STRONG VARIATIONS OF ADIABATIC MASS PARAMETERS

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It is well established [1] that the main features of the collective nuclear dynamics at low excitation energy are globally described within the so-called Bohr Hamiltonian approach [2] involving five components of the quadrupole deformation tensor. A considerable effort has been devoted to obtain, in a microscopic fashion, seven functions of two intrinsic deformations (e.g., the β and γ parameters) entering the Bohr Hamiltonian. One way to tackle the problem has taken the time-dependent Hartree – Fock – Bogolyubov (TDHFB) approximation in the adiabatic limit (ATDHFB) as a starting point. It was initiated in the pairing plus quadrupole approach of Kumar and Baranger [3] and cast later in a broader perspective by Baranger and Veneroni [4]. The other class of approaches has made use of the generator coordinate method (GCM) with further approximations of the Gaussian overlap approximation (GOA) type [5 – 8]. In all practical realistic applications so far, using full-fledged effective interactions of the Skyrme or Gogny type, one has limited oneself either to zero-pairing cases in the so-called adiabatic time-dependent Hartree – Fock (ATDHF) limit (see, e.g., [9]) or to perturbative mass parameter calculations of the Inglis – Belyaev type [10, 11], i.e., neglecting the so-called Thouless – Valatin self-consistent terms [12] generating the time-odd part of Hartree – Fock – Bogolyubov potentials through the time-odd part of the density matrices. The results discussed here belongs to the last category. Starting from the more general point of view of the full ATDHFB method, we present recent advances made in the understanding of current versions of the Inglis – Belayev mass problem. We focus mainly on many cases where such mass parameters exhibit strong variations over an interval of the considered collective variable which is small with respect to a characteristic range of variation of the associated potential energy curve. In that context, we discuss two origins for such a behavior as well as their physical consequences. This will be illustrated in the generic case of axial quadrupole motion.

The starting point is the matrix expression of the TDHFB equation of motion in a doubled space [13, 14]:

$$i\hbar \frac{\partial R}{\partial t} = [H, R], \qquad (1)$$

with the generalized Hamiltonian matrix H and density R denned from the Hartree – Fock h and pairing fiedls Δ, on the one hand, and from the normal ρ and abnormal density matrices k, on the other hand, with usual notation as:

$$R = \begin{pmatrix} \rho & k \\ -k^* & 1-\rho^* \end{pmatrix}, \quad H = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \qquad (2)$$

For a Bogolyubov quasi-particle vacuum, it is known [15] that R is Hermitian idempotent (i.e., projector) operator. This allows one, as noted in [4] and explicated in [16], to make use of the so-called Baranger – Veneroni theorem [4]:

$$R(t) = \exp(i\chi(t)) R_0(t) \exp(-i\chi(t)), \qquad (3)$$

where both R_0 and χ are Hermitian and time-even, allowing thus an expansion of R in terms of χ as performed in the Hartree – Fock case within the normal (i.e., non-doubled) space.

We perform now the same set of further approximations which were made in the nonpairing-correlated case (see, e.g., [17]), namely:

1. adiabatic expansion of R around R_0 up to the second order in χ,
2. dynamical reduction of the time-dependence of the TDHFB solution through only one (here) or a few collective variables,
3. *a priori* choice of this collective variable to keep contact with the original Bohr Hamiltonian approach, for example, the expectation value q of the axial quadrupole moment operator Q_{20}.

Upon making the adiabatic expansion mentioned above (approximation 1), one can split the TDHFB equation of motion, Eq.(1), into a time-even part and a time-odd part. Again as in the ATDHF case, we further assume that the R_0-part of the solution of the

time-even equation of motion is given by a constrained HFB (CHFB) problem where the time-even constraining field is precisely the operator whose expectation value is the chosen collective variable (approximations 2 and 3), i.e., Q_{20} in the above example. Then it is obvious to generalize the result of, e.g., [9] to show that once the set of q-dependent R_0 matrices is known, one gets R_1, the first order (time-odd) part of R, by solving a double CHFB equation:

$$\delta\langle\Psi|\, H - \lambda Q - 2\,\frac{dq}{dt}P|\,\psi\rangle = 0 \tag{4}$$

with a generalized cranking operator P defined as

$$P = \frac{i\hbar}{2}\left[\frac{\partial R_0}{\partial q}, R_0\right]. \tag{5}$$

