3.15)$$

whose hyperbolic character $\langle X'|(E+i\Gamma-H)|X\rangle$ is explicit. The extremum generated by Eqs.(2.2.10) thus seems to be a saddle point, which may disappear when the functional is restricted to just products of orbitals, Eq.(2.3.1). While an iterative algorithm starting from a high-energy limit, first guess

$$|\varphi_i^{(1)}\rangle = (E-t)^{-1}\ |t_i\rangle\ , \qquad (2.3.16)$$

would be a reasonable calculation to undertake, the sequence of second guess $\Phi^{(2)}$, third guess $\Phi^{(3)}$... and so on deduced from Eqs.(2.3.14) may have no chance to converge.

Nonetheless the patterns shown by the orbitals in that sequence $\Phi^{(n)}$ have a physical interest. For nothing prevents to define, in a

second round of the variational calculation, a new trial function with correlations

$$|\phi> = \sum_n c_n \, |\phi^{(n)}> \quad , \tag{2.3.17}$$

where now the linear coefficients c_n are the variational parameters. While Eq.(2.3.1) makes a non linear ansatz, this Eq.(2.3.17) restores the linearity of the theory. An insertion of Eq.(2.3.17) into Eq.(2.2.10) provides a linear discretization of Eq.(2.2.10), hence a set of linear equations for the c_n. It is trivial to solve these equations and obtain a unique estimate for ΔT, despite the lack of convergence of the non linear algorithm. More important, if the patterns shown by the orbitals $\varphi_i^{(n)}$ are explicit enough to suggest reaction mechanisms, then the linear superposition, Eq.(2.3.17), does provide an *interference* between these mechanisms.

This interpretation of the theory in terms of interference of mechanisms can be pushed further. It could also happen, indeed, that Eqs.(2.3.14) have *many* solutions rather than none (or one). These many solutions would of course be obtained with different initial guesses, $\phi_\alpha^{(o)}$, for the iterative algorithm. Let $\{\phi_\alpha\}$ be these different solutions. The obvious generalizations of Eq.(2.3.17) are the ansatz

$$|\phi> = \sum_\alpha c_\alpha \, |\phi_\alpha> \, , \tag{2.3.18}$$

and the ansatz

$$|\phi> = \sum_{\alpha,n} c_\alpha^{(n)} \, |\phi_\alpha^{(n)}> \quad . \tag{2.3.19}$$

The latter obviously combines different solutions and their successive guesses.

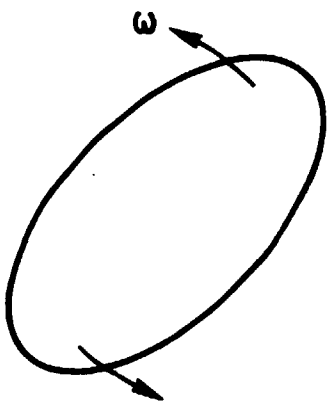
2.4 *All boson* correlations

There could be cases where the mean field equations might be too cumbersome, or their interpretation in terms of reaction mechanisms might be difficult. Nothing then prevents to feed the variational principle with explicit trial functions, such as those shown by Fig.1.

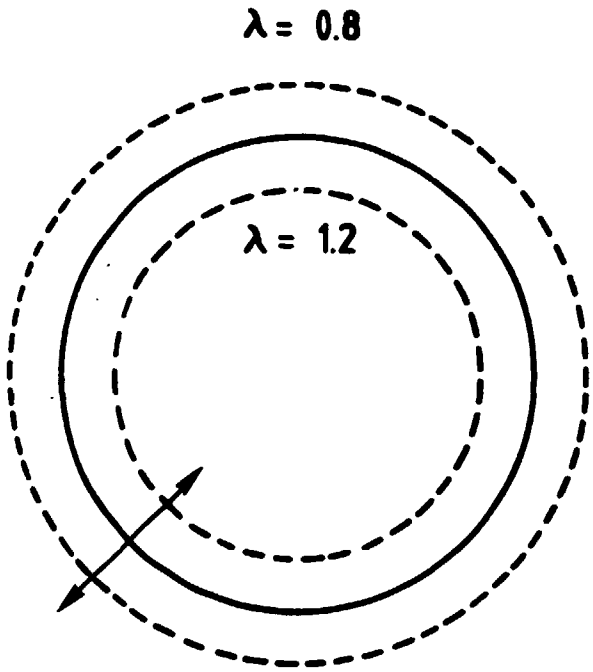
For instance, one may consider solutions ϕ_ω of the cranking model, or also quadrupole-boosted states

$$\phi_\beta = \exp\left[i \sum_{\mu=-2}^{+2} \beta_\mu \, Q_\mu \right] \phi_o \quad , \tag{2.4.1}$$

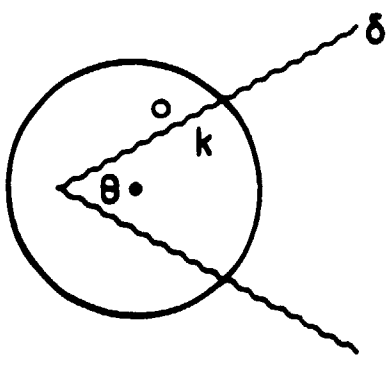
where the 5 parameters β_μ can be complex and ϕ_o is a static shell model



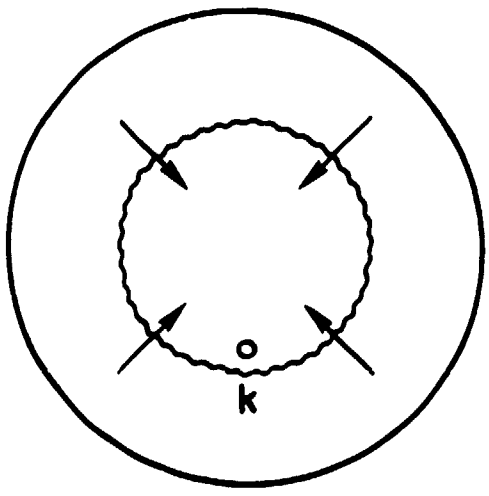
Rotation



Breathing



Shock



Implosion

Fig. 1

state, with or without a reference deformation.

The variational principle will then select values of ω and β_μ which are privileged in the reaction mechanism.

When nuclear compression is at stake, trial functions Φ_λ, where orbitals $\varphi(\lambda\vec{x})$ just exhibit a scale factor λ (preferably complex in analytical models) are certainly in order.

Shock waves can also be investigated in a self consistent way. Given an orbital φ_o of a reference state Φ_o, nothing prevents to define

$$\varphi_{\theta,\vec{k}}(\vec{x}) = \begin{cases} \exp(i\vec{k}.\vec{x})\ \varphi_o(\vec{r}) & \text{inside } \theta \\ \varphi(\vec{x}) & \text{outside } \theta \end{cases} , \qquad (2.4.2)$$

where the phrase "inside" and "outside" θ refer to the cone with angle θ at its tip. For the sake of smoothness of the wave function the boost factor should actually read something like

$$\exp \frac{i\vec{k}.\vec{x}}{1 + \exp\left(\frac{\alpha-\theta}{\delta}\right)}$$

where α is the polar angle of $\vec{x}$ as referred to $\vec{k}$ and the tip of the cone and δ defines the width of the transition zone. Again the variational principle will select dominant values for the cone angle θ and the discontinuity boost $\vec{k}$.

An implosion model is also available. It consits in boosting inwards an outer ring of nuclear matter. The ansatz looks like

$$\varphi_K(\vec{x}) = \exp\left(-\frac{iKr}{1 + \exp\left(\frac{r_o - r}{\delta}\right)}\right)\ \varphi_o(\vec{x}) \qquad (2.4.3)$$

where r_o is the inner radius of the implosing shell and δ again defines a smooth but narrow transition zone.

