The cranking formula and the spurious behaviour of the mass parameters

B. Mohammed-Azizi
University of Bechar, Bechar, Algeria

Abstract

We discuss some aspects of the approach of the mass parameters by means of the simple cranking model. In particular, it is well known that the numerical application of this formula is often subject to ambiguities or contradictions. It is found that these problems are induced by the presence of two derivatives in the formula. To overcome these problems, we state a useful ansatz and we develop a number of simple arguments which tend to justify the removal of these terms. As soon as this is done, the formula becomes simpler and easier to interpret. In this respect, it is shown how the shell effects affect the mass parameters. A number of numerical tests help us in our conclusions.

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*Electronic address: aziziyoucef@voila.fr

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I. INTRODUCTION

Under the assumption of the adiabaticity of the nuclear motion (the shape variations are slower than the single-particle motion), a collective Hamiltonian can be defined as the sum of the kinetic and potential energy of deformation [1]:

\[ H_{\text{collective}} = \frac{1}{2} \sum_i \sum_j D_{ij} \{ \beta_1, \ldots, \beta_n \} \frac{d\beta_i}{dt} \frac{d\beta_j}{dt} + U \{ \beta_1, \ldots, \beta_n \} \]

(1)

In this paper we consider only the deformation of the nucleus neglecting thus the rotational degrees of freedom. The set \{ \beta_1, \ldots, \beta_n \} specifies a set of deformation parameters of the nuclear surface. They constitute the dynamical variables of the motion. The functions \( D_{ij} \{ \beta_1, \ldots, \beta_n \} \) represent the so-called mass parameters or the tensor of inertia, and \( U \{ \beta_1, \ldots, \beta_n \} \) is the potential energy of deformation. Both of these functions depend on the deformation of the nucleus. These two quantities are especially important in the study of the dynamic of the nucleus such as the nuclear fission (lifetime estimates) [1] and the collective levels of the nucleus [2].

Usually, the quantity \( U \{ \beta_1, \ldots, \beta_n \} \) can be evaluated in the framework of the constrained Hartree-Fock theory or by the phenomenological shell correction method. The mass parameters \( D_{ij} \{ \beta_1, \ldots, \beta_n \} \) are often approximated by the cranking formula [3] or in the self consistent approaches by other models [4]-[6].

The present work focuses mainly on the drawbacks of the numerical aspect of the calculation of the mass parameters on the basis of the cranking formula. In particular, it is well known that cranking procedure is somewhat delicate and in some cases can even lead to singular unphysical values for the mass parameters. One of the goals of the present work is precisely to discuss this point and to propose a correction to this formula. First and foremost, to our point of view, it seems that the main mistake is the presence in the formula of the derivatives of the gap parameter and the Fermi level. Therefore, the main part of this work will be devoted to the looking for the arguments (or proofs) which could justify the removing of these terms. On the basis of theoretical as well as numerical approaches, this survey will also be very useful to demonstrate the relative importance of the different terms entering into the calculations and also to show how the shell effects affect precisely the mass parameters. We realize that we criticize an old and well-established formula, but it is only "the bad" part of the formula which is called into question, not the formula itself. This "bad part" is the main source of the problems of the formula. We are intimately convinced that this criticism will be very useful and will bring new insight to this subject.

II. THE INGLIS-BELYAEV OR CRANKING FORMULA

A. The Cranking or Inglis formula for the mass parameters

The mass (or vibrational) parameters are given by the Inglis formula [1, 3]:

\[ D_{ij} \{ \beta_1, \ldots, \beta_n \} = 2\hbar^2 \sum_{M \neq 0} \frac{\langle O | \frac{\partial}{\partial \beta_i} | M \rangle \langle M | \frac{\partial}{\partial \beta_j} | O \rangle}{E_M - E_O} \]

(2)

Where \( | O \rangle , | M \rangle \) are respectively the ground state and the excited states of the nucleus. The quantities \( E_M, E_O \) are the associated eigenenergies. In the independent-particle model, whenever the state of the nucleus is assumed to be a Slater determinant (built on single-particle states of the nucleons), the ground state\( | O \rangle \) will be of course the one where all the particles occupy the lowest states. The excited states \( | M \rangle \) will be approached by the one particle-hole configurations. In that case, Eq. (2) becomes (see appendix A):

\[ D_{ij} \{ \beta_1, \ldots, \beta_n \} = 2\hbar^2 \sum_{l>\lambda, k<\lambda} \frac{\langle k | \frac{\partial}{\partial \beta_i} | l \rangle \langle l | \frac{\partial}{\partial \beta_j} | k \rangle}{\epsilon_l - \epsilon_k} \]

(3)

\( \lambda \) denotes the Fermi level. The above expression can be simplified further if the following simple property is used: \( (\epsilon_k - \epsilon_l) \langle k | \frac{\partial}{\partial \beta_j} | l \rangle = \langle k | [H_{sp}, \frac{\partial}{\partial \beta_j}] | l \rangle = - (\langle k | H_{sp} \frac{\partial}{\partial \beta_j} | l \rangle) \) for \( k \neq l \) so that Eq. (3) becomes

\[ D_{ij} \{ \beta_1, \ldots, \beta_n \} = 2\hbar^2 \sum_{l>\lambda, k<\lambda} \frac{\langle k | \frac{\partial}{\partial \beta_i} | l \rangle \langle l | \frac{\partial}{\partial \beta_j} | k \rangle}{(\epsilon_l - \epsilon_k)^2} \]

(4)
where $H_{sp}$ is the single-particle Hamiltonian. The single particle states are given by the Schrödinger equation of the independent-particle model.

$$H_{sp} |\nu\rangle = \epsilon_{\nu} |\nu\rangle$$  \hfill (5)

B. The Inglis-Belyaev or cranking formula with pairing correlations

It must be noted that in Eq. (4) the denominator $\epsilon_{\nu} - \epsilon_{k}$ vanishes in the case where the Fermi level coincides with two or more degenerate levels. This is the major drawback of the formula. It is possible to overcome this difficulty by taking into account the pairing correlations. This can be achieved through the BCS approximation by the following replacements in Eq. (2):

i) the ground state $|O\rangle$ by the BCS state $|BCS\rangle$.

ii) the excited states $|M\rangle$ by the two quasiparticle excitations states $|\mu, \nu\rangle$ (here we consider only the even-even nuclei).

This led Belyaev [7] to two types of non-vanishing matrix elements (see also the demonstration given in the appendix B):

$$\langle \mu, -\nu | \partial / \partial \beta | \nu \rangle = (u_{\nu}v_{\mu} + u_{\mu}v_{\nu}) \langle \nu | \frac{\partial}{\partial \beta_{i}} | \mu \rangle \quad \nu \neq \mu$$ \hfill (6)

$$\langle \nu, -\nu | \partial / \partial \beta | \nu \rangle = - \frac{1}{v_{\nu}} \frac{\partial u_{\nu}}{\partial \beta_{i}}$$ \hfill (7)

The later is due to the changing of the occupations probabilities with the deformation, i.e. with $u_{\nu}$ and $v_{\nu}$:

iii) the energy $E_{0}$ by $E_{BCS}$ and $E_{M}$ by the energy of the two quasiparticles, i.e., by $E_{\nu} + E_{\mu} + E_{BCS}$. The quasiparticle energy being $E_{\nu} = \sqrt{(\epsilon_{\nu} - \lambda)^{2} + \Delta^{2}}$ and the BCS state is defined from the "true" vacuum $|0\rangle$ by:

$|BCS\rangle = \Pi_{k} (u_{k} + v_{k}a_{k}^{+}a_{-k}) |0\rangle$.

The Belyaev formulation for the mass parameters (formula (B3) of the appendix B) is then:

$$D_{ij} \{ \beta_{1}, .., \beta_{n} \} = 2h^{2} \sum_{\nu} \sum_{\mu \neq \nu} \frac{(u_{\nu}v_{\mu} + u_{\mu}v_{\nu})^{2}}{E_{\nu} + E_{\mu}} \langle \nu | \frac{\partial}{\partial \beta_{i}} | \mu \rangle \langle \mu | \frac{\partial}{\partial \beta_{j}} | \nu \rangle + h^{2} \sum_{\nu} \frac{1}{v_{\nu}} \frac{\partial u_{\nu}}{\partial \beta_{i}} \frac{\partial u_{\nu}}{\partial \beta_{j}}$$ \hfill (8)

Beside this formula, there is an other more convenient formulation due to Bes [8] modified slightly by the authors of Ref. [1]. In the latter, the above two types of matrix elements have been cast under a more explicit form (see again the demonstrations in appendices C and D).

$$\langle \nu, -\mu | \partial / \partial \beta | \nu \rangle = \frac{u_{\nu}v_{\mu} + u_{\mu}v_{\nu}}{E_{\nu} + E_{\mu}} \langle \nu | \frac{\partial H_{sp}}{\partial \beta_{i}} | \mu \rangle \quad \nu \neq \mu$$ \hfill (9)

$$\langle \nu, -\nu | \partial / \partial \beta | \nu \rangle = - \Delta \langle \nu | \frac{\partial H_{sp}}{\partial \beta_{i}} | \nu \rangle + \Delta \frac{\partial \lambda}{\partial \beta_{i}} + (\epsilon_{\nu} - \lambda) \frac{\partial \Delta}{\partial \beta_{i}}$$ \hfill (10)

The final formula of the mass parameters takes now the form (cf. formula (D1) of the appendix D):

$$D_{ij} \{ \beta_{1}, .., \beta_{n} \} = 2h^{2} \sum_{\nu} \sum_{\mu \neq \nu} \frac{(u_{\nu}v_{\mu} + u_{\mu}v_{\nu})^{2}}{(E_{\nu} + E_{\mu})^{3}} \langle \nu | \frac{\partial H_{sp}}{\partial \beta_{i}} | \mu \rangle \langle \mu | \frac{\partial H_{sp}}{\partial \beta_{j}} | \nu \rangle + 2h^{2} \sum_{\nu} \frac{\Delta^{2}}{8E_{\nu}^{2}} R_{\nu}^{i} R_{\nu}^{j}$$ \hfill (11)

where

$$R_{\nu}^{i} = - \langle \nu | \frac{\partial H_{sp}}{\partial \beta_{i}} | \nu \rangle + \frac{\partial \lambda}{\partial \beta_{i}} + \frac{(\epsilon_{\nu} - \lambda) \partial \Delta}{\Delta}$$ \hfill (12)

The two quantities of the r.h.s of Eq. (11) are in the adopted order, the so-called "non-diagonal" and the "diagonal" parts of the mass parameters. The derivatives are contained in the above diagonal term $R_{\nu}^{i}$. When the derivatives $\partial \lambda / \partial \beta_{i}, \partial \Delta / \partial \beta_{i}$ cancel the diagonal term reduce simply to the diagonal matrix element $- \langle \nu | \partial H_{sp} / \partial \beta_{i} | \nu \rangle$. In order to facilitate the comparison with other papers, we recall that the cranking formula is usually cast under a slightly different form:
\[
D_{ij} \{ \beta_1, \ldots, \beta_n \} = 2\hbar^2 \sum_{\nu} \sum_{\mu} \left( \frac{(u_{\nu}v_{\mu} + u_{\mu}v_{\nu})^2}{(E_{\nu} + E_{\mu})} \right) \langle \nu | \frac{\partial H_{sp}}{\partial \beta_i} | \mu \rangle \langle \mu | \frac{\partial H_{sp}}{\partial \beta_j} | \nu \rangle + P_{ij}
\]

where the quantity \( P_{ij} \) enclose all (and only) the derivatives [1] because the product of matrix element of \( R^i_\nu R^j_\mu \) is "displaced" to the first term of the r.h.s. of Eq. (13).

III. SOME PRECISIONS ON THE MICROSCOPIC MODEL

A. The Schrodinger equation

In this work the numerical tests are based on a microscopic hamiltonian (represented by \( H_{sp} \) in the previous formulae). The latter is defined starting from a deformed Woods-Saxon potential. In order to obtain a realistic model, a spin-orbit and a Coulomb (protons case) terms are also taken into account in the hamiltonian.

Since in the hamiltonian the kinetic energy operator does not depend on the deformation and since the deformed average potential is the most important term compared to the spin-orbit and coulomb interactions, the derivative of the single-particle hamiltonian (appearing in the above cranking formula) will be approximated by the one of the average potential as in Ref. [1]:

\[
\langle \nu | \frac{\partial H_{sp}}{\partial \beta_i} | \mu \rangle \approx \langle \nu | \frac{\partial V}{\partial \beta_i} | \mu \rangle
\]

where \( V \) denotes the deformed Wood-Saxon potential. In our work, the deformation of the nuclear surface and hence the one of the mean field \( V \) is of the quadrupole type and is given by the well known Bohr parameters \((\beta, \gamma)\). These quantities are connected to the elongation and the axial asymmetry of the nucleus. In this special case, our notation reduces here to these two deformations parameters:

\[
\{ \beta_1, \ldots, \beta_n \} = \{ \beta, \gamma \}
\]

The solution of the eigenvalues problem is obtained as follows:

(i) The eigenfunctions \( |\nu\rangle \) of this hamiltonian are expanded onto the basis’ functions of the three dimensional anisotropic harmonic oscillator. The representative matrix of this hamiltonian is then effectively built in this basis.

(ii) This matrix is then diagonalized by using a large basis (\( \sim 16 \to 20 \) major shells of the oscillator basis).

One obtains in this way, the single-particle energies spectrum \( \{\epsilon_{\nu}\} \) and the set of the components of associated eigenfunctions \( \{|\nu\rangle\} \) on the oscillator basis. All the details of our microscopic model and the corresponding FORTRAN program have been given in Ref. [9].

Knowing the single-particle spectrum, the next step is to find the gap parameter \( \Delta \) and the Fermi level \( \lambda \) by solving the standard BCS equations. Technical details of these calculations can be found from Ref [10]. As soon as \( \Delta \) and \( \lambda \) are known, it becomes easy to deduce the BCS amplitudes \( v_{\nu}, u_{\mu} \) associated with the energy level \( \epsilon_{\nu} \). Thus, at this stage, all the quantities such as \( \epsilon_{\nu}, |\nu\rangle, \Delta, \lambda, u_{\nu}, v_{\mu} \) which are necessary in Eq. (11) are known.

B. Deformation dependence of \( \Delta \) and \( \lambda \)

Due to the fact that the single-particle hamiltonian \( H_{sp} \) depends explicitly on the deformation, its eigenenergies and its eigenfunctions will be also explicitly deformation dependent. To keep in mind that the deformation dependence comes only from the Schrodinger equation, it is useful to highlight this explicit dependence:

\[
H_{sp}(\beta, \gamma) |\nu; (\beta, \gamma)\rangle = \epsilon_{\nu}(\beta, \gamma) |\nu; (\beta, \gamma)\rangle
\]

Although being explicit, the above notation is somewhat cumbersome, therefore, for brevity the dependence on the deformation of the above quantities is usually omitted.

Starting from the single-particle spectrum the gap parameters \( \Delta \) and the Fermi level \( \lambda \) are solved from the BCS equations (17) and (18) as soon as the single-particle spectrum \( \{\epsilon_{\nu}\} \) is known.

\[
\frac{2}{G} = \sum_{\nu=1}^{N_{px}} \frac{1}{\sqrt{(\epsilon_{\nu} - \lambda)^2 + \Delta^2}}
\]
N or \( Z = \sum_{\nu=1}^{N_N} \left( 1 - \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}} \right) \)

Of course, the deformation dependence of the eigenenergies \( \epsilon_\nu(\beta) \) involves the ones of \( \Delta \) and \( \lambda \). However, this dependence is not obtained “straightforwardly” from the single particle model itself, that is, from the Shroedinger equation (15), but from the BCS equations (17) and (18). From this point of view, these two quantities (i.e. \( \Delta \) and \( \lambda \)) must not be linked to the deformation as the eigenenergies and eigenfunctions of \( H_{sp} \) do. Nevertheless, usually they are considered “explicitly” deformation dependent through the expression of their derivatives obtained by the so-called lowest-order expansion [12, 1]:

\[
\frac{\partial \lambda}{\partial \beta} = \frac{ac_\beta + bd_\beta}{a^2 + b^2}, \quad \frac{\partial \lambda}{\partial \gamma} = \frac{ac_\gamma + bd_\gamma}{a^2 + b^2} \quad (19)
\]

\[
\frac{\partial \Delta}{\partial \beta} = \frac{b c_\beta - a d_\beta}{a^2 + b^2}, \quad \frac{\partial \Delta}{\partial \gamma} = \frac{b c_\gamma - a d_\gamma}{a^2 + b^2} \quad (20)
\]

with

\[
a = \sum_\nu \Delta E_\nu^{-3}, \quad b = \sum_\nu (\epsilon_\nu - \lambda) E_\nu^{-3}, \quad (21)
\]

\[
c_\beta = \sum_\nu \Delta (\epsilon_\nu - \lambda) \frac{\partial H_{sp}}{\partial \beta} |\nu\rangle \langle \nu| E_\nu^{-3}, \quad d_\beta = \sum_\nu (\epsilon_\nu - \lambda) \langle \nu| \frac{\partial H_{sp}}{\partial \beta} |\nu\rangle E_\nu^{-3} \quad (22)
\]

\[
c_\gamma = \sum_\nu \Delta (\epsilon_\nu - \lambda) \frac{\partial H_{sp}}{\partial \gamma} |\nu\rangle \langle \nu| E_\nu^{-3}, \quad d_\gamma = \sum_\nu (\epsilon_\nu - \lambda) \langle \nu| \frac{\partial H_{sp}}{\partial \gamma} |\nu\rangle E_\nu^{-3} \quad (23)
\]

In the following the expression “the derivatives” which will be used many times in the text means simply the both derivatives given by Eq. (19) and (20).

IV. THE PROBLEM OF THE PHASE TRANSITION: THE SINGULARITY IN THE MASS PARAMETERS OR THE PARADOX OF THE CRANKING FORMULA

The transition between the normal and the superfluid phase affects generally the spherical magic nuclei under changing deformation [12]. As we shall see, this phenomenon causes the most serious problem to the mass parameters. For convenience, in the following, we choose to discuss just only one parameter, namely \( D_{\beta\beta}(\beta, \gamma) \). This does by no means restrict the conclusions of this study.

It is well known that the BCS equations have non-trivial solutions only above a critical value of the strength \( G \) of the pairing interaction. The trivial solution corresponds theoretically to the value \( \Delta = 0 \) of an unpaired system. In this case, the mass parameters given by (11) reduces to the ones of the formula (4), i.e. the cranking formula of the independent-particle model. Indeed, when \( \Delta = 0 \) it is clear that the quasi-particle energies of (11) become \( E_\nu = |\epsilon_\nu - \lambda| \), and the quantities \( u_\nu, v_\nu \) are then either 0 or 1 so that the non-diagonal part of the right hand side of this formula reduces to:

\[
\lim_{\Delta \to 0} 2\hbar^2 \sum_{\nu, \mu \neq \nu} \frac{(u_\nu v_\mu + u_\mu v_\nu)^2}{(E_\nu + E_\mu)} \langle \mu| \frac{\partial H_{sp}}{\partial \beta} |\mu\rangle \langle \mu| \frac{\partial H_{sp}}{\partial \beta} |\nu\rangle = 2\hbar^2 \sum_{\nu > \lambda \nu \leq \lambda} \frac{1}{(\epsilon_\nu - \epsilon_\mu)} \langle \nu| \frac{\partial H_{sp}}{\partial \beta} |\mu\rangle \langle \mu| \frac{\partial H_{sp}}{\partial \beta} |\nu\rangle
\]

which is the same formula that the one given by Eq. (4). This implies the important fact that in this limit (\( \Delta \to 0 \)), the diagonal part (i.e. the second term) of the right hand side of Eq. (11) must vanish. However in a few cases for which \( \Delta \approx 0 \), contrary to all expectations, it happens that this diagonal term leads to very large numerical values near some “critical deformation”. This well-known singular behaviour constitutes undoubtedly unphysical and undesirable effects. This is the main paradox of the formula.

Because the diagonal matrix element \( \langle \nu| \frac{\partial H_{sp}}{\partial \beta} |\nu\rangle \) are finite and relatively small (cf. to the numerical examples given below), it is immediately clear from Eq. (12) that it is the derivatives of \( \Delta \) and \( \lambda \) which cause the problem.
In this respect, the formulae \([19]\) and \([20]\) are subject to a major drawback due to the fact that their common denominator can vanish. This can be easily explained because on the one hand, \(a\) is proportional to \(\Delta\) (see Eq. \([21]\)) and therefore vanishes with it and because on the other hand \(b\) is defined as a "random" sum of postive and negative values (see again Eq. \([21]\)) depending on whether the terms are below or above the Fermi level. In the literature, this problem has been reported many times \([1, 11, 13]\), but no solution has been proposed. The authors of Ref. \([1]\) and \([12]\) claim that for sufficiently large pairing gaps \(\Delta\) the total mass parameter is essentially given by the diagonal part without the derivatives, whereas those of Ref. \([13]\) affirm that the role of the derivatives is by no mean small in the fission process. Other studies \([14]\) neglect the derivatives without any justification. Even if in some cases the derivatives introduce small differences, in others, this is not true at all. In fact, it is easy to realize that these terms involve serious and insoluble problems. Therefore, after intensive numerical calculations, we have led to ask ourselves if their presence could be called into question. If so, their removal should be justified. Consequently, the problem amounts to find good arguments for that. This constitutes the first step of this work. Without further ado, let us examine this point in the next section.

V. ANSATZ AND CORRECTION OF THE CRANKING FORMULA OF THE MASS PARAMETERS

To overcome "the paradox" of the previous section, we need to start from an ansatz or assertion which justify the removal of the derivatives of \(\lambda\) and \(\Delta\). Before that, we want to recall some important points. First, the derivatives of \(\lambda\) and \(\Delta\) come from the derivatives of the probabilities in the formula \([8]\). It is then worth to recall their expressions:

\[
u_k = \frac{1}{\sqrt{2}} \left( 1 + \frac{\epsilon_k - \lambda}{\sqrt{\epsilon_k^2 - \lambda^2 + \Delta^2}} \right)^{1/2}
\]

\[
u_k = \frac{1}{\sqrt{2}} \left( 1 - \frac{\epsilon_k - \lambda}{\sqrt{\epsilon_k^2 - \lambda^2 + \Delta^2}} \right)^{1/2}
\]

These quantities depend implicitly on the deformation \(\beta\) through the level \(\epsilon_k(\beta)\) of the spectrum and also through \(\lambda\) and \(\Delta\) which themselves depend implicitly on the entire spectrum \(\{\epsilon_0(\beta), \epsilon_1(\beta), \ldots\}\) via the non linear equations of the BCS theory. First, we will proceed from a point of view which somewhat looks like the Virtual works principle. The following ansatz contains two points:

1) Thus, we suppose a "virtual change in deformation" \(\delta\beta\) in such a way that one and only level undergoes change, namely the level \(\epsilon_k\). Therefore the "virtual change" of the probabilities would be in this case.

\[
\delta \nu_k = \frac{\partial \nu_k}{\partial \epsilon_k} \delta \epsilon_k + \frac{\partial \nu_k}{\partial \lambda} \frac{\partial \lambda}{\partial \epsilon_k} \delta \beta + \frac{\partial \nu_k}{\partial \Delta} \frac{\partial \Delta}{\partial \epsilon_k} \delta \beta
\]

\[
\delta \nu_k = \frac{\partial \nu_k}{\partial \epsilon_k} \delta \epsilon_k + \frac{\partial \nu_k}{\partial \lambda} \frac{\partial \lambda}{\partial \epsilon_k} \delta \beta + \frac{\partial \nu_k}{\partial \Delta} \frac{\partial \Delta}{\partial \epsilon_k} \delta \beta
\]

This is very logical because the changes of \(\lambda\) and \(\Delta\) are basically due the change of the deformation, not straightforwardly but through the change of the single-particle levels. In other words we have to write \((\partial \lambda/\partial \epsilon_k)(\partial \epsilon_k/\partial \beta)\) instead \((\partial \lambda/\partial \beta)\) because the changes of \(\lambda\) and \(\Delta\) are determined from the knowledge of the spectrum \(\{\epsilon_k\}\) which depends itself on the deformation of the nucleus. Thus from our "principle" the "virtual change of the probability", i.e. \(\delta \nu_k\), is due to only one level, namely "the corresponding" level \(\epsilon_k\).

2) It is well known from the BCS theory that the quantities \(u_k, v_k, \lambda, \Delta\) are related to each other self-consistently so that the change of \(\delta u_k\) would depend on its own change through \(\lambda\) and \(\Delta\). For example in the BCS theory we have \(\Delta = G \sum u_k v_k\) and \(\delta \Delta\) would depend on the changes \(\delta u_k\) and \(\delta v_k\) which in turn depend on \(\delta \Delta\). This constitutes an illogical consequence. To overcome this problem, we state the following intuitive assertion which avoid such a problem and hence the "initial" problem of the derivatives of \(\lambda\) and \(\Delta\): "Between two infinitely close "virtual" deformations \(\beta\) and \(\beta + \delta \beta\), the quantities \(u_k, v_k, \lambda\) and \(\Delta\) must verify the simple (but not so obvious) following conditions":

\[
\frac{\partial u_k}{\partial \lambda} \frac{\partial \lambda}{\partial \epsilon_k} + \frac{\partial u_k}{\partial \Delta} \frac{\partial \Delta}{\partial \epsilon_k} = 0
\]

\[
\frac{\partial v_k}{\partial \lambda} \frac{\partial \lambda}{\partial \epsilon_k} + \frac{\partial v_k}{\partial \Delta} \frac{\partial \Delta}{\partial \epsilon_k} = 0
\]

in such a way that Eq. \([27]\) and \([28]\) reduce to:

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\[ \delta u_k = \frac{\partial u_k}{\partial \beta} \delta \beta \]

Implying that:

\[ \delta \nu_k = \frac{\partial \nu_k}{\partial \beta} \delta \beta \]

Must be employed instead

\[ \frac{\partial u_k}{\partial \beta} = \frac{\partial u_k}{\partial \beta} \delta \beta + \frac{\partial u_k}{\partial \lambda} \frac{\partial \lambda}{\partial \beta} + \frac{\partial u_k}{\partial \Delta} \frac{\partial \Delta}{\partial \beta} \]

In fact a real change of the deformation implies "all the levels of the spectrum". Consequently the "virtual" changes \( \delta u_k \) and \( \delta \nu_k \) must be applied "successively" to all the levels (\( u_k = u_1, u_2, \ldots \)). We recall the important fact that Eq. (35) is used in appendix D to obtain the formula (11) whereas Eq. (33) leads to the following more simple result (which consists of simply ignoring the derivatives of the "old" formula):

\[ D_{\beta \beta} = 2\hbar^2 \sum_{\nu \neq \mu} \frac{(u_{\nu \nu} + u_{\mu \mu})^2}{(E_\nu + E_\mu)} \langle \nu | \partial H_{sp} / \partial \beta_i | \mu \rangle \langle \mu | \partial H_{sp} / \partial \beta_i | \nu \rangle + 2 \hbar^2 \sum_{\nu \neq \mu} \frac{\Delta^2}{s E_\nu} \langle \nu | \partial H_{sp} / \partial \beta_i | \nu \rangle^2 \]

In this case, it is very important to note that Eq. (37) reduces to Eq. (4) of an unpaired system and removes the previous "paradox" of the "old" formula.

Furthermore, for convenience it is to be noted that it is possible to collect the both terms in the right hand side of the above formula, say, the non-diagonal and the diagonal parts in only one term. Indeed, with the identity

\[ \frac{(u_{\nu \nu} + u_{\mu \mu})^2}{(E_\nu + E_\mu)} = \frac{(\Delta E_\nu)^2}{(2 E_\nu)^3} = \frac{\Delta^2}{s E_\nu} \]

so that the missing term in the "non-diagonal part" is precisely the second contribution of the right hand side of Eq. (37). Consequently Eq. (37) can be cast under the more compact form:

\[ D_{ij}(\beta) = 2\hbar^2 \sum_{\nu \neq \mu} c_{\nu \mu} \langle \nu | \partial H_{sp} / \partial \beta_i | \mu \rangle \langle \mu | \partial H_{sp} / \partial \beta_i | \nu \rangle \]

with

\[ c_{\nu \mu} = \frac{(u_{\nu \nu} + u_{\mu \mu})^2}{(E_\nu + E_\mu)^3} \]

Thus, the only difference between the two versions of the mass parameters Eq. (11) and Eq. (37) or Eq. (39) is the absence of the derivatives \( \partial \lambda / \partial \beta_i \) and \( \partial \Delta / \partial \beta_i \) in the second version of the formula. The latter constitutes for us the cranking formula without derivatives or the "corrected" formula. In the following \( c_{\nu \mu} \) will be called simply "the coefficient", and for \( \nu = \mu, \langle \nu | \partial H_{sp} / \partial \beta_i | \mu \rangle^2 \) will be referred to as "the squared matrix element".

VI. NUMERICAL EXAMPLES AND OTHER ARGUMENTS IN FAVOUR OF THE "CORRECTED" CRANKING FORMULA (I.E., WITHOUT DERIVATIVES)

A. Comparisons between the two variants of the formula for \( \Delta \approx 0 \)

In the present section we will try to prove that the modified or "corrected" cranking formula for the mass parameters is consistent with "reasonable" results. In this respect, we have first looked for a "critical" case where there is no
BCS solution apart from the trivial solution ($\Delta = 0$) and applied then the both formulae. Such situation is obtained generally for a magic neutron or proton number. Here, we use the nuclei $^{136}_{54}Xe_{82}$ for which we have plotted in fig. 1-bottom the neutrons’ contribution ($N = 82 = magic$) to the mass parameters vs the quadrupole deformation $\beta$ in the two versions of the formula.

In these calculations the deformation parameter of the axial asymmetry is fixed to the value $\gamma = 0^\circ$ (prolate shape). The mention ”with” between parentheses signifies that the calculations are performed with the formula (11) including $\partial\lambda/\partial\beta_i$ and $\partial\Delta/\partial\beta_i$, and by ”without” the same ones done with the formula Eq. (37) without these terms. From this example, it is clear that whenever the gap parameter $\Delta$ becomes small (here $\Delta \lesssim 0.2$ MEV) the two formula give very different results for the mass parameters. The major difference is reached for $\beta \sim 0.1$ (for which $\Delta \approx 0.004$) where we obtain values about $6.000000 \text{ MEV} \hbar^{-1}$ and $25 \text{ MEV} \hbar^{-1}$ for the two versions of the formula of the mass parameter $D_{\beta\beta}$. This singular behaviour (of course within the version including the derivatives) has obviously nothing to do with reasonable physical values for the mass parameters. However, both formula give close, though non-identical, results as soon as $\Delta > 0.2$ MEV. Thus, this simple numerical test confirms that it is the derivatives which appear in the formula (11) that are responsible of the divergence character of the mass parameters for the case where the valid BCS solution breaks down.

More precisely, we have checked that it is the common denominator in Eq. (19) and (20) which causes the problem. Indeed, in this denominator the quantities $a$ and $b$ defined by (21) vanish simultaneously. On this point, we give in the following table further details concerning the numerical values of $a$, $b$, $c_\beta$, $d_\beta$ which intervene in the quotients of the derivatives in Eq. (19), and Eq. (20).

Of course, it is to be noted that numerically $\Delta$ does not vanish rigorously for the trivial solution. This is due to the occupations probabilities which are numerically not exactly equal to 0 or 1. As mentioned before, the large values of the derivatives are due to the denominator $a^2 + b^2$ which is very small (For explanations see section IV). As already noted, this constitutes the main defect of the formula including the derivatives. On the other hand, we have also verified that there is no crossing levels near the Fermi level for this case ($\beta = 0.1$). Thus the derivatives can diverges without
any problem of the so-called crossing levels, as it is often claimed. Indeed, from fig. 1-bottom as soon as $\nu = 41$ the third contribution is small near the Fermi level, $\epsilon_{\nu}$ which does not depend on the level $\nu$ which is responsible of the singularity $(\Delta \approx 0)$ whereas it is $\partial \lambda / \partial \beta_i$ which modifies the results for valid BCS solutions. Thus, in all the case of a valid BCS state. Further checkings have shown that it is $\partial \Delta / \partial \beta_i$ which is defined from Eq. (12). Indeed, the quantity, $R^\nu_i$ is the contribution of three terms which are summarized with their most important corresponding coefficient in the table II. The energy levels $\epsilon_{\nu}$ are labeled by $\nu$ according to an increasing order as already précised and the associated eigenfunctions are noted by $|\nu\rangle$. In this particular case, we have took $N = 82$ neutrons. There is thus 41 pairs of particles in time-conjugate states. For this reason the Fermi level is close to the $41^{th}$ level, i.e., the last filled level. This explains why the most important levels are labeled with indices $\nu$ which are close to 41. From this table it is clear that the third contribution is small near the Fermi level, $\partial \Delta / \partial \beta_i$ being also relatively small for such a value of the pairing gap $(\Delta = 0.90 \text{ MeV})$. On the other hand, the contribution $\partial \lambda / \partial \beta_i$ which does not depend on the level $\nu$ is by no means so small $(\sim 7.66 \text{ MeV})$ compared to the matrix element. This result contradicts some works in which the derivatives are neglected, claiming that the derivatives are small in the case of a valid BCS state. Further checkings have shown that it is $\partial \Delta / \partial \beta_i$ which is responsible of the singularity $(\Delta \approx 0)$ whereas it is $\partial \lambda / \partial \beta_i$ which modifies the results for valid BCS solutions. Thus, in all the cases the derivatives modify the results. In fact, in terms of physical arguments, we can say that the derivative $\partial \lambda / \partial \beta_i$ perturbs or "masks" the shell effects of the diagonal matrix element (see the next subsection) and this constitutes an additional physical argument in favour of the removal of the derivatives.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
$\beta$ & $\gamma$ & $a(MEV^{-2})$ & $b(MEV^{-3})$ & $c_{\beta}(MEV^{-1})$ & $d_{\beta}(MEV^{-1})$ & $\Delta(MEV)$ & $\frac{\Delta}{90}(MEV)$ & $\frac{\Delta}{90}(MEV)$ \\
\hline
0.1 & 0 & 0.0096 & 0.0034 & 0.0190 & -25.7134 & 0.0044 & 2366.3 & -832.6 \\
\hline
\end{tabular}
\caption{Some numerical details concerning the calculations of the derivatives given by the formulae (19) and (20).}
\end{table}

\section*{B. Single-particle contributions to the "element" $R^\nu_i$}

For a valid BCS solution (i.e. for $\Delta \gg G$, or approximately $\Delta \gtrsim 0.80$ in our examples) the problem of the divergence disappears. Indeed, from fig. 1-bottom as soon as $\beta$ exceeds 0.3 the gap parameter reaches its normal value and the divergence is no more present, the both formulae with and without derivatives give close results.

Unlike the closed shell, the mid-shell regions (neutrons or protons) are characterized by a very regular behaviour of the pairing $\Delta$ and hence of the mass parameters. This is the case in fig. 1-top for the neutron number $N = 70$ of the nuclei $^{136}$Xe$^{70}$. However, as in the preceding example, the both formulae (with and without derivatives) do not give the same results. This is entirely due to the derivatives contained in the expression of $R^\nu_i$ which is defined from Eq. (12). Indeed, the quantity, $R^\nu_i$ is the contribution of three terms which are summarized with their most important corresponding coefficient in the table II. The energy levels $\epsilon_{\nu}$ are labeled by $\nu$ according to an increasing order as

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
$\nu$ & $\beta = 0.50, \gamma = 0^\circ, \Delta = 0.90 \text{ MeV}$ & $\text{coeff.}$ & $\text{first contrib.}$ & $\text{second contrib.}$ & $\text{third contrib.}$ \\
\hline
level number $\nu$ & $\frac{2\hbar^2 c_{\nu \nu}}{\epsilon_{\nu \nu}}$ & $\langle \nu \rangle \frac{\partial H}{\partial \beta_i} | \nu \rangle$ & $\frac{\partial \lambda}{\partial \beta_i}$ & $\frac{\partial \lambda - \Delta}{\Delta} \frac{\partial \lambda}{\partial \beta_i}$ \\
\hline
40 & 0.117 & -0.81 & 7.66 & 1.03 \\
41 & 0.292 & -14.19 & 7.66 & 0.38 \\
42 & 0.186 & -14.50 & 7.66 & -0.75 \\
43 & 0.108 & 0.72 & 7.66 & -1.07 \\
\hline
\end{tabular}
\caption{The most important single-particle contributions to the term $R^\nu_i$ given by the formula (12). Note that the derivative $\partial \lambda / \partial \beta_i$ is not so small compared to the diagonal matrix elements of the derivative (cf. text).}
\end{table}

C. Matrix elements: comparison between the diagonal and the non-diagonal parts. The shell effects lie in the diagonal part

At this stage, the effects of the "perturbations" involved by the derivatives are known. Therefore, from now, we will concentrate only on the formula of the cranking without derivatives. It is interesting to compare the magnitude of the contributions of the diagonal and non-diagonal parts given by Eq. (37). These two contributions are plotted in fig. 2 for a magic number of neutrons $N = 82$ (bottom) and for a mid-shell neutron number $N = 70$ (top). In the both
cases, the diagonal contribution is dominant (about 10 times larger) if we except the region of the spherical shape \((\beta = 0)\) for \(N = 70\) which seems to be very particular. Apart from the noted special spherical case, the explanation of these results can be easily understood. Indeed, first, the diagonal matrix elements are always by far more important than the other because in the integrand the derivative of the potential are multiplied by a squared wave function,

\[
\langle \nu | \frac{\partial H_{sp}}{\partial \beta} | \nu \rangle \approx \langle \nu | \frac{\partial V}{\partial \beta} | \nu \rangle = \int |\varphi_\nu(\mathbf{r}, \beta, \gamma)|^2 \frac{\partial V(\mathbf{r}, \beta, \gamma)}{\partial \beta} d^3 r
\]

whereas for the non-diagonal matrix elements, i.e., for

\[
\langle \nu | \frac{\partial H_{sp}}{\partial \beta} | \mu \rangle \approx \langle \nu | \frac{\partial V}{\partial \beta} | \mu \rangle = \int \varphi_\nu^*(\mathbf{r}, \beta, \gamma) \frac{\partial V(\mathbf{r}, \beta, \gamma)}{\partial \beta} \varphi_\mu(\mathbf{r}, \beta, \gamma) d^3 r
\]

the two radial wave functions are not always in phase, their product \(\varphi_\nu^*(\mathbf{r}, \beta, \gamma) \frac{\partial V(\mathbf{r}, \beta, \gamma)}{\partial \beta} \varphi_\mu(\mathbf{r}, \beta, \gamma)\) has not a definite sign, the contributions to the integral will have tendency to cancel each other, or at least to lead to a small values.

It is clear that the more important coefficients \(c_{\nu \mu}\) (diagonal and non diagonal) are those which are the closest to the Fermi level. Indeed, these coefficients are which given by (see Eq. (40)), are maximums when the quasiparticle energy \(E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}\) reaches its minimal value, i.e. for \(\epsilon_\nu \approx \epsilon_\mu \approx \lambda\). The few important non-diagonal coefficients are generally multiplied by weak matrix elements. Indeed, for closed levels \((\nu \approx \mu, \nu \neq \mu)\), the radial wave functions are often in ”opposite” phase (like two ”consecutives” wave functions of the one dimensional infinite square well) so that the contribution to the integral will be necessarily very small. This explains why the diagonal part is dominant. Before closing this paragraph, we would like to add an important remark concerning the shell effects. The latter are of course due to quantum mechanics. They involve sudden variations in the mass parameters with the number of particles. They appear when a few states contribute essentially to the mass parameters. In fact, for the mass parameters, we have a very limited number of diagonal matrix elements which contribute essentially to the mass parameters opposed to an admixture of a large number of small non-diagonal matrix elements. Consequently, it is clear that the shell effects will be contained in the diagonal part (of course without the derivatives).

FIG. 2: (Bottom and Top) same as fig 1; Here, the figure details the diagonal contribution without derivatives and the non-diagonal one; Apart from the spherical case \((\beta = 0)\) for \(N = 70\) which constitutes a ”special case”, the diagonal part is by far always more important.
D. Magnitude of the different terms

We have found numerically that when there is not BCS solution the diagonal term (without derivatives) is practically equal to zero ($\sim 10^{-6} MEV$) so that the mass parameters reduce only to the non-diagonal part of the formula. In this case the mass parameters are very small. Because the values and the fluctuations of the mass parameters are mostly due to the diagonal contribution, our numerical study will concern exclusively this term. In the following, once more, we will concentrate obviously on the version of the formula without derivatives. The "simple" diagonal part can be cast under the following form:

$$D_{\beta\beta}(\text{diagonal part}) = \sum_{\nu} c_{\nu\nu} \langle \nu| \frac{\partial V}{\partial \beta_i}|\nu \rangle^2$$  \hspace{1cm} (43)

with,

$$c_{\nu\nu} = (\frac{\hbar^2}{4}) \frac{\Delta^2}{\sqrt{(\epsilon_{\nu} - \lambda)^2 + \Delta^2}}$$  \hspace{1cm} (44)

As mentioned before, only few (about two up to five at all) energy levels contribute really to the final value of the mass parameters. Indeