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AN INTRODUCTION TO THE ADIABATIC TIME-DEPENDENT HARTREE-FOCK METHOD

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IPNO/TH 84-38 May 1984

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Contribution to the International Conference on Theoretical Approaches to Heavy Ion Reaction Mechanisms (Paris, May 1984).

AN INTRODUCTION TO THE ADIABATIC TIME-DEPENDENT HARTREE-FOCK METHOD

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The aim of the adiabatic time-dependent Hartree-Fock method is to investigate the microscopic foundations of the phenomenological collective models. We briefly review the general formulation, which consists in deriving a Bohr-like Hamiltonian from a mean field theory, and discuss the limiting case where only a few collective variables participate to the motion. Some applications to soft nuclei and heavy ion collisions are presented.

Among the quantum mechanical systems possessing many degrees of freedom, the atomic nucleus is one of those capable of the most extravagant variety of behaviours. During a long period in the development of Nuclear Theory, this "multivaluate" identity of the nucleus, reflecting a high degree of complexity, gave rise to the simultaneous elaboration of several models inspired from different and even contradictory pictures of the system : ensemble of non-interacting particles evolving in a one-body potential or, at the opposite, liquid drop whose strongly coupled constituents are capable of coherent motion. The successes of these descriptions raised the question of conciliating the conflicting aspects of nuclear motion, i.e. of understanding the interplay between collective and individual degrees of freedom.

Numerous "tentative marriages" of the independent particle description with the collective phenomenological model have in common the same "philosophy" : take for granted the validity of the macroscopic interpretation of the studied collective mode, and estimate the parameters entering in the Bohr Hamiltonian by means of some mean field approximation. Such a procedure basically suffers from an intrinsic inconsistency : the Bohr Hamiltonian is there introduced as a "magic recipe" ! However, its ability to describe a large class of phenomena suggests that in some circumstances, a large number of nucleons are really capable of moving so coherently as to "produce themselves" a Bohr Hamiltonian, and a fascinating theoretical problem is to understand how such a mechanism can be built from the short range mutual interactions between nucleons. A tempting way to explore this question would be to *derive a collective Bohr Hamiltonian*

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from a microscopic theory, i.e. starting from the internucleon interactions. One step in this direction has been achieved a long time ago, at least formally. Indeed, the Random Phase Approximation (RPA) can merely be viewed as a search for the normal modes of the nucleus, using microscopic ingredients ; and the success of the now fully self-consistent RPA calculations in the study of giant resonances has reinforced the macroscopic image of the nucleus as a classical object capable of shape vibrations. However, the RPA is typically a small amplitude approximation, and cannot describe collective processes during which the nuclear wave function undergoes important alterations, such as fission, fusion, heavy ion reactions, low energy vibrations (and even ground state dynamical features) of soft nuclei.

A natural, and still almost unavoidable microscopic framework to study dynamics of large amplitude collective motion is the time-dependent Hartree-Fock method (TDHF). However, it is hopeless to derive a collective Hamiltonian from TDHF without any further assumption (see below). An adequate hypothesis for this purpose is to introduce *two time-scales* in the nucleus, one characterizing the rapid single particle excitations, the other one being associated with the slower collective modes. This *adiabatic approximation* to TDHF was initiated independently by Villars[1] and by Baranger and Véneroni[2]. The two formalisms share some points of view, but follow rather different paths, and I shall remain here in the spirit of Ref. 2.

1. THE ADIABATIC TIME-DEPENDENT HARTREE-FOCK FORMALISM (ATDHF)

First, let us explain in a few words the key point of the ATDHF procedure, that is how and in which sense one can hope to get a collective Hamiltonian from a time-dependent mean field approximation. Consider the TDHF energy

$$E = \langle \Phi(t) | H | \Phi(t) \rangle, \tag{1}$$

where H is the Hamiltonian of the nucleus (sum of a kinetic term and of a two-body interaction), and where $\Phi(t)$ is a Slater determinant, solution of the TDHF equation of motion at any time t ; we recall that this total energy E is a *constant of motion.* The idea is then to extract from Φ a set of variables $\{q_i(t), p_i(t)\}$ such that the TDHF energy takes the form

$$E = \frac{1}{2} \sum_i p_i \dot{q}_i + \mathcal{V}(\{q_i\}) \tag{2-a}$$

$$= \frac{1}{2} \sum_{ij} m_{ij}(\{q_k\}) \dot{q}_i \dot{q}_j + \mathcal{V}(\{q_i\}) \equiv \mathcal{H}_{c\ell}. \tag{2-b}$$