And so on. All these mechanisms can be made to interfere in a combined ansatz

$$\Phi = \int d\omega\ f(\omega)\ \Phi_\omega + \int d\beta\ g(\beta)\ \Phi_\beta + \int d\lambda\ h(\lambda)\ \Phi_\lambda + \int d\theta\ d\vec{k}\ i(\theta,\vec{k})\ \Phi_{\theta,\vec{k}} + \int dK\ j(K)\ \Phi_K \ , \qquad (2.4.4)$$

where the mixture amplitudes $f,g,h,i,j,\ldots$ are now governed by linear

integral equations deduced trivially from the projection of Eqs.(2.2.10) into the subspace spanned by $\Phi_\omega, \Phi_\beta \ldots, \Phi_K$.

Time dependent Hartree-Fock states Φ_t could also be used as a basis. The ansatz is

$$\Phi = \int dt\ f(t)\ \Phi_t \quad , \tag{2.4.5}$$

where $\{\Phi_t\}$ is taken for times where the nuclei remain in the interaction region. The variational equation related to Eq.(2.2.10) is then the integral equation

$$\int dt\ \langle \Phi_t, | (W-H)\ | \Phi_t \rangle\ f(t) = \langle \Phi_t, | \Psi \rangle \quad . \tag{2.4.6}$$

This is just an inhomogeneous generalization of the Griffin-Hill-Wheeler equation [6,7]. The matrix elements $\langle \Phi_t, | \Phi_t \rangle$, $\langle \Phi_t, | \Psi \rangle$ and $\langle \Phi_t, | H | \Phi_t \rangle$ shown by Eq.(2.4.6) involve factorized states and stay therefore within the domain of practical calculations. Then the manipulation of Eq.(2.4.6) is very close to the manipulations which have become familiar in the generator coordinate theory of collisions [8,9].

2.5 Back to plane waves and on shell amplitudes

This is a problem which has not yet been faced numerically in the present theory. For the one shell amplitude is actually

$$\Delta T_{ex} = \lim_{\Gamma \to 0} \left(\lim_{b \to \infty} \Delta T \right) \quad , \tag{2.5.1}$$

where b means the ranges of the wave packets for relative motion. The limits must be taken in that order, namely first $b \to \infty$ then $\Gamma \to 0$, for the range of the Green function goes to infinity when $\Gamma \to 0$, while the theory demands that the wave packet cut-off should not be artificial.

Returning to Eq.(2.2.6), however, we see that, in the case of two-fragment channels, the multiplication of $|\chi\rangle$ by V makes anyhow $|\Psi\rangle$ a short range state. In that sense the limit $b \to \infty$ might not be critical.

In any case we can remember that a wave packet χ (or χ') depends on many labels. One sees explicitly in Eq.(2.1.4) the boost labels $\vec{k}', \vec{k}'', \ldots$, etc but there are also parameters inside the shell model wave functions $\varphi'_{sm}, \varphi''_{sm}, \ldots$, etc.

Let π be the set of all these labels. Nothing prevents to expand

$|\chi_{ex}>$ as

$$|\chi_{ex}> = \int d\pi \; f(\pi) \quad |\chi_{\pi}> \quad , \tag{2.5.2}$$

where a discrete set of values of the parameters π can be used for simplicity, the subscript π has been added to the wave packet χ for the sake of clarity and $f(\pi)$ is a suitable mixture amplitude. Nothing prevents in particular to select $f(\pi)$ in such a way that the relative momentum be defined much sharper than in the initial wave packet χ.

Then, after a similar manipulation for χ', one finds

$$\Delta T_{ex} = \lim_{\Gamma \to 0} \int d\pi \; d\pi' \; <\chi'_{\pi'}, | V'(E-H+i\Gamma)^{-1} \; V|\chi_{\pi}> f'^{*}(\pi') f(\pi) \quad . \tag{2.5.3}$$

In other words, and this will be the conclusion of the present chapter, the boosted shell model theory of collisions is just a change of representation for the calculation of transition amplitudes. As seen in the previous paragraph, this change of representation opens the way to a large body of numerical calculations and physical interpretations in terms of reaction mechanisms. All the methods used in the calculation of bound states now become available for the calculation of collisions.

3. Time Dependent Hartree-Fock Theory of Collective Motion

3.1 Time dependent Hartree-Fock

There are many ways to introduce TDHF. One of the most ambitious ways is to use the fact that the set of all Slater determinants ϕ for N fermions makes an over complete set in the corresponding Hilbert space, in order to prove that there exists a measure $d\mu(\phi)$ for which the identity operator resolves[10] as

$$I = \int d\mu(\phi) \; |\phi><\phi| \quad . \tag{3.1.1}$$

This leads to a functional integral[10,11] representation of the matrix elements of the evolution operator

$$<\phi_f|\exp(-i\,Ht)|\phi_i> = \int \mathcal{D}[\phi(\tau)] \exp\left[i \int_0^t d\tau \; L(\tau) \right] \quad , \tag{3.1.2}$$

where $\phi(\tau)$ is any path in the space of Slater determinants with boundary

conditions

$$\phi(0) = \phi_i \quad , \quad \phi(t) = \phi_f \quad , \tag{3.1.3}$$

and $\mathcal{D}[\phi(\tau)]$ is the functional measure. The Lagrangian density is defined as

$$L(\tau) = i\langle\phi(\tau)|\frac{d}{d\tau}\phi(\tau)\rangle - \langle\phi(\tau)|L|\phi(\tau)\rangle \tag{3.1.4}$$

The stationary phase approximation to eq. (3.1.2) selects as "least action path" the TDHF path, with the equation of motion

$$i\frac{d}{d\tau}|\phi\rangle = H(\phi)|\phi\rangle \quad , \tag{3.1.5}$$

where $H(\phi)$ is the usual Hartree-Fock Hamiltonian

$$H = T+U \ , \tag{3.1.6}$$

with T and U the N-particle kinetic energy $T = \sum_{i=1}^{N} t_i$ and average potential energy $U = \sum_{i=1}^{N} u_i$, respectively. The mean field u acting on the orbitals of ϕ is defined, as usual in Hartree-Fock theory, by

$$\langle\vec{x}|u|\vec{x}'\rangle = \delta(\vec{x}-\vec{x}')\int d\vec{x}''\ v(\vec{x}-\vec{x}'')\rho(\vec{x}'',\vec{x}'') - v(\vec{x}-\vec{x}')\rho(\vec{x},\vec{x}') \quad , \tag{3.1.7}$$

where the one-body density matrix ρ is obtained trivially from the orbitals φ_i which make ϕ,

$$\rho(\vec{x},\vec{x}') = \sum_{i=1}^{N} \varphi_i(\vec{x})\varphi_i^*(\vec{x}') \quad . \tag{3.1.8}$$

One recognizes in eq. (3.1.7) the local two-body potential v introduced in eq. (2.2.2), hence a local direct term and a non local exchange term in u (locality of v is a simplification, not a mandatory element of the theory). Again one neglects the subtraction of T_{cm}, in order to simplify eq. (3.1.6). This detail will be understood in the following.

The functional integral approach has at least one serious drawback, namely the contradiction between Eqs. (3.1.3) and Eq. (3.1.5). For the latter is a first order differential equation with respect to time. Hence only *one* out of the two boundary conditions Eqs. (3.1.3) can be normally satisfied in a generic situation, not both. Improvements of the theory are possible[12], at the cost of introducing an additional evolution equation, namely that of a measure operator in a Heisenberg

representation. But these improvements are not yet related to the finding of collective modes and will not be discussed here, although they will be stimulating in the near future.

Returning to traditional TDHF, the simplest way to justify Eq. (3.1.5) is admit that since we do not know how to solve accurately on a computer the realistic time dependent Schrödinger equation (TDSE),

$$i \frac{d}{d\tau} \Psi = H\Psi \quad , \qquad (3.1.9)$$

one may replace Ψ by a Slater determinant ϕ in first approximation, and then just remember that, by Thouless' theorem, an infinitesimal variation of ϕ is just a one-particle, one-hole vector. Thus Eq. (3.1.9) can be projected in the particle-hole space,

$$i\langle ph|\dot{\phi}\rangle = \langle ph|H|\phi\rangle \quad ,$$

This is nothing but Eq. (3.1.5) since the very definition of the Hartree-Fock Hamiltonian $H(\phi)$ provides that

$$\langle ph|H|\phi\rangle \equiv \langle ph|H|\phi\rangle \quad .$$

It could be pointed out that the infinitesimal variation $i\dot{\phi}dt$ has also a component proportional to ϕ itself. This raises interesting questions of phase evolution of ϕ and gauge invariance[13] of the theory. The relation between Eq. (3.1.9) and Eq. (3.1.5) must therefore just be completed by a prescription such as

$$i\langle\phi|\dot{\phi}\rangle = \langle\phi|H|\phi\rangle + \mu(\tau) \quad ,$$

where $\mu(\tau)$ is a suitable phase. This question, however, does not seem yet to be full correlated to the subject of collective motion and will not be discussed further, although it was shown[13] to play a role in the search for *periodic* TDHF solutions and their quantization.

Let us come to the point. When is a TDHF (numerical) solution of any interest for a collective (nuclear) motion ?

And what is collectivity in the first place ? This question will be faced later in this lecture. For the present paragraph, we shall be satisfied with two empirical criteria, as follows.

A TDHF solution will first be found to be interesting for collective motion if its time evolution reads

$$\phi(\tau) \simeq \prod_{\mu=1}^{R} \exp[i\, a_\mu(\tau) X_\mu]\phi(0) \quad , \tag{3.1.10}$$

where $a_\mu(\tau)$ is any function of time which helps fitting the evolution of ϕ, and X_μ is among the collective one-body operators one finds in the nuclear zoology. The ideal case occurs of course when the R operators X_μ make a (closed) Lie algebra and when the approximate equality sign $\simeq$ is a true equality sign.

The relation between " collective" TDHF and "collective" operators is not a circular argument. For if X_μ coincides with, e.g., angular momentum operators, or quadrupole operators or higher multipoles, one stays on the firm ground of the many-year success of the collective model of Bohr and Mottelson.

A second, weaker condition for the pertinence of a TDHF solution is to obtain a time independent collective state

$$\Psi = \int dt\, f(\tau)\phi(\tau) \quad , \tag{3.1.11}$$

after using time[14] as a generator coordinate. The condition is weaker than Eq. (3.1.10) for it is the linear subspace spanned by the set $\{\phi(\tau)\}$ which then makes sense rather than each individual $\phi(\tau)$. Again the argument is not completely circular, for there is a large consensus in the literature about which states Ψ in the spectrum of a nucleus are collective and which are not.

Some practical examples are now in order. They are the subject of the next paragraph.

3.2 Two elementary cases of TDHF collectivity

The first elementary case is that of translation. Consider a doubly even nucleus and any of its static Hartree Fock solutions ϕ_o. We will now prove, as a theorem, that if we label $\varphi_{io}(\vec{p})$ in momentum representation the orbitals which make ϕ_o, then the translated and boosted orbitals

$$\varphi_i(\vec{p},\tau) = \exp\left[i\left(\frac{k^2}{2} - \varepsilon_i - \vec{k}.\vec{p}\right)\tau\right]\varphi_{io}(\vec{p}-\vec{k}) \quad , \tag{3.2.1}$$

where ε_i is the static self energy of φ_{io}, make a determinant $\phi(\tau)$

which is a TDHF solution.

For that purpose, we first notice that the transformation, Eq. (3.2.1), is indeed a relation between the hole states as referred to ϕ and ϕ_o as vacuums, respectively, but also that the same relation holds for the relation between *particle* states. Let i and i', then i_o and i'_o, respectively denote two orbitals (particle or hole states) of ϕ and ϕ_o. With the convention that Planck's constant ħ and nucleon mass m are unity, the one-body kinetic energy t shows the following relation for its matrix elements

$$\langle i'|t|i\rangle = \langle i'_o|\left(t+\vec{k}.\vec{p}-\frac{k^2}{2}\right)|i_o\rangle \exp[i(\varepsilon_{i'}-\varepsilon_i)\tau] \quad . \tag{3.2.2}$$

This is because $t = p^2/2$, which commutes with the phase exponential found in the right hand side of Eq. (3.2.1).

Then we consider the equivalent of Eq. (3.2.1) in coordinate representation

$$\varphi_i(\vec{x},\tau) \equiv \exp\left[i\left(\frac{k^2}{2}-\varepsilon_i\right)\tau+\vec{k}.(\vec{x}-\vec{k}\tau)\right]\varphi_{io}(\vec{x}-\vec{k}\tau) \quad . \tag{3.2.3}$$

This induces for the density matrices ρ and ρ_o of ϕ and ϕ_o, respectively, the relation

$$\rho(\vec{x},\vec{x}') = \exp[i\,\vec{k}.(\vec{x}-\vec{x}')]\,\rho_o(\vec{x}-\vec{k}\tau,\vec{x}'-\vec{k}\tau) \quad . \tag{3.2.4}$$

Hence the corresponding mean field potentials u and u_o verify

$$\langle\vec{x}|u|\vec{x}'\rangle = \exp[i\,\vec{k}.(\vec{x}-\vec{x}')]\langle\vec{x}-\vec{k}\tau|u_o|x'-\vec{k}\tau\rangle \quad . \tag{3.2.5}$$

As a consequence one finds the relation between matrix elements,

$$\langle i'|u|i\rangle = \langle i'_o|u_o|i_o\rangle \exp[i(\varepsilon_{i'}-\varepsilon_i)\tau] \quad . \tag{3.2.6}$$

From Eqs. (3.2.2) and (3.2.6) one now obtains

$$\langle i'|(t+u)|i\rangle = \langle i'_o|(t+u_o)|i_o\rangle\exp[i(\varepsilon_{i'}-\varepsilon_i)\tau] \tag{3.2.7}$$

$$+\langle i'_o|\left(\vec{k}.\vec{p}-\frac{k^2}{2}\right)|i_o\rangle \exp[i(\varepsilon_{i'}-\varepsilon_i)\tau] \quad .$$

Since ϕ_o is a static Hartree-Fock solution, $|i_o\rangle$ is an eigenstate of $(t+u_o)$ with that static self energy ε_i, hence

$$\langle i'|(t+u)|i\rangle = \langle i'_o|\left(\varepsilon_i+\vec{k}.\vec{p}-\frac{k^2}{2}\right)|i_o\rangle \exp[i(\varepsilon_{i'}-\varepsilon_i)\tau] \quad . \tag{3.2.8}$$

We now return to eq. (3.2.1) to find the time derivative of $|i>$,

$$i \frac{d}{d\tau} |i> = \left(\varepsilon_i + \vec{k}.\vec{p} - \frac{k^2}{2}\right)|i> \quad , \tag{3.2.9}$$

and also notice that

$$<i'|i> = <i'_o|i_o>\exp[i(\varepsilon'_i - \varepsilon_i)\tau] \quad , \tag{3.2.10a}$$

$$<i'|\vec{p}|i> = <i'_o|\vec{p}|i_o>\exp[i(\varepsilon_{i'} - \varepsilon_i)\tau] \quad . \tag{3.2.10b}$$

Hence the expected theorem,

$$<i'|(t+u)|i> = <i'|\left(\varepsilon_i + \vec{k}.\vec{p} - \frac{k^2}{2}\right)|i> = <i'|i \frac{d}{d\tau}|i> . \tag{3.2.11}$$

In other words, the boosted static Hartree-Fock determinants propagates linearly with a fixed velocity and *no spreading* as a TDHF solution. This lack of spreading is a typical solitonic behaviour. As usual, the trend towards spreading induced by the Laplacian t is compensated by the trend towards shrinking induced by the cubic non linearity $u\varphi$, since u, Eq. (3.1.7), is quadratic with respect to φ, see Eq. (3.1.8).

It is amusing to realize that spreading does occur is TDHF with an initial condition such that shown on fig. 2a. In that situation, one has on purpose switched off the non linearity, upon inducing no overlap between the initial orbitals. This cancels the potential u, and only the Laplacian t is active.

There is no need to stress that Eqs. (3.2.1) and (3.2.3) are perfect illustrations of Eq. (3.1.10). The operators X_μ are here, obviously, the total center of mass coordinate and momentum. Furthermore it is here obvious that Eq.(3.1.11) amounts to projection of the total linear momentum, in the Peierls-Yoccoz way. For the time τ occurs inside ϕ via combinations $\vec{x}-\vec{k}\tau$, hence it is as well a position index in a sequence of translated states.