This operator P assumes, of course, the same 2×2 matrix structure as the density R, for instance, and can be shown to be of the form:

$$P = \frac{i\hbar}{2}\begin{pmatrix} p^h & p^\Delta \\ p^{\Delta^*} & p^{h*}\end{pmatrix}. \tag{6}$$

We will now perform two last approximations. The first consists in neglecting the Thouless – Valatin corrections that is the self-consistent response H_1 due to the R_1 part of the generalized density matrix (leaving thus the time-odd constraint $q\,P$ as the only time-odd operator in the variational problem). In a second step, we approximate the static solution R_0 by a self-consistent BCS solution at each time as defined and justified in [7].

We have calculated all matrix elements in the canonical basis (the basis of the eigenstates of ρ_0). Therefore, our results, for the mass parameters in particular, are given in terms of single particle energies (of the Hartree – Fock type) and pairing gaps, making them rather transparent and easy to compare with results obtained in their approaches. This feature makes our approach different from the work of Dobaczewski and Skalski [18] which have presented potentially similar results (apart from the self-consistency of our approach with the restriction, however, that theirs have included in some approximate way the Thouless – Valatin corrections) in a matricial form which is rather compact and then somewhat hard to connect with usual single particle spectroscopic properties.

Neglecting, as mentioned above, the Thouless – Valatin self-consistency, a solution of the time-odd part of the ATDHFB equations of motion can be obtained explicity. It is formally a system of two coupled equations giving ρ_1 and k_1 in a matricial form as functions of the p^h and p^Δ constraining operators:

$$[h_0, \rho_1] - \Delta_0 k_1^* + k_1\Delta_0^* =$$

$$= i\hbar\, q\{|\, p^h, \rho_0|\, - p^\Delta k_0^* + k_0\, p^{\Delta^*}\},$$

$$-\,\Delta_0\,\rho_1^* - \rho_1\Delta_0 + h_0 k_1 + k_1 h_0^* =$$

$$= i\hbar\, q\{\, p^h, k_0 - k_0\, p^{h^*} + p^\Delta - p^\Delta\rho_0^* - \rho_0\,\rho^\Delta\}, \tag{7}$$

which we have to project onto four subspaces labelled with obvious notations (μ, ν), $(\bar\mu, \nu)$, $(\mu, \bar\nu)$, $(\bar\mu, \bar\nu)$, where $|\,\bar\mu\rangle$ is the time-reversed of the state $|\,\mu\rangle$.

Out of some manipulation which will be detailed in a forthcoming publication, one can express the matrix elements of ρ_1 and k_1 in terms of matrix elements of the p^h and p^Δ operators which themselves may be expressed in terms of matrix elements of the derivative of ρ_0 with respect to q so that:

$$\rho_{1\mu\nu} = \rho_{1\bar\mu\,\bar\nu} = \frac{i\,\hbar\, q}{E_\mu + E_\nu}\, p^H_{\mu\nu} =$$

$$= \frac{i\,\hbar\, q}{E_\mu + E_\nu}\,\frac{(\upsilon_\mu^2 - \upsilon_\nu^2)}{(u_\mu\upsilon_\nu + u_\nu\upsilon_\mu)^2}\left(\frac{\partial\rho_0}{\partial q}\right)_{\mu\nu}, \tag{8}$$

$$k_{1\mu\bar\nu} = -\,k_{1\bar\nu\mu} = \frac{i\,\hbar\, q}{E_\mu + E_\nu}\, p^\Delta_{\mu\nu} =$$

$$= \frac{i\,\hbar\, q}{E_\mu + E_\nu}\,\frac{(u_\mu\upsilon_\mu + u_\nu\upsilon_\nu)}{(u_\mu\upsilon_\nu + u_\nu\upsilon_\mu)^2}\left(\frac{\partial\rho_0}{\partial q}\right)_{\mu\nu}. \tag{9}$$

The mass parameter which we note $M^P(q)$ is deduced from the part of the total energy which depends quadratically on the collective velocity and may be written as:

$$M^P(q) = \frac{1}{q}\,\mathrm{tr}\,(R_1 P). \tag{10}$$

Making use of the above-summarized results, one may show that

$$M^P(q) = 2\hbar^2 \sum_{\mu,\,\nu}{}' \left(\frac{1}{E_\mu + E_\nu}\right)\frac{1}{(u_\mu\upsilon_\nu + u_\nu\upsilon_\mu)^2}\left(\frac{\partial\rho_0}{\partial q}\right)^2_{\mu\nu}, \tag{11}$$

where the summation $\sum_{\mu\nu}'$ restricts the considered space to half of the one-particle space[1].

In the particular case of global rotation, where the cranking operator is well known [12] and given within the so-called Routhian approach, it is easy to show that one retrieves the Belyaev [11] version of the Inglis [10] cranking formula.

Upon solving the static HFB equation associated with Eq.(1) by using a time-even constraint $(-\lambda Q)$ or, in other words, with a vanishing collective velocity $(q = 0)$, one gets two independent equations relating the matrix elements of the Hartree–Fock and pairing fields (h_0, Δ_0) and those of the normal and abnormal associated densities (ρ_0, k_0). Using the projector equation $(R^2 = R)$, after differentiating them with respect to q, one finally gets the following relations expressing the matrix elements of $\partial\rho_0/\partial q$ as functions of $\partial\Delta_0/\partial q$ and $\partial h_0/\partial q$:

$$\left(\frac{\partial\rho_0}{\partial q}\right)_{\mu\nu} = -\frac{(u_\mu v_\nu + u_\nu v_\mu)^2}{E_\mu + E_\nu}\left\{\left(\frac{\partial h_0}{\partial q}\right)_{\mu\nu} - \right.$$

$$\left. - \frac{1 - v_\mu^2 - v_\nu^2}{(u_\mu v_\mu + u_\nu v_\nu)}\left(\frac{\partial\Delta_0}{\partial q}\right)_{\mu\nu}\right\}, \qquad (12)$$

from which one may express the mass parameter as

$$M^P(q) = 2\hbar^2 \sum_{\mu,\nu}' \frac{1}{(E_\mu + E_\nu)^3}\left\{(u_\mu v_\nu + u_\nu v_\mu)\left(\frac{\partial h_0}{\partial q}\right)_{\mu\nu} - \right.$$

$$\left. - (u_\mu v_\nu + u_\nu v_\mu)\left(\frac{\partial\Delta_0}{\partial q}\right)_{\mu\bar{\nu}}\right\}^2. \qquad (13)$$

The presentation of this second form of the mass parameter has three purposes:

i) First, since it involves derivatives of potentials and not of the normal density as in Eq.(11), upon comparing both results for mass parameters, it allows one to assess the accuracy of the numerical calculation of these derivatives.

ii) Moreover, it provides a theoretical frame in which one can compare our mass parameter M^P of Eqs.(11) and (13) with the one (noted here M^Q) consistently used over the years by some groups (as the group in Bruyeres-le-Chatel) which have developed microscopic approaches to large-scale collective modes in nuclei [7, 8, 20, 21], using the Gogny force [22] in the HFB approximation as a starting point. In the noncorrelated case, it was shown [23, 24] for fully self-consistent ATDHF solutions that the mass parameter is given by

$$M^{\mathrm{ATDHF}}(q) = \frac{\hbar^2}{2}\,\frac{M_{-3}^{\mathrm{RPA}}(Q)}{[M_{-1}^{\mathrm{RPA}}(Q)]^2}. \qquad (14)$$

The approximation used in the above-referred papers consists in replacing the RPA moments $M_{-3}^{\mathrm{RPA}}(Q)$ and $M_{-1}^{\mathrm{RPA}}(Q)$ in Eq.(14) by their perturbative value (i.e., neglecting the rearrangement effects both static and of the Thouless-Valatin type), namely, for BCS wavefunctions:

$$M_n(Q) = \sum_{\mu,\nu}' (u_\mu v_\nu + u_\nu v_\mu)^2 (E_\mu + E_\nu)^n |\langle\mu|Q|\nu\rangle|^2, \qquad (15)$$

writing therefore:

$$M^Q(q) = \frac{\hbar^2}{2}\,\frac{M_{-3}(Q)}{2[M_{-1}(Q)]^2}. \qquad (16)$$

It is clear that, when suppressing a part of self-consistency, the above and our approach have no longer to yield identical results. It is easy to check that this mass M^Q [Eq.(16)] is nothing but our mass M^P if one neglects all static rearrangements in the potentials so that the only non-vanishing term in Eq.(13) is due to the time-even constraint λQ.

iii) Thirdly, starting from the expression of Eq.(13), we will be able below to trace back the microscopic origins of the observed violent fluctuations of the mass parameters as functions of the collective variables.

For the rest of the paper, we will limit ourselves to the study of the axial quadrupole mode, using the *D*1*S* parametrization [25] of the Gogny force. Tests of numerical accuracy will be detailed in a forthcoming publication. We simply mention here that the CHFB calculations have been performed by projection of single-particle states on an axially symmetric harmonic oscillator basis whose spring constant has been optimized for each deformation, while its deformation parameter was interpolated from optimized values on a loose mesh [the basis size corresponds to 11 (13, resp.) major shells for rare earth (actinide, resp.) nuclei]. The numerical derivatives (of the normal densities) have been performed by a three-point formula taking into account the results of three self-consistent calculations performed in the vicinity of the deformation under scrutiny. Their accuracy has been assessed by the existence of a plateau of the mass parameter in terms of the chosen quadrupole moment intervals which are involved as well as by comparing,

[1] In a preliminary account [19] of these results, a mishandling of the time reversal properties of the matrix elements of the p^{11} operator has lead to introducing an erroneous very small corrective term in the expression of the mass as given in Eq.(11).

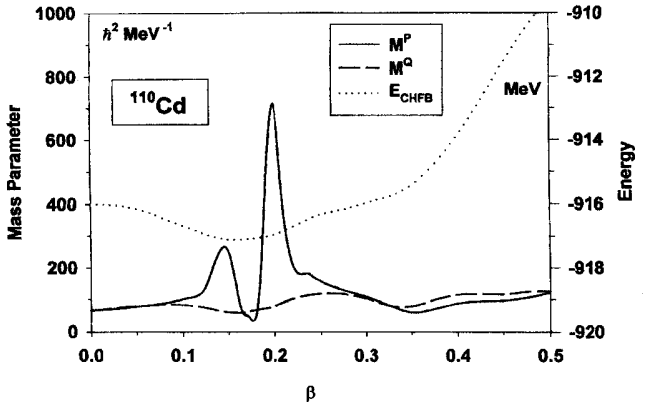

Fig.1. Quadrupole axial vibrational mass parameters $M^P(\beta)$ and $M^Q(\beta)$ for the usual quadrupole deformation parameter β taken as a collective variable are displayed (scale on the left) together with the total energy E_{CHFB} (scale on the right) for the ^{110}Cd nucleus as functions of β

as already mentioned, the masses resulting from Eqs.(11) and (13). As a result, it may be evaluated to be much less than one percent in regions where the mass is moderately varying with deformation and up to some percent in regions of strong variations (peak regions).

One sees that violent variations of the mass parameters are expected either when the pairing field or the Hartree ¯ Fock field is rapidly changing. We illustrate below each of these two situations. In Fig.1, the masses M^P and M^Q are shown for the nucleus ^{110}Cd where the usual deformation parameter β is deduced from the calculated quadrupole moment of the mass distribution. The total energy is also displayed, showing that large oscillations of the mass M^P occur close to the equilibrium deformation of this rather solf nucleus. It clearly appears that M^P exhibits variations which are absent in M^Q. In the upper part of Fig.2, the proton contribution to M^P is compared with its neutron counterpart for prolate deformations. The former is responsible for two peaks appearing at $\beta \approx 0.14$ and $\beta \approx 0.20$. The explanation for these peaks lies, as shown also in Fig.2, in the existence of an unpaired region for protons. In quite general terms, one may show that the peaks occur near the transition on the superfluid side (here slightly above $\beta \approx 0.14$ and slightly below $\beta \approx 0.20$). The fact that the derivative of the pairing field $\partial\Delta_0/\partial q$ is responsible for the discussed structure is also demonstrated in this figure where its contribution to the proton component of the mass parameter M^P is separated from the contribution of $\partial\Delta_0/\partial q$.

A similar situation is found for the rare earth nucleus ^{150}Gd. One observes three extremely high peaks in

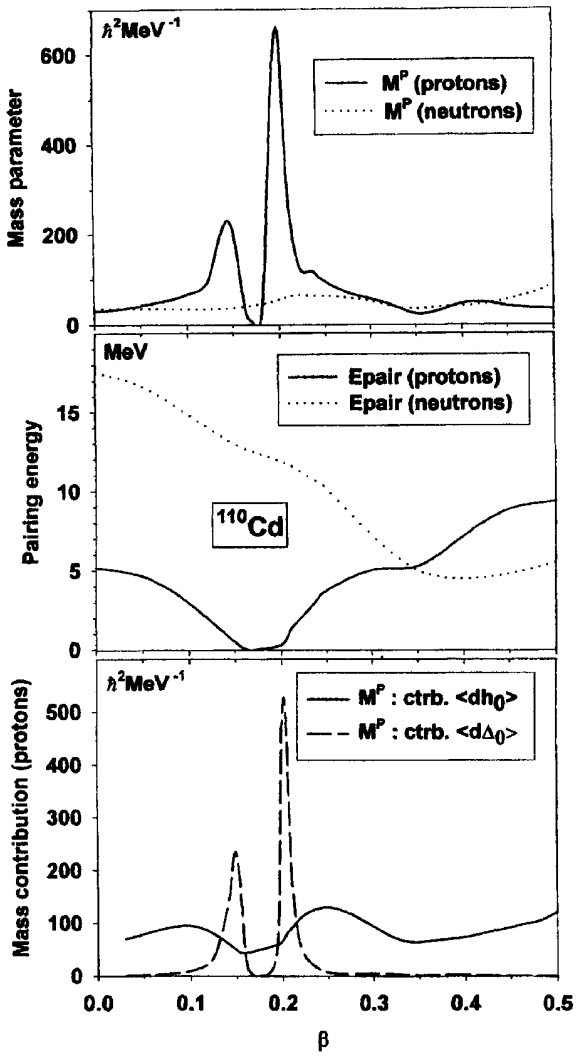

Fig.2. For the ^{110}Cd nucleus, as functions of the deformation β, the proton (dotted line) and neutron (solid line) components of the β-vibrational mass parameter $M^P(\beta)$ are displayed in the upper part, while the medium part shows the corresponding proton (resp., neutron) pairing energies expressed as $-\,\mathrm{tr}\Delta_0 k_0$. Contributions of the type $\langle dh_0\rangle$ (solid line) and $\langle d\Delta_0\rangle$ (dashed line) to the proton component of $M^P(\beta)$ are displayed in the lower part

M^P in the upper part of Fig.3 near the deformation $\beta \sim 0.7$ and culminating more than one order of magnitude above the peaks observed in neighboring nuclei or in other deformation regions in the same nucleus. Again, M^Q does not exhibit such dramatic variations. As shown in the medium and lower parts of Fig.3, these peaks are also correlated with pairing phase transitions, but now for both protons and neutrons. Furthermore, one notices an accidental conjunction of the disappearance of neutron pairing