In Eqs. (2), $\mathcal{V}(\{q_i\})$ depends only on the q_i's, and the p_i's are *linear* functions of the q_k's, as seen by passing from (2.a) to (2.b). The expression (2.b) of E evoques a classical Hamiltonian $\mathcal{H}_{cl}$, with $\{q_i\}$ as coordinates, $m = [m_{ij}]$ as mass tensor, and $\mathcal{V}$ as potential energy. For such an identification of E with $\mathcal{H}_{cl}$ to be "seriously" supported, one has to require the *classical* equations of motion for the coordinates and momenta (q_i, p_i) to be consistent with the *quantal* TDHF equation. One can convince oneself that such a program is not feasible without introducing a supplementary approximation ; the reason for this is that it is impossible to find a set $\{q_i, p_i\}$ such that the momenta p_i behave linearly in the velocity $\dot{q}_i$, which is an absolute requirement to define mass parameters. As we shall see now, this obstacle is overcome in the adiabatic limit.

1.1. The general ATDHF method

Let us consider the one-body reduced density matrix $\rho(t)$, solution of the TDHF equation :

$$\rho(t) = \sum_{h=1}^{A} |h(t)\rangle\langle h(t)| \ , \tag{3}$$

which is the projector onto the A-dimensional subspace of single particle states $|h(t)\rangle$ being occupied in the A-particle determinant $|\phi(t)\rangle$ (these states are supposed to satisfy $\langle h|h'\rangle = \delta_{hh'}$) :

$\rho|h\rangle = |h\rangle$ if $|h\rangle$ is occupied in $|\phi\rangle$ (hole state)

$\rho|p\rangle = 0$ if $|p\rangle$ is unoccupied in $|\phi\rangle$ (particle state).

Baranger and Vénéroni introduced the following decomposition of ρ :

$$\rho(t) = e^{i\chi(t)}\rho_0(t)e^{-i\chi(t)} \ , \tag{4-a}$$

where ρ_0 and χ are hermitian and time-reversal invariant operators :

$$\rho = \rho_0^{+} = \rho_0^{T} = \rho_0^{2} \ , \tag{4-b}$$

$$\chi = \chi^{+} = \chi^{T} . \tag{4-c}$$

Given any projector ρ, the existence of such a decomposition can be shown under rather unrestrictive hypothesis[3] : in the present context, the main limitation is that this applies only for even-even nuclei (the decomposition theorem leading to Eqs. (4) is essentially a refined version, of Thouless theorem for determinants). To make the set of operators (ρ_0, χ) unique, one can add the supplementary condition that the operator χ has no particle-particle and hole-hole matrix elements in any basis of eigenvectors of ρ_0 (i.e. is "antidiagonal" with respect to ρ_0) :

$$\rho_o = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & 0 \end{array}\right] \qquad \chi = \left[\begin{array}{c|c} 0 & K \\ \hline K^+ & 0 \end{array}\right] . \tag{4-d}$$

We now formulate the adiabatic assumption by assuming the operator χ to be "small", i.e. to have its eigenvalues small compared to unity. Why this is a slow motion hypothesis is by no means trivial at this stage, and let us for the moment take this requirement as a trick, leaving for later on the understanding of its physical content, and also of the opportunity of introducing the decomposition (4).

The next steps are to get the TDHF equations of motion in the limit of a small χ, and to investigate their classical underlying structure. In doing this, we shall follow the scheme proposed in Ref. 4, which differs from 2 essentially by adopting the Hamiltonian, rather than the Lagrangian point of view, and whose advantage is to make manifest the classical structure from the very beginning, i.e. at the variational source of the TDHF equation. Indeed, consider the integral

$$I = \int_{t_1}^{t_2} \langle \Psi \mid i\hbar \frac{\partial}{\partial t} - H \mid \Psi \rangle \, dt = \int_{t_1}^{t_2} \mathcal{L} \, dt \tag{5}$$

and the stationarity condition

$$\delta I = 0 \tag{6-a}$$

where the functions Ψ and Ψ^* are to be varied independently, with the end point conditions