The case of translations having been dealt with, we now turn to a second elementary case, that of vibrations. As studied by Bonche, Doubre and Quentin[15], let $\phi(0)$ be a static HF solution ϕ_o, boosted in a quadrupole mode however

$$\varphi_i(\vec{x},0) = \exp[i\,\varepsilon q(\vec{x})]\varphi_{io}(\vec{x}) \quad . \tag{3.2.12}$$

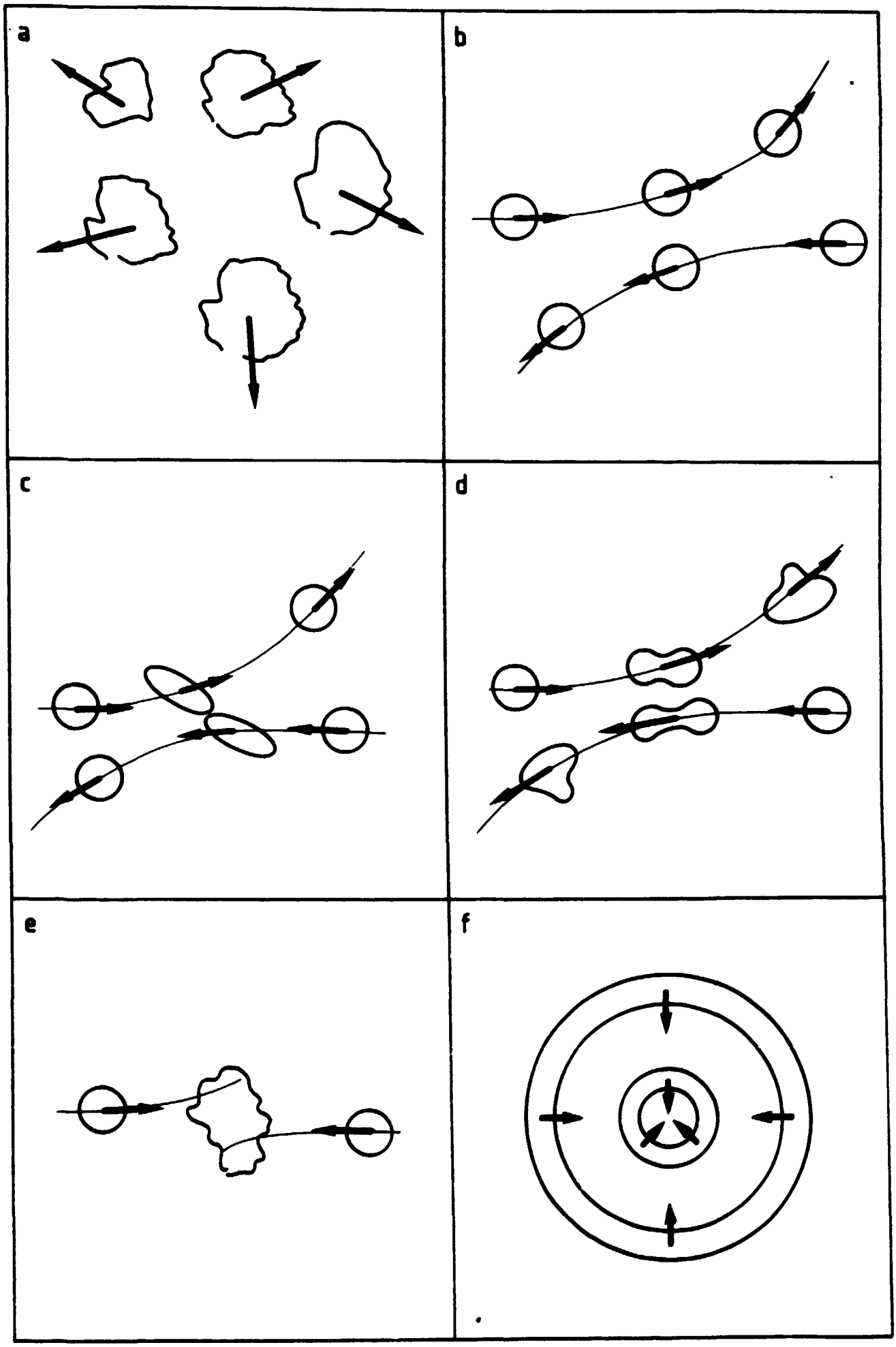


Fig.2

Here $q(\vec{x})$ is the usual quadrupole, and ε is an adjustable parameter. One selects ε such that εq be small within the range of the (bound) orbits φ_{io}.

The initial condition $\phi(o)$ built by the orbitals φ_i, Eq.(3.2.12) does induce a TDHF evolution $\phi(\tau)$ which was found in Ref.[15] to be strongly harmonic for several periods. This harmonicity can be proved to be of a RPA type if ε is sufficiently small [15]. For large values of ε, however, the RPA limit may be more difficult to justify. Nonetheless, the numerical plot of the expectation value of the quadrupole

$$\langle Q\rangle(\tau) = \sum_i \langle \varphi_i(\tau)|q|\varphi_i(\tau)\rangle \quad , \tag{3.2.13}$$

does show a very regular harmonic behavior. This is strong evidence of quadrupole vibration, although the conjugate operator with respect to q is not known explicitly from first principles, hence Eq.(3.1.10) cannot be used easily. The frequency shown [15] by $\langle Q\rangle(\tau)$, however, is strongly reminiscent of the frequencies obtained by elementary (shell model) calculations of the 2^+ vibrational spectrum. It is then most likely that Eq.(3.1.11) would have provided such vibrational time independent states Ψ. In any case, it is remarkable that the cubic TDHF equation can provide such a harmonic behavior, since the initial condition, Eq.(3.2.12), was plugged directly into a numerical time evolution code without any a priori linearization for small values of ε. This second elementary application of TDHF is both a simple and intringuing case of collective behaviour.

3.3 Transition from TDHF collectivity to TDHF chaos

The two simple examples described in the previous paragraph were one-center problems. Most of the TDHF calculations actually deal with two-center cases, namely the collision of two nuclei. For a good sample of the zoology of solutions, the reader may refer to Sandhya Devi et al [16], Cusson et al [17] and Grammaticos [18] for example. There is no unique classification of the increasing complexities of the patterns obtained, but an attempt is proposed by Fig.2.

We first put aside the initial conditions 2a (maximum spreading) and 2f (implosion of two shells), which have never been investigated numerically. They would be interesting, however. Indeed, some overlap between the "orbitals" shown by Fig.2a would be built up after some

spreading, hence the non linearity would be partly restored. It is an open question whether critical values of this overlap would occur. On the other hand the implosion geometry, Fig.2f, is ideally suited to the study of partial waves, for the angular momentum is far better defined [14] than in the usual impact parameter [16-18] initial condition. Besides, if the outer shell is a photon shell and the inner shell an atomic shell rather than nuclear shells, this geometry provides a simulation of laser compression experiments (the modification of mean field equations to include bosons is straightforward).

The initial conditions 2b-e correspond to the impact parameter representation. Namely the initial orbitals read

$$\varphi_i(\vec{p},\tau=0) \equiv \exp(\mp i \frac{\vec{b}}{2} \cdot \vec{p})\, \varphi_{io}(\vec{p} \mp \vec{k}) \quad , \qquad (3.3.1)$$

where the $\mp$ sign refers to the projectile and target, respectively, and φ_{io} is a static orbital like that considered for Eq.(3.2.1). The vector $\vec{b}$ has a component along $-\vec{k}$, which shifts the nuclei apart before the collision, and a component perpendicular to $\vec{k}$, which defines an impact parameter.

Many cases occur. The simplest case correspond to propagation of the nuclei along curved trajectories, but without distorsion. This case, Fig.2b, has been analytically investigated [19]. Then some simple distorsions may occur, first in the intermediate stages only, see Fig.2c, and then also in the final stages, see Fig.2d. Last but not least the distorsions can be so large that a parametrization in terms of low order multipoles (quadrupole , octupole...) is no more possible. This is the case of Fig.2e, where a fusion situation is reached. Some chaotic limit may thus have been reached.

We have no a priori rigorous criterion for the classification of some TDHF evolutions as more collective than others. The visual observation of density patterns for the time-dependent orbitals is a largely *subjective* method for such an analysis. This is why we have added at the end of these lectures a provocative section on the subject of pattern discrimination by the nervous system. Before going into much speculations, however, we shall dedicate the next two paragraphs to more elementary approaches for the recognition of collectivity : a metric approach and an adiabatic non metric approach.

3.4 Metric collectivity

Let us try to make advantage of the fact, that our wave functions $\phi(\tau)$ are just defining a trajectory on the unit sphere of the Hilbert space. It is not difficult to define the rate $\frac{d\ell}{d\tau}$ at which this wave function evolves as a function of time,

$$\left(\frac{d\ell}{d\tau}\right)^2 \equiv < \frac{d\phi}{d\tau} \mid \frac{d\phi}{d\tau} > \quad . \tag{3.4.1}$$

The physical meaning of this rate, an inverse time, is obviously given by the energy of propagation. Renormalization of $d\phi/d\tau$ by $\frac{d\ell}{d\tau}$ then provides the basic unit vector

$$\mid \frac{d\phi}{d\ell} > = \left(\frac{d\ell}{d\tau}\right)^{-1} \mid \frac{d\phi}{d\tau} > \quad , \tag{3.4.2}$$

which is nothing but the unitary tangent to the trajectory.

The next step is, obviously, to consider the derivative of this tangent and observe that the length of this derivation is nothing but the curvature

$$C^2 = <\frac{d^2\phi}{d\ell^2} \mid \frac{d^2\phi}{d\ell^2} > \quad . \tag{3.4.3}$$

How can this formal quantity C be interpreted in terms of collectivity ? On one hand, it is obvious that $C^2 \geq 1$, because the propagation occurs on the unit sphere in the Hilbert space, the curvature of which being obviously 1. On the other hand, it is intuitive that if the trajectory $\phi(\tau)$ generates a very large curvature, in other words winds very rapidly, the algebra $\{X_\mu\}$, see Eq.(3.1.10), which one would try for a collectivity parametrization would be fairly complicated. This complicated situation would not be very interesting and would rather indicate chaos rather than order. As defined by Eq.(3.4.3), C is a dimensionless number. Since the two limits C=1 and C infinite are found to be improper, the range of C to be investigated is likely to be a few units.

In order to refine our intuition let us consider again the heuristic ansatz for collectivity, Eq.(3.1.10), in its simplest form (one linear term for the argument of the exponential)

$$\phi(\tau) = \exp(i\tau X)\ \phi(0) \quad . \tag{3.4.4}$$

It is trivial to check from Eqs.(3.4.1) and (3.4.3) that

$$\left(\frac{d\ell}{d\tau}\right)^2 = \langle\phi(o)|X^2|\phi(o)\rangle \tag{3.4.5}$$

and

$$C^2 = \frac{\langle\phi(o)|X^4|\phi(o)\rangle}{\langle\phi(o)|X^2|\phi(o)\rangle^2} \quad , \tag{3.4.6}$$

with X hermitian of course. It is now seen that the curvature is 1 if and only if $\phi(o)$ is an eigenstate of X^2, for otherwise the fourth moment $\langle X^4\rangle$ is larger than the square of the second moment $\langle X^2\rangle$. For such an eigenstate the time evolution, Eq.(3.4.4), reduces to an uninteresting phase.

More interesting is the case where $\phi(o)$ is a coherent state with respect to X. Namely, let us assume there exists a set of commuting observables $\underline{\Xi}$, which commute with X and which provide a complete basis $|x\ \xi\rangle$ of the Hilbert space (here x and ξ are eigenvalues of X and $\underline{\Xi}$ respectively). If then a Gaussian approximation is possible,

$$\langle x\ \xi|\phi(o)\rangle \propto \exp[-(x-z)^2/\beta^2]\ \alpha(\xi) \quad , \tag{3.4.7}$$

where z is any complex number, β is some width and $\alpha(\xi)$ takes care of the degrees of freedom which differ from X, then $\phi(o)$ appears like a Glauber coherent state with respect to X. In our heuristic search for collectivity, such coherent states make sense, for several reasons. First, they make an over complete basis, like that discussed in paragraph 2.1. Second, they are often the starting point of a classical approximation, and collective motion is often associated to the dominance of one degree of freedom, with large quantum numbers, all the other degrees of freedom having been averaged out. This is a typical classical limit. Third, and maybe more important, a large class of representations in group theory can be constructed from maximum weight states, which are indeed coherent states.

As a matter of fact, the value $C = \sqrt{3}$, corresponding to coherent states, seems to be a critical value for the collectivity of a trajectory. This value comes obviously from the fact that the 4^{th} moment of a Gaussian equals 3 times the square of the 2^{nd} moment. But it was also found [20] to occur for Slater determinants when the generator X, Eq.(3.4.4), is a particle-hole operator with maximum sharing of the

particle-hole strength between all available particle-hole components. This even spreading of the strength is the usual criterion retained in Tamm-Dancoff or RPA calculations to give evidence of collectivity. This critical value $C = \sqrt{3}$ was also found [21] to be the limit curvature of geodesics on orbits of Lie group (special unitary and symplectic) which are familiar in the traditional theory of collective motion (SU(3), SP(1,R), etc...).

Thus, given a numerical TDHF trajectory $\phi(\tau)$, it is interesting to calculate at each time the curvature $C(\tau)$ and give a close look at these periods when $C \simeq \sqrt{3}$. But of course other criteria are possible. Nothing yet is known about the information contained in higher derivatives $d^n\phi/d\ell^n$. Nothing is known about the relaxation times for these curvatures ; how long will a $C \simeq \sqrt{3}$ survive the non linearity of the TDHF dynamics ? How stable with respect to the initial condition $\phi(o)$ is the existence of such a "collective" portion of a TDHF trajectory ?

To summarize this paragraph, elementary geometrical considerations can be deduced from the metric of the Hilbert space in which time dependent trajectories $\phi(\tau)$ are embedded. There seems to be a connection between the curvature properties of these trajectories and their physical meaning : triviality ($C\simeq 1$), collectivity ($C\simeq\sqrt{3}$) and chaos ($C>>1$). But the nature of this connection, the nature of the collective degrees of freedom themselves and a complete set of geometrical criteria are still unknown.

3.5 Adiabatic collectivity

As pointed out by Kerman and Koonin [22], the TDHF equation (3.1.5) is strictly equivalent to an infinite set of Hamilton equations. In other words, let the orbitals φ_i which make ϕ be expanded on a complete basis $\{u_n\}$ of single particle functions

$$|\varphi_i\rangle = \sum_n c_{in} |u_n\rangle \ . \qquad (3.5.1)$$

The energy functional

$$E(\phi) = \langle\phi|H|\phi\rangle \qquad (3.5.2)$$

is then a 4^{th} degree polynomial with respect to the coefficient c_{in}, or their real and imaginary parts $\sqrt{2}q_{in}$ and $\sqrt{2}p_{in}$. It is then equivalent

to solve Eq.(3.1.5) or to solve

$$\frac{d}{d\tau} q_{in} = \frac{\partial E}{\partial p_{in}} \quad , \tag{3.5.3a}$$

$$\frac{d}{d\tau} p_{in} = -\frac{\partial E}{\partial q_{in}} \quad . \tag{3.5.3b}$$

The question of collective coordinates is thus raised in a classical phase space rather than in a Hilbert space. The metric used in paragraph 3.4 is lost however. Generally, there is not in that phase space a sufficient number of conserved quantities J_μ (and conjugate coordinates α_μ) to make Eqs.(3.5.3) an analytically integrable system whereby the collective classical degrees of freedom would be, trivially, the J_μ, α_μ. In general Eqs.(3.5.3) are not an analytically integrable Hamilton system.

Let us concentrate, for a while, on the search for collectivity in a classical unintegrable problem. *Since collectivity is an attempt to model the system by a smaller number of degrees of freedom* (and actually just one in the simplest case), a possible answer is provided by the search for adiabaticity.

We define here adiabaticity by *two* criteria, namely

i) limit of low velocities and/or momenta and
ii) large amplitudes for positions.

This definition is more restrictive than it looks at first. For it actually breaks the Hamilton invariance of the theory. Indeed, criteria i) and ii) handle momenta and positions separately. The textbook canonical transformation $q \to p$ and $p \to -q$, which conserves Poisson brackets, is thus forbidden. In other words, this definition of adiabaticity tolerates canonical transformations which mix positions among themselves only. Furthermore, the limit of low velocities may technically differ from that of low momenta. This subtle point will not be discussed in the following, where we shall restrict ourselves to a representation where the dynamics could actually be formulated by a Lagrangian L which is just quadratic in the velocities and a Hamiltonian just quadratic in the momenta, with strictly positive masses

$$\begin{aligned} L &= \frac{1}{2} \sum_\nu m_\nu \dot{q}_\nu^2 - W(\vec{q}) \\ E &= \frac{1}{2} \sum_\nu \frac{p_\nu^2}{m_\nu} + W \quad , \; p_\nu = m_\nu \dot{q}_\nu \; . \end{aligned} \tag{3.5.4}$$

Since momenta and positions cannot be mixed, the coordinate (hyper) plane, defined by all $p_\nu=0$, is invariant under the residual transformation allowed, namely the mixing of the q_ν among themselves into a new set of positions X, $\underline{\Xi}$ (here we assume X to be of dimension 1 and $\underline{\Xi}$ to take care of all the other degrees of freedom). We now look in that plane for a line $\underline{\Xi} = \underline{\Xi}_o$, namely all degrees of freedom constant except X and want this line to be a candidate for a collective path according to criteria i) and ii). It must be pointed out here, for the sake of clarity, that this path is not a trajectory in the phase space, since momenta and velocities always vanish on that path. Rather, the path is the projection on the coordinate hyperplane of trajectories in the phase space.

The situation described by Eqs.(3.5.4) is not the most general, but it has a large validity range. Then Eqs.(3.5.3) become, trivially

$$m_\nu \dot{q}_\nu = p_\nu \quad , \tag{3.5.5a}$$

$$\dot{p}_\nu = -(\text{grad } W)_\nu \quad , \tag{3.5.5b}$$

where the gradient is taken with respect to $\vec{q}$. We now take advantage of criteria i) to initiate a trajectory from the coordinate hyperplane and find that the projection of trajectory has a cusp, since $\dot{\vec{q}} = 0$, whose tangent is given by the next derivative, namely Newton's equation

$$m_\nu \ddot{q}_\nu = -(\text{grad } W)_\nu . \tag{3.5.6}$$

Unsurprisingly, gradient lines (tangent to the force) thus appear like candidates for collective path. We now ask whether there are many trajectories in phase space whose projections on the coordinate hyperplane is the same gradient line. If so, criterion ii) will be satisfied to some extent at least, for the coordinate along the gradient line will be taken as X, orthogonal coordinates will be taken as $\underline{\Xi}$, the multiplicity of trajectories projecting along the same path will mean decoupling between X and $\underline{\Xi}$, and the various kinetic energies in that multiplicity will provide various propagation ranges, hence a chance for the large amplitudes required by criterion ii).

Two trajectories projecting along the same path differ by their momentum only. According to Eq.(3.5.5b), the next trajectory to consider after that which starts with $\vec{p}=0$ is a *boosted* trajectory which starts at the same $\vec{q}$, but with an infinitesimal momentum proportional

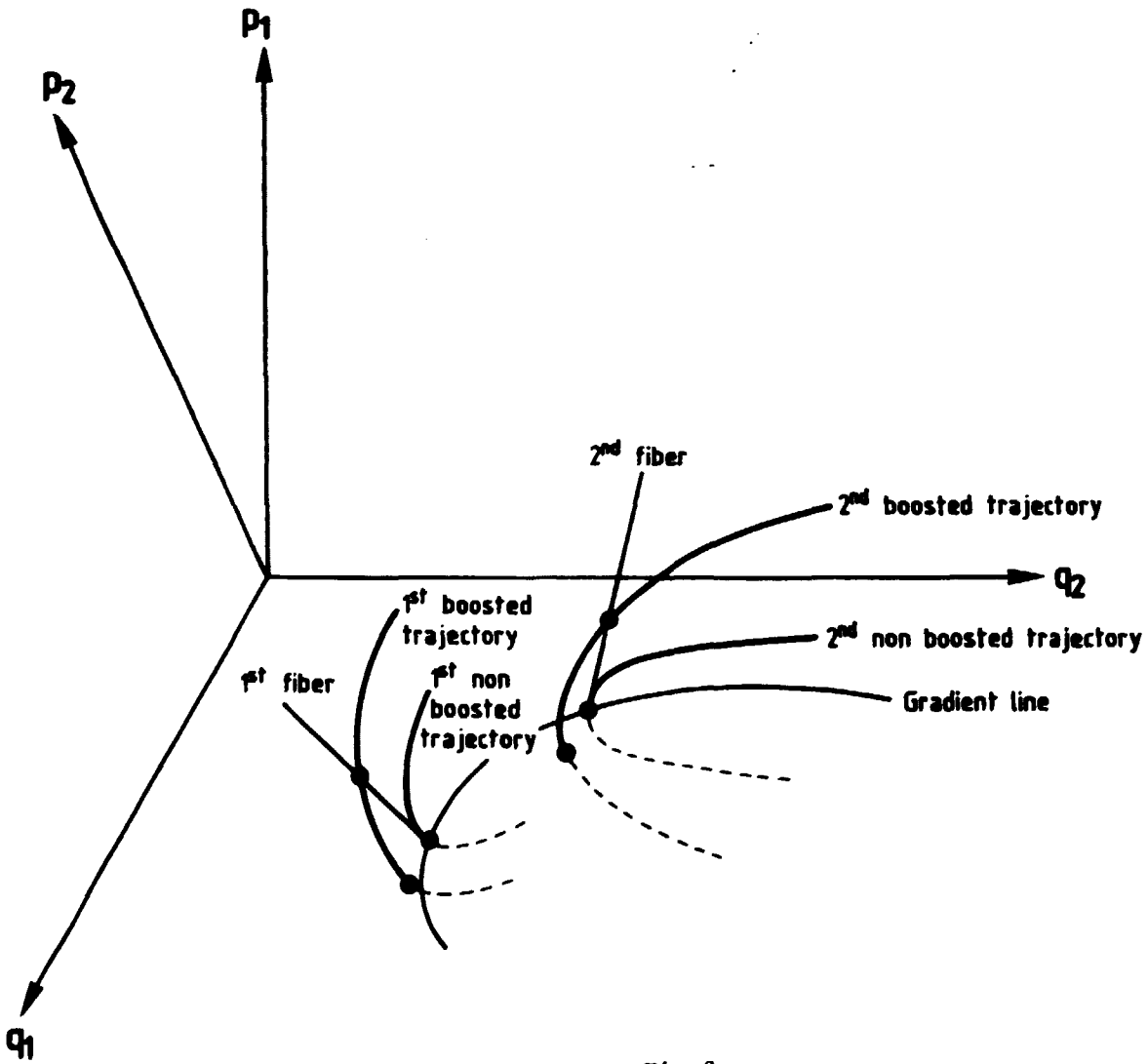

p_1
p_2
q_1
q_2
2nd fiber
2nd boosted trajectory
2nd non boosted trajectory
Gradient line
1st boosted trajectory
1st non boosted trajectory
1st fiber

Fig.3

to $-\overrightarrow{\text{grad}}\, W$. According to Eq.(3.5.5a) this second trajectory projects with the same tangent as the first one, see Eq.(3.5.6). We have found two trajectories which, at least locally, project along the same path.

The process must be reinstated all along the gradient line which is a candidate to be the path. The algorithm can be phrased into the language of fiber bundles, in the following steps

a) select any gradient line in the position hyperplane. The line is the candidate for collective path. It is the base of the fiber bundle which will be defined now ;

b) as the fiber for any point $\vec{q}$ of the gradient line consider the points for which $\vec{p}$ is small and proportional to $\ddot{\vec{q}}$, where $\ddot{\vec{q}}$ is calculated from the equations of motion for that value of $\vec{q}$ and for $\vec{p}=0$;

c) consider all the trajectories in phase space whose initial conditions are taken from the fiber bundle ;

d) these trajectories make a 2-parameter family, hence span a 3-dimensional hypersurface, which is very close to the 2-dimensional bundle ;

e) adiabatic collectivity, namely selection of the best path, is obtained when the deviation of the 3-dimensional hypersurface away from the 2-dimensional bundle is minimal.

This scheme is summarized by Fig.3. It is a very simple and realistic scheme, but it can be critized on several grounds. First, the Lagrangian and/or Hamiltonian may be more complicated than those shown by Eqs.(3.5.4). In particular, velocity dependent forces may distort the boosted trajectories away from the non boosted ones. Nonetheless, in a natural representation where the $\vec{q}$ and $\vec{p}$ are single particle coordinates and momenta, the initial directions of trajectories initiated with $\vec{p}=0$ still make a vector field which deserves investigation even though it may not be a gradient field. It is still tempting to construct a bundle out of a line tangent to that vector field and fibers which are related to a natural boost.

A second criticism is that the fibers must be truncated at some strength of the boost, and also the trajectories must be interrupted after some time. Also the width Δ of the 3-dimensional hypersurface with respect to the 2-dimensional bundle must be estimated by an a priori arbitrary rule. We notice, however, that although the phase space has

no natural metric, the position space and the momentum space may often have natural metrics. Hence, although the width Δ will be parameter dependent (with respect to the truncations listed above), the likely behaviour of Δ with respect to these parameters will be exponential. It is the coefficients of these exponents which are expected to be model independent and which can then be used as criteria for collectivity.

We now return to TDHF and briefly recall the considerations of Ref.[19]. The line of the argument is very close to the scheme a) to e).

We first use the projection theorem by Baranger and Veneroni [15]. Each complex determinant ϕ is *projected* into a position-like, time even (real) determinant ϕ_o along a *fiber* defined by a particle hole operator χ as a generator

$$\phi = e^{i\chi} \phi_o \tag{3.5.7}$$

The technical rules for the unicity of χ and ϕ_o are described in that Ref.[15] and will not be recalled here. The point of interest is that now the set of real determinants ϕ_o play the rôle of a position hyperplane, although it is in fact a *curved* hypersurface.

A trajectory initiated from a real determinant ϕ_o is then found, just from the TDHF algebra, to define [19] a sequence of particle-hole operators W_o, W_1, W_2 ... etc. These operators just occur when the equation of motion is expanded in powers of an adiabaticity parameter ε. In other words, W_o is the Hartree-Fock Hamiltonian of ϕ_o

$$W_o = H(\phi_o) \quad , \tag{3.5.8}$$

one considers the fiber

$$\phi(o) = \exp[i\varepsilon W_o(\phi_o)]\, \phi_o \tag{3.5.9}$$

and the TDHF trajectories initiated from $\phi(o)$. It turns out that the time evolution brings both real and imaginary variations into the determinants $\phi(\varepsilon)$. The fiber, with generator W_o, corresponds to imaginary variations (momentum-like). Position-like variations are found at the next order in ε, and provide the tangent to the candidate for collective path. Except for technical corrections [19], this tangent is defined by the particle hole operator W_1, hence the (approximate) path equation

$$\frac{d|\phi_o\rangle}{dx} = W_1(\phi_o)|\phi_o\rangle \quad , \tag{3.5.10}$$

where the label x just reminds that we are looking for a collective degree of freedom X.

The solution of Eq.(3.5.10) plays the rôle of a gradient line. Alternately, a more direct definition of a gradient line is given by the equation

$$\frac{d|\phi_c>}{dx} = W_o(\phi_o)|\phi_o> \quad . \tag{3.5.11}$$

These two equations (3.5.10) and (3.5.11) are usually not compatible. Their compatibility is a condition for the selection of the best candidate for collective path.

The use of Eq.(3.5.9) for the fibers and of Eq.(3.5.10) or (3.5.11) for the base provides a fiber bundle. The minimization of the deviations of the TDHF trajectories, initiated from that bundle, away from the bundle, is a second condition for the selection of the best collective path. The reader is referred to Ref.[19] for more technical details, or for the generalization to more than one collective degree of freedom.

The physical summary of this long argument is in fact simple. A two-parameter family of TDHF trajectories normally makes a 3-dimensional hypersurface. If there exists situations where the hypersurface is very thin in one coordinate-like dimension, if one of the other two dimensions is coordinate-like and the second momentum-like, these latter two dimensions are in fact analogous to the phase space of just one degree of freedom, now labelled collective. The width is due to the residual coupling of this not-quite-isolated degree of freedom to all the other degrees of freedom to be neglected in a collective model.

4. Order from Chaos : Pattern Discrimination

4.1 Signal screening

There is at least one part of the nervous system which a few specialists have dared to modelize and which is of special interest in a discussion of collective motion. For this part, the cerebellum , has been proved by many medical evidences to play an important role in the control of motricity. There is no need to stress that motricity is based on the coherent action of many a priori independent motor units as individual degrees of freedom. Hence motricity gives typical cases of collective motion.

The point is, many signals are carried to the cerebellum, from most parts of the body, by nerve fibers, the so-called mossy fibers. Some of these signals can be pertinent for the control of a given element of muscular action. Most of these signals may not be pertinent. The extraordinary complexity of the incoming influxes of signals look a priori like a chaos. If the task of a given major element of the cerebellum, the so called Purkinje cell, is to provide a significant output, some screening of the input is mandatory.

This section deals with the theories proposed by Marr [23] and Albus [24] for the functionning of the cerebellum. We will only sketch their arguments, and will bring no personal view, except the hope that some day a better understanding of living systems could help the physicist with a better understanding of what physical collectivity is (and conversely). In what follows we focus only on that aspect of Marr's and Albus' theories which deal with pattern discrimination, and neglect the rest, although it is as important (theory of learning, stabilization of the system, etc.). For a less simplistic approach the interested reader will refer to the original papers [23-24].

The next paragraph will now describe the system which connects mossy fibers to much more numerous relay cells, the so called grain cells. As a matter of fact, to *one* Purkinje cell one estimates that about 7000 mossy fibers send messages via 200.000 relay cells and their corresponding fibers.

Since the 200.000 relay fibers (named the parallel fibers in the physiology literature) can carry obviously more information than the 7000 mossy fibers, it will be shown that pattern discrimination is possible.

4.2 The mossy fiber-parallel fiber system

The system is schematized in an ultra simplified way in Fig.4. The orders of magnitudes are of course taken from Refs.[23-24]. As far as one Purkinje cell is concerned, a mossy fiber connecting to that cell does so via many paths, an average of 130 paths. In other words, a mossy fiber like fiber I of Fig.4 is connected to as many as 130 grain cells whose parallel fibers reach a given Purkinje cell. This is a considerable convergence-divergences ratio. Conversely, a grain cell is usually connected to an average of 4 to 5 mossy fibers, see grain cell n°1 on Fig.4.

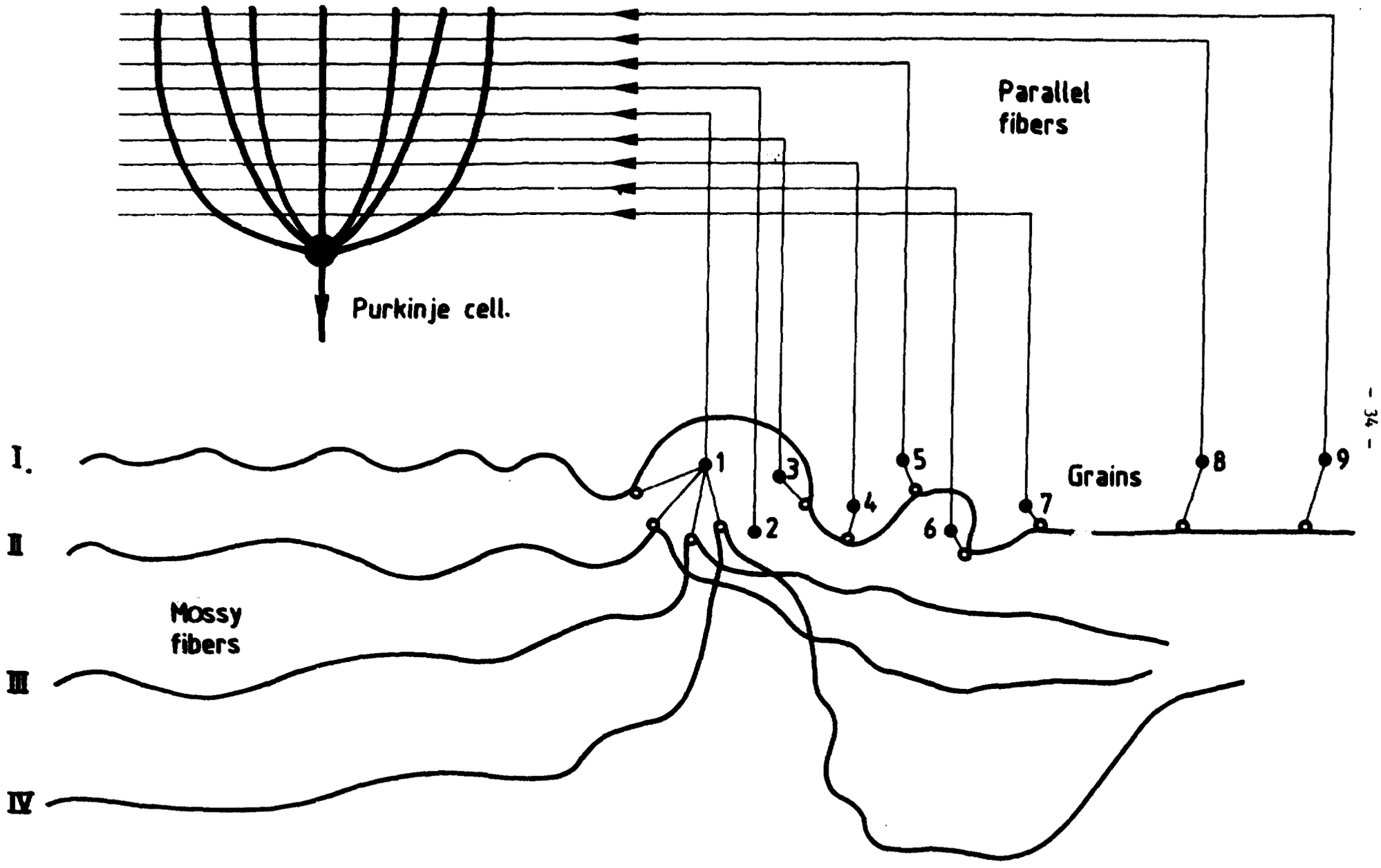

Parallel
fibers
Purkinje cell.
I.
II
III
IV
Mossy
fibers
Grains
1
2
3
4
5
6
7
8
9

Fig. 4

Let us count the number of connections (synapses) between mossy fibers and grain cells. Viewed from the relevant parallel fibers or grains, this number is

$$N \simeq 200.000 \times 4.5 \simeq 900.000 \ . \qquad (4.2.1)$$

Viewed from the point of view of mossy fibers, this number is as well

$$N \simeq 7000 \times 130 \simeq 900.000 \ . \qquad (4.2.2)$$

The average ratio of 130 between parallel fibers and mossy fibers leads to one of the major proposals of the theories of Marr and Albus, namely that the system acts as an expansion recoder. More precisely, patterns of active mossy fibers which are very much alike can be converted into patterns of active parallel fibers which are very different. Hence a significant discriminatory power of the system. A seemingly random activity in the mossy fibers is translated into a contrasted pattern of parallel fibers, some of them collectively active, some of them collectively silent.

The algebraic details of this mechanism will now be sketched in the next paragraph.

4.3 Statistics of the contrast generator

Assume that a sensory message of the body to the cerebellum involves the activity of L mossy fibers among the 7000 under consideration. There is physiological evidence that L may vary between a few tens and 1000 or 2000, but that the maximum of 7000 is not reached (otherwise the system would saturate).

Assume another (pertinent ?) message also involves a pattern of $L' \simeq L$ mossy fibers. This second pattern differs from the first one, but both may have W active fibers in common.

If W is not negligible with respect to L, the ratio W/L has the meaning of a ratio of confusion. Indeed if W/L is larger than 0.5 for instance, a distinction between the two patterns may be difficult.

We now remember that each grain is connected to C = 4 or 5 mossy fibers and will assume, for the sake of simplicity, that a parallel fiber will be active if, and only if, the 4 to 5 mossy fibers to which the corresponding grain is connected are active.

There are a priori

$$N' = \frac{L!}{C!(L-C)!} \qquad (4.2.3)$$

ways of combining the L mossy fibers of the first pattern in order to obtain activity of N' grains (or parallel fibers). There are also the same number N' of ways to convert the second pattern of mossy fibers into a pattern of parallel fibers. Because the two sets of mossy fibers have W fibers in common, the two sets of ways have now a number

$$N'' = \frac{W!}{C!(W-C)!} \qquad (4.2.4)$$

of common ways. The ratio

$$N''/N' = \frac{W!(L-C!)}{(W-C)!L!} = \frac{W(W-1)\ldots(W-C+1)}{L(L-1)\ldots(L-C+1)} \qquad (4.2.5)$$

measures now the probability of confusion between the corresponding patterns of parallel fibers.

In so far as

$$C << W < L \quad , \qquad (4.2.6)$$

the new confusion ratio verifies the condition

$$N''/N' \simeq \left(\frac{W}{L}\right)^C << \frac{W}{L} \quad . \qquad (4.2.7)$$

The contrast between the two patterns of active parallel fibers is then much higher than the contrast between the two initial patterns of active mossy fibers.

If one of these mossy fibers patterns is interpreted, for physiological reasons, as "noise" and the other as "pertinent", the system is thus able to take advantage of the improved contrast at the level of parallel fibers and use it for motricity control.

4.4 Discussion

The $\binom{7000}{C}$ connection schemes which are possible between mossy fibers and grains are not all actually realized. Nor are the $\binom{L}{C}$ schemes realized in general. For there are only 200.000 grains involved, which is large but not as large as the total number of schemes. Thus the 200.000 grains provide only a sampling of these combination ways.

Whether the sampling is just random, or shows some trend to an order parameter like a spin glass model or even exhibits a strong ordered structure is not known. Since anyhow there is strong evidence of motricity control by the cerebellum, it is reasonable to conclude that this biological structure hides a very elaborate processing of data in order to sort out collective behavior from non collective one.

The hunt for collectivity criterion which was the main subject of the previous section, section 3, could only benefit from the perspective offered by section 4. One-body densities which have little contrast could correspond to highly discriminating many-body correlations (this reminds us also of the search for order parameters in spin glasses). This is an open, but very stimulating question.

5. GENERAL CONCLUSION AND ACKNOWLEDGMENTS

The ideas proposed in these lectures are in fact fairly simple and should not be obscured by the mathematical or numerical apparatus which follows them. For the theory of collisions, we have just proposed that there is a representation (the boosted shell model) in which matrix elements of the T-matrix are easier to evaluate, via a variational principle. For the theory of collective motion we have stressed that there is a certain amount of arbitrariness in the way collectivity is defined. In the various geometrical approaches to collectivity (restriction to a Lie group, curvature properties with a given metric, dissymetry between momenta and coordinate in an adiabatic theory, etc), it is the physicist himself who selects, to a large extent, the geometry he likes for reasons of simplicity. And if some day biological models are better understood, they could also provide us with clues for what we call simple collective behaviour of a physical system and what we still classify as chaos.

It is pleasure to thank the organizers of this School for the opportunity of so many stimulating meetings and discussions. Part of this work results from the hospitality of the Laboratoire de Physiologie de la Faculté de Médecine Pitié-Salpétrière, which is gratefully acknowledged.

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