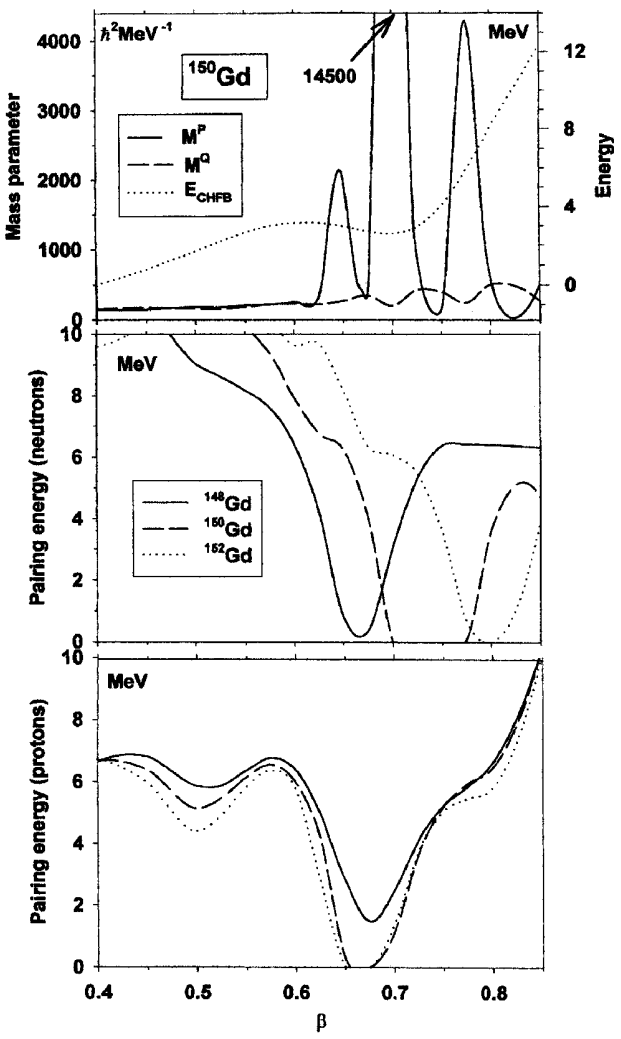

Fig.3. In the upper part, for the ^{150}Gd nucleus, β-vibrational mass parameters $M^P(\beta)$ (solid line) and $M^Q(\beta)$ (dashed line) corresponding to the left hand side scale are displayed as functions of the deformation parameter (β), together with the total energy E_{CHFB} (dotted line) corresponding to the right-hand side scale. Pairing energies (here defined as $\tilde{}\mathrm{tr}\Delta_0 k_0$) of ^{148}Gd (solid lines), ^{150}Gd (dashed lines), and ^{152}Gd (dotted lines) related to neutron (resp., proton) distributions are displayed on the medium (resp., lower) part of this figure as functions of the deformation parameter β

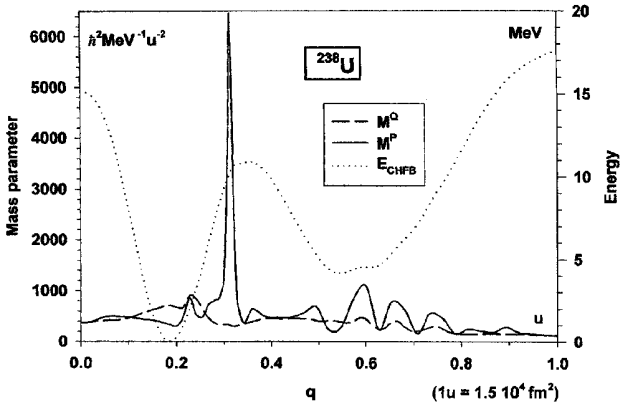

Fig.4. For the ^{238}U, as functions of the quadrupole moment in units 1.510^4 fm^2, the quadrupole vibrational mass parameters $M^P(q)$ (solid line) and $M^Q(q)$ (dashed line) are displayed together with the total energy. Here and in the following figure, contrarily, to what was the case in previous ones, the retained collective variable is the quadrupole moment q of the mass distribution

with the reappearance of the proton pairing which yields a pile-up of two peaks, thus resulting in a strong middle peak. The fact that this phenomenon occurs precisely in phase with the calculated superdeformed secondary minimum may entail amusing consequences. One expects indeed that the corresponding collective wavefunction will be anomalously squeezed. It is worth noting that such double phase transitions and therefore such strong peaks, as already mentioned, are not observed in neighboring Gd isotopes (see Fig.3) in the superdeformation region. Taking into account roughly the Coriolis antipairing effect, such a double phase transition is also possible at a medium spin in ^{148}Gd and may be in ^{152}Gd but not in other isotopes in the superdeformed region. It so happens, on the other hand, that the rather elusive phenomenon of staggering in the gamma rays of some superdeformed bands is only found near this ^{150}Gd isotope [26, 27]. As a possible explanation for such a staggering, the authors of [28] have proposed a zero point motion associated with the quantization of intrinsic vortical modes in highly rotating nuclei. On the other hand, through an analogy [29] with the Aharonov – Bohm phase effect at work in the persistent currents observed in mesoscopic rings (see [29] for references), they have related the scarcity of this staggering with a damping effect due to the spreading in the deformation space of the intrinsic superdeformed wave function. In this context, the reduction of the width of the superdeformed collective wave function precisely near the ^{150}Gd isotope is to be mentioned. It may be also interesting to note that such strong peaks have not been found in our calculations for nuclei where such a staggering has been finally excluded as in the $A \sim 190$ region (see, e.g., [30]) or is only tentatively proposed with irregular behavior as in the superdeformed states of nuclei with $A \sim 130$ [31].

Let us illustrate now the appearance of structures in the mass parameters related with variation of the Hartree – Fock field. In Fig.4, one shows that they exist for M^P, and again not for M^Q, in the case of the ^{238}U nucleus on the prolate side of the deformation energy curve specifically near the first fission barrier (i.e., for a value of the mass quadrupole moment

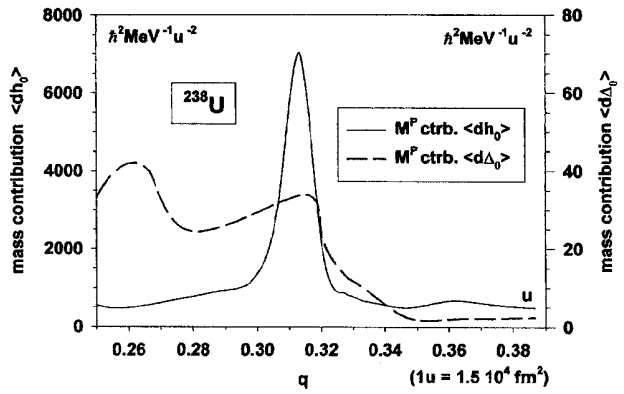

Fig.5. Contribution of the $\langle dh_0 \rangle$ (resp., $\langle d\Delta_0 \rangle$) type to the quadrupole vibrational mass parameter $M^P(q)$ as a function of the quadrupole moment q in units $u = 1.5104$ fm^2 are displayed around the top of the first fission barrier of ^{238}U in dashed line (resp., solid line) and corresponding to the left-hand scale (resp., right-hand scale)

slightly below 5000 fm^2). Equating the contribution of the derivative of the pairing field to zero, one retrieves most of the mass parameter (see Fig.5) which demonstrates that this peak stems from a rapid variation of the Hartree – Fock field. As a matter of fact, the latter is due to the conjunction of many single-particle crossings for both proton and neutron mean fields around this particular deformation. Such a dramatic situation is by all means not generally encountered near the top of fission barriers in other actinide nuclei. Strong peaks in the mass under fission barriers can, of course, yield a significant change in the collective lifetime for the fission isomer decay into the ground state valley. As an example, upon using the actual approximate expression M^P of the ATDHFB mass parameter for ^{238}U instead of M^Q in the calculation of the $E2$ isomeric transition rate (according to the method of [32], equivalent in this one-dimensional case to what is used in [33] taking apart the question of the choice made for the mass parameter), one decreases the corresponding lifetime by slightly less than two orders of magnitude. Most of this can be related to the peak under the barrier, the rest being due to other variations of the mass M^P in the second well introducing a change in the relevant collective wave function model structure.

As a conclusion, M^P mass parameters do exhibit strong variations which can be correlated to rapid variations of either pairing correlations or single particle properties near the Fermi surface. The physical consequences are governed by the time scale for the collective modes. In general, the width of the collective wave function is relatively larger than the characteristic collective extension of such mass variations, so that they are just smeared out fluctuations and therefore not significant. This remark is relevant for most of the cases studied in the microscopic approaches of [20, 21], where the smoothing expression M^Q of the mass parameters is used. In few cases, corresponding to longer collective times, however, such a structure in the mass parameter may be of importance. Nevertheless, it is clear that the present work needs to be pursued into fully selfconsistent ATDHFB calculations, i.e., including Thouless – Valatin corrective terms, and it must be considered in this perspective as providing good starting grounds for a more comprehensive account of the low-energy collective dynamics. While doing so, some approximations would still remain. One of the most stringent could be the limited number of chosen collective variables. In this respect, the existence of peaks in the mass parameters might give a hint of the usefulness of introducing other paths in the collective motion. Consequently, even though our work is limited to a one-dimensional collective dynamics, the fact that we demonstrate the existence of such unexpected structures is of relevance for a possible extension to a larger number of coupled collective modes.

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