$$\delta\Psi(t_1) = \delta\Psi(t_2) = 0 . \tag{6-b}$$

When no restriction is made on the variational space, the conditions (6) lead to the Schrödinger equation. Now, if one constrains the trial function Ψ to remain a Slater determinant during the variation (i.e. the associated one-body density operator ρ to remain a projector), one gets from (6) the TDHF equation. Let us now see what happens when making the adiabatic hypothesis into (5-6). To do this, we introduce the expression (4) for the density operator associated with Ψ, and keep, in the expansion of the integrant $\mathcal{L}$ in powers of the small operator χ, all terms up to the second order in χ. After some manipulations, one gets for the adiabatic limit of (6-a)

$$\delta I_a = \int_{t_1}^{t_2} \{ \operatorname{tr} \hbar \chi \dot{\rho}_o - E_a(\rho_o, \chi) \} \, dt = \delta \int_{t_1}^{t_2} \mathcal{L}_a \, dt = 0 , \tag{7}$$

where "tr" stands for the trace, and where $E_a(\rho_o, \chi)$ results from the expansion of the TDHF energy

$$E[\rho] = \operatorname{tr} t\rho + \frac{1}{2} \operatorname{tr}_1 \operatorname{tr}_2 \rho(1) \tilde{V}(1,2) \rho(2) \tag{8}$$

up to second order in χ. In Eq. (8), t is the kinetic energy operator, $\tilde{V}(1,2)$ is the antisymmetrized two-body interaction, and $tr_1 tr_2$ stands for the double trace over the single particle spaces of particles (1) and (2). To get E_a from E_1 we replace ρ in (8) by its expression (4), and drop terms of orders greater than two. Due to the time-reversal invariance of ρ_o and χ, terms of first order in χ vanish identically, and one obtains for E_a

$$E_a = E_0[\rho_0] + E_2[\rho_0, \chi] , \qquad (9)$$

where

$$E_0 = E[\rho_0] = tr\, t\rho_0 + \frac{1}{2} tr_1 tr_2\, \rho_0(1)\, \tilde{V}(1,2)\, \rho_0(2) \qquad (10)$$

is the value of the Hartree-Fock energy for the independent particle state $|\phi_0>$ associated with the one-body density operator ρ_0, and where the term $E_2[\rho_0, \chi]$ is *quadratic in* χ. Now, the classical analogy becomes apparent : the integrant $\mathcal{L}_a$ in (7)

$$\mathcal{L}_a = tr\, \hbar\chi\, \dot{\rho}_0 - E[\rho_0] - E_2[\rho_0, \chi] \qquad (11\text{-a})$$

has exactly the same structure as a classical Lagrangian

$$\mathcal{L}_{cl} = \sum_i p_i \dot{q}_i - V(q_i) - T(q_i, p_i) = \sum_i p_i \dot{q}_i - H_{cl}(q_i, p_i), \qquad (11\text{-b})$$

the matrix elements of ρ_0 *and of* $\hbar\chi$ in a time-independent basis playing the roles of the *coordinates and of their conjugate momenta respectively*. The variational principle can be viewed as a classical action principle, and we expect to get Hamilton-like equations by varying independently ρ_0 and χ in (7), just in the same way as the classical Hamilton equations emerge from independent *variations** of p_i and q_i in the action principle $\delta \int_{t_2}^{t_1} \mathcal{L}_{cl}\, dt = 0$. In a symbolic notation, these equations are

$$\dot{\rho}_0 = \frac{\delta E_a}{\delta(\hbar\chi)} \qquad (12\text{-a}) \quad , \qquad \hbar\dot{\chi} = -\frac{\delta E_a}{\delta \rho_0} \qquad (12\text{-b})$$

analogous to

$$\dot{q}_i = \frac{\partial H_{cl}}{\partial p_i} \quad , \qquad \dot{p}_i = -\frac{\partial H_{cl}}{\partial q_i} .$$

As in the classical case, the first set (12-a) provides linear relations between the "velocities" (i.e. the matrix elements of $\dot{\rho}_0$) and the "conjugate momenta"

* For the sake of simplicity, we just draw a sketch of the variational procedure, and of the classical analogy. The situation is, in fact, complicated by the relations (4-b) and (4-d) which need to be put as constraints during the variation. It has been proved that the existence of such constraints depending both on the "coordinates" and on the "momenta" does not destroy the classical Hamiltonian character of the problem, and in particular is not an obstacle for the ultimate requantization of the system [6,7].

(i.e. the matrix elements of χ), the matrix of this linear system playing the role of the mass tensor. Using this set of linear relations, one can show that the "kinetic term" $\frac{1}{2}\mathrm{tr}\,\hbar\chi\dot{\rho}_o$ is actually quadratic in the velocities, and equal to $E_2[\rho_o,\chi]$, which demonstrates the complete consistency of the classical analogy. We will not write the explicit expressions for all the quantities introduced in this section, and we refer the reader to Refs. 2,4-6 for technical details. We shall rather try to summarize some important features of the formalism

Comments

i) In the classical analogy, the matrix elements of the operator χ are identified with the conjugate momenta, the coordinates being the matrix elements of ρ_o. When written in explicit form, the first set (12-a) of equations of motion obtained in the limit of small χ shows that the matrix elements of $\dot{\rho}_o$ are linear in χ, i.e. that the velocities are small, whereas from the second set (12-b) one can see that the density operator ρ_o almost satisfies a static Hartree-Fock equation. The physical meaning of these two properties is that the motion is slow (adiabatic) and that the restoring force acting on the system remains weak during the motion. As a consequence of the adiabatic hypothesis, the collective "kinetic" energy is found to be small compared to a typical single particle energy times the number of degrees of freedom contributing to the collective motion, and this property illustrates how the hypothesis of smallness of χ leads to distinguish between two time-scales.

ii) The Hamilton equations (12) are a set of coupled equations which provide —as in the classical Hamiltonian case— both the "*path*" $\rho_o(t)$ and the associated *mass parameters*. In the particular cases of pure translations or rotations of the nucleus, Eqs. (12) lead to the Thouless-Valatin mass and moment of inertia, and the cranking result for the mass parameters appears as a non self-consistent approximation to the ATDHF value.

iii) Of course, the ATDHF equations in their Hamiltonian form (12) are equivalent to the TDHF equation in the limit of small χ. Since the RPA can be derived from TDHF by imposing small amplitudes, it is also a by-product of ATDHF.

iv) The condition (4-d) ensuring the uniqueness of the decomposition (4-a, b,c) may appear as an artificial device. In fact, the "superiority" of this particular choice of the "gauge" is that the operator χ having no particle-particle and hole-hole matrix elements contains the right number of degrees of freedom of the system (i.e. the initial number,

reduced by the number of independent constraints contained in the condition for $|\phi_o>$ to remain a determinant), and this property makes the classical analogy more illuminating. However, the Hamiltonian structure of the equations can also be proved for any other choice of the decomposition (4-a,b,c). Moreover, the equations of motion are shown to be "gauge invariant", which ensures that the physical properties are unaffected by relaxing the condition (4-d).

v) *Finally, let us mention that the formalism sketched in this Section in the* framework of the TDHF approximation can be extended without any difficulty to include pairing correlations, i.e. in the framework of the Hartree-Fock-Bogolyubov approximation.

1.2. Reduction of the number of degrees of freedom

In the preceding approach, all degrees of freedom are taken into account, and the equations of motion contain implicitly the "key" of the collective path and parameters .In a first stage, one would like to treat the simplest problem of one (or a few(*)) collective variable. In doing so, we shall make a drastic approximation, which consists in guessing a choice for the collective variable q and its dynamical path $\rho_o(q)$ .To get the equations of motion, we come back to the stationarity principle (7), where $\dot{\rho}_o$ has to be replaced by $\dot{q}\frac{\partial\rho_o}{\partial q}$, and perform independent variations with respect to i) the *scalar* q (which is now the only degree of freedom of ρ_o) and ii) the *operator* χ . From the variation ii), we recover the first Hamilton-like equation (12-a), which defines the operator χ in terms of $\frac{\partial\rho_o}{\partial q}$, whereas the variation i) leads to a scalar equation which is useless for the purpose of deriving the parameters of the Bohr Hamiltonian. The kinetic energy takes the form

$$\mathcal{K} = \frac{1}{2}\,\mathrm{tr}\,\hbar\chi\dot{\rho}_o = \frac{1}{2}\dot{q}\,\mathrm{tr}\,\hbar\chi\frac{\partial\rho_o}{\partial q}\,, \qquad (13)$$

where $\mathrm{tr}\,\hbar\chi\frac{\partial\rho_o}{\partial q}$ appears as the conjugate momentum p of the collective coordinate q. The mass parameter is therefore given by

$$M(q) = \frac{p}{\dot{q}} = \mathrm{tr}\,\frac{\hbar\chi}{\dot{q}}\,\frac{\partial\rho_o}{\partial q}\,. \qquad (14)$$

Thus, the calculation of the mass parameter requires i) to evaluate the operator $\frac{\partial\rho_o}{\partial q}$ from the knowledge of $\rho_o(q)$, and ii) to compute χ by solving Eq.(12-a). From Eqs. (10-11), the potential term of the Bohr Hamiltonian is simply the expectation value of the "microscopic" Hamiltonian H in the Slater determinant $\Phi_o(q)$ associated with the density $\rho_o(q)$:

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* In the following, we present the case of one degree of freedom ; the generalization to several variables is straightforward.

$$V(q) = \langle \Phi_o(q) \mid H \mid \Phi_o(q) \rangle \ . \qquad (15)$$

Let us now investigate two particular choices of the trajectory $\rho_o(q)$.

a) "Scaling" path

When studying electric isoscalar multipole modes of the nucleus, the most simple choice of the path is suggested by the macroscopic image of the nucleus whose density oscillates according to a scaling law. For instance the scaling path for isoscalar quadrupole oscillations is defined as

$$\rho_o(\alpha;x,y,z) = \rho_{SHF}(\alpha x, \alpha y, \frac{z}{\alpha^2}) \ , \qquad (16)$$

where $\rho_o(\alpha;x,y,z)$ is the density (diagonal element of the operator ρ_o in $\underset{\sim}{r}$-representation) as function of the scaling parameter α, and where $\rho_{SHF}(x,y,z)$ is the static Hartree-Fock equilibrium density. Instead of α, let us take as collective variable the quadrupole moment of the nucleus in the independent particle state Φ_o corresponding to ρ_o :

$$q = \langle \Phi_o | \hat{Q}_{20} | \Phi_o \rangle = \mathrm{tr}\, \hat{Q}_{20}\, \rho_o = \int (3z^2 - r^2)\, \rho_o(\alpha; x,y,z)\, d\underset{\sim}{r} \qquad (17)$$

The mass parameter is then given by [7]

$$M_{SC}(q) = m / [\, 4(2A\langle r^2 \rangle + q)] \ . \qquad (18)$$

In Eq. (18), m is the nucleon mass, A is the nucleon number, and $\langle r^2 \rangle$ is the mean square radius of the nucleus in the state Φ_o.

b) "Constrained Hartree-Fock" path (CHF)

Another possible choice of the trajectory $\rho_o(q)$, which is expected to contain more "microscopic information" on the system, consists in defining the operator ρ_o as the solution of the constrained Hartree-Fock problem

$$\delta \langle H - \lambda \hat{Q} \rangle = 0 \ , \qquad (19)$$

the collective variable being

$$q = \mathrm{tr}\, \hat{Q}\, \rho_o \ . \qquad (20)$$

In this case, one can show that solving the Hamilton equation (12-a) is equivalent to solve the doubly-constrained Hartree-Fock equation :

$$\delta \langle H - \lambda \hat{Q} - \dot{q}\, \hat{P} \rangle = 0 \ , \qquad (21)$$

where the (time-odd) operator $\hat{P}$, generating the dynamics of the system, is given by

$$\hat{P} = i\hbar \left[\frac{\partial \rho_o}{\partial q} \ , \rho_o \right] \qquad (22)$$

and where $\dot{q}$ is a small parameter (linear response). The (CHF) mass parameter $M_{CHF}(q)$ associated with the collective variable q is then the *polarizability* of

of the nucleus with respect to the constraining field $\hat{Q}$. The cranking value

$$M_{ICR}(q) = 2\hbar^2 \sum_{ph} \frac{|\langle h(q)|\partial/\partial q|p(q)\rangle|^2}{\varepsilon_p - \varepsilon_h} \qquad (23)$$

of the mass parameter is obtained at the first numerical iteration of Eq. (21), i.e. it does not include the effects of the rearrangement of the density under the influence of the time-odd part of the Hartree-Fock field.

2. APPLICATIONS

2.1 The isoscalar quadrupole mode

The first applications of the method presented in 1.2 concerned the isoscalar quadrupole mode[7]. Here we shall focus our attention on the two following points : i) comparison of the mass parameters $M_{SC}(q)$ and $M_{CHF}(q)$ obtained for the two paths considered in 1.2, and ii) study of the discrepancy between the non-self-consistent mass $M_{ICR}(q)$ and the ATDHF mass $M_{CHF}(q)$. All the calculations reported here were done with Skyrme interactions.

As shown in Fig.1, the scaling and CHF paths are practically equal for the nucleus ^{40}Ca. This property can be simply understood in terms of sum rules[8] ; essentially it is due to the fact that the quadrupole strength is totally concentrated in 2-$\hbar\omega$ particle-hole excitations for spin-saturated nuclei. There-

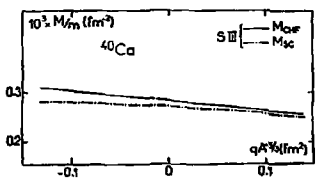

FIGURE 1
Adiabatic mass parameters of ^{40}Ca as functions of the collective variable $q = \langle \hat{Q}_{20} \rangle$. M_{CHF} is obtained from the CHF path with $\hat{Q}_{20}$ as constraining operator ; M_{SC} is obtained from the scaling path (see Eq. (18)). [taken from Ref. 8]

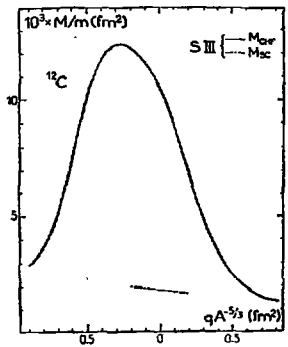

FIGURE 2
Same as Fig. 1, for ^{12}C [taken from Ref. 7]

fore, the CHF path carries information only on the high energy part of the spectrum, as is also expected for the hydrodynamical scaling path. In this case, the quantization of the Bohr Hamiltonian would lead, for both paths, to the hydrodynamical estimation of the mean energy of the giant resonance, which is known as a good approximation to the RPA value. For non-spin-saturated nuclei, on the contrary, one expects the CHF mass to be dominated by 0-$\hbar\omega$ single particle excitations. The case of ^{12}C is particularly illustrative (see Fig. 2) : the CHF mass parameter has a strong structure with respect to the deformation, which is a signature of anharmonic motion. It is peaked on a negative value of q, its maximum value being $\sim$6 times larger than M_{SC}. The occurence of the bump for M_{CHF} can be attributed to the rapid variation with q of the particle-hole $1p^{3/2}-1p^{1/2}$ energy (see the cranking formula (23)). Whereas the equilibrium static Hartree-Fock wave function is found spherical (for the same interaction SIII), one expects a concentration of the intrinsic wave function (obtained from a quantization of the Bohr Hamiltonian) around the value of q corresponding to the maximum of the mass M_{CHF} ; this generates in the ground state an oblate deformation of *purely dynamical origin*, in qualitative agreement with experiment.

As already mentioned, the difference between the self-consistent and the

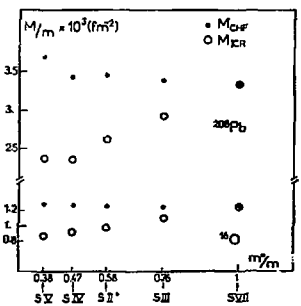

FIGURE 3

Quadrupole mass parameters of ^{208}Pb and ^{16}O (at spherical equilibrium) as functions of the Skyrme interactions characterized by their effective mass. The dots represent self-consistent masses M_{CHF}, and the open circles correspond to cranking masses M_{ICR}. [taken from Ref. 8]

cranking mass parameters $-M_{CHF}$ and $M_{ICR}-$ for the CHF path is generated by the time-odd Hartree-Fock field. In the case of Skyrme interactions, one can show[8] that the parameter governing the intensity of this field is the effective mass m^*/m of the force (the time-odd field is proportional to (m/m^*-1)). In Fig. 3 are displayed the mass parameters M_{CHF} and M_{ICR} for ^{208}Pb and ^{16}O. The discrepancy between the two masses is a decreasing function of m^*/m, and vanishes for $m^*/m = 1$, as expected from the known m^*- dependence of the time-odd field. Among the Skyrme forces considered here, SIII is probably the best adapted to the study of the quadrupole mode (see Ref. 9, where an estimation of the value of m^* is deduced from the energy of the quadrupole giant resonance), which allows to consider, at least for the quadrupole mode, the cranking as a rather good approximation.

2.2 Heavy ion collision.

The next example we consider, taken from Ref. 10, is a calculation of the fusion cross section for the collision $^{40}Ca - ^{40}Ca$. The collective variable is the quadrupole moment of the system, and the parameters entering in the Bohr Hamiltonian are obtained for the CHF path (with $\hat{Q}_{20}$ as constraining operator). Notice that for the Bonche-Koonin-Negele interaction, used here, the cranking mass M_{ICR} is exactly equal to the self-consistent mass M_{CHF}. The interaction potential is shown on the lower part of Fig. 4 as a function of the variable $R = (2q/A)^{1/2}$, which is the interdistance between the nuclei when the two fragments are well-separated. The kink at the top of the barrier corresponds to formation of the neck between the two nuclei (see Fig. 5). The mass parameter (upper part of Fig. 4) is equal to the reduced mass of the system for large interdistances. In the region where the ions are touching, it displays a large peak, whose origin is the following : when nuclei begin to overlap too much, the Pauli principle induces rapid modifications of the single-particle wave functions, i.e. of the operator $\hat{P}$ (Eq. (22)), and consequently of the mass parameter, which is the polarizability with respect to $\hat{P}$. In terms of the cranking formula (23), this structure of the mass is therefore due to fast variations of the *numerator*, whereas a similar effect (Fig.2) was found to originate from fast variations of the *denominator* for the quadrupole mode of ^{12}C. The effect of this structure of $M_{CHF}(R)$ is very important. As can be seen from Fig. 6, where classical trajectories obtained with the ATDHF mass M_{CHF} and with the (constant) reduced mass are compared, the peak in $M_{CHF}(R)$ constrains the fragments to remain in contact for a longer time, and leads to a deflection angle which is larger by 60° compared to the case of a constant mass. After quantization of the collective Bohr Hamiltonian, the fusion cross section can be calculated using a barrier penetration method. The agreement with experimental data is found noticeably better for the adiabatic mass than for the

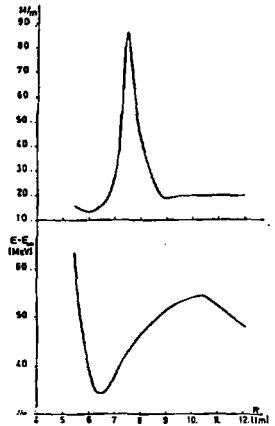

FIGURE 4
CHF mass parameter (upper part) and interaction potential (lower part) for the collision of two calcium-40 nuclei (the constraining operator is the quadrupole moment Q_{20}) [taken from *Ref.10*]

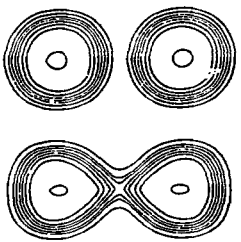

FIGURE 5
Contour lines of the density integrated over the coordinate normal to the scattering plane at R = 10.42 fm (top) and R = 10.38 fm (bottom) [taken from Ref.10]

reduced mass (See Fig. 7).

Similar structures in the mass parameters obtained from the CHF path have been found for other heavy ion collisions[12], and are in disagreement with results of other calculations[13] using a prescription to determine the path. It would be interesting to know whether such a discrepancy also occurs for the $^{40}Ca - ^{40}Ca$ collision, and to compare the fusion cross sections obtained by the two methods in the energy range corresponding to the data of Fig. 7.

2.3 Vibrational and rotational spectra.

Let us finally report some recent calculations[14] of spectra of soft nuclei. The path is obtained by solving a doubly constrained Hartree-Fock Bogolyubov equation for the β-γ degrees of freedom. Mass parameters are evaluated in the cranking approximation, and the spectra are computed by quantizing the Bohr Hamiltonian with zero point energy corrections for the five quadrupole degrees

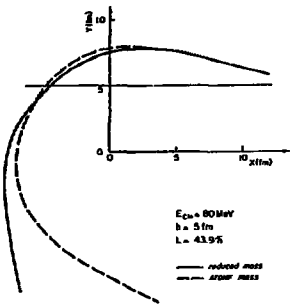

FIGURE 6
Classical trajectories calculated for the collision of two calcium-40 nuclei. The impact parameter is b=5fm and the c.m. energy is E = 80 MeV. The solid curve is calculated with a constant mass equal to the reduced mass while the dashed curve is obtained with the adiabatic mass M_{CHF} [taken from Ref.10]

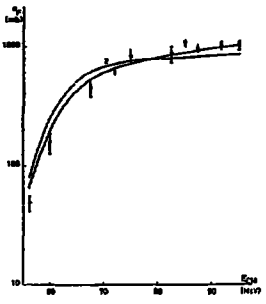

FIGURE 7
Fusion cross sections for two calcium 40 nuclei, calculated with the reduced mass (2) and with the ATDHF mass (1) are compared with the experimental data of Ref. 11 . [taken from Ref. 10]

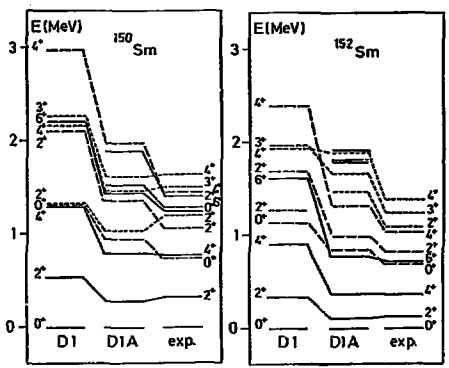

FIGURE 8
Ground state, β and γ bands of ^{150}Sm and ^{152}Sm. Theoretical spectra are obtained with D1 and D1A Gogny interactions [taken from Ref. 14]

of freedom as described in Ref. 15. Calculations are performed with Gogny D1 and D1A interactions (The D1A effective force[16] is a modified version of D1, fitted to better reproduce even-even and even-odd binding energy differences). On Fig. 8, are displayed the ground state, β and γ bands for the nuclei ^{150}Sm and ^{152}Sm. Comparison of the spectra obtained with D1 and D1A interactions shows the strong effects of the pairing properties. The differences between the two interactions have negligible influence on the collective potential, and the modification of the spectra can be completely attributed to the sensitivity of the mass parameters to the smoothing pairing effects at single particle level crossings. The D1A results support the comparison with experimental data at an unexpected level of quality, in view of the degree of complexity of the properties under study and of the parameter-free character of the theoretical method. Another remarkable agreement with experiment is obtained for the first 0^+ and 2^+ excited states of the nucleus ^{68}Ni (Fig. 9). The position of the first 0^+ excited state is found to be largely influenced by the slope of the potential energy in the vicinity of the shape isomer, as can be seen in Fig. 10.

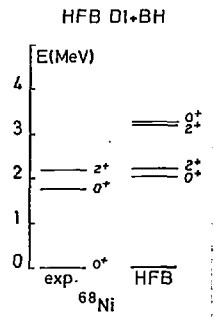

FIGURE 9
Experimental and theoretical (HFB) first excited states of the nucleus ^{68}Ni. The theoretical results are obtained with the D1A interaction [Experimental levels are taken from Ref. 17. Theoretical results are taken from Ref. 14]

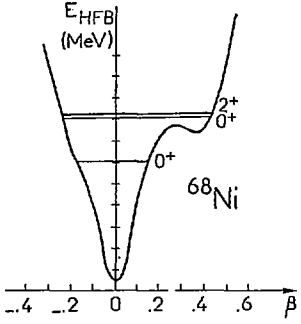

FIGURE 10
Collective potential as a function of the shape parameter β for ^{68}Ni. [Taken from Ref. 14]

Concluding remarks

All the calculations presented in Sect. 2 illustrate the essential improvements gained by calculating in a consistent way both the collective potential and the inertial parameters of the Bohr Hamiltonian. The method used has no

adjustable parameters, and in this respect the results are quite promising. However, the reduction of the general ATDHF method to a few collective variables requires the drastic simplifications of guessing a collective path and assuming its decoupling with intrinsic excitations. As discussed in Ref. 18, getting rid of this disadvantage is not a simple problem, and certainly implies involved numerical calculations. Also related to the reduction of the number of degrees of freedom is the problem of dissipation, which is not discussed in the formalism reported here ; and though the semi-phenomenological attempts in this direction are clearly in progress, the question of deriving a transport equation with collision terms in a completly self-consistent way remains so far unsolved.

ACKNOWLEDGEMENTS

I am indebted to D.M. Brink, H. Flocard, P.H. Heenen, P. Quentin, and D. Vautherin for numerous discussions, and to D. Gogny and M. Girod for permission to present results prior to publication. I am most grateful to M. Véneroni, who initiated and followed with constant interest part of the works reported in this talk.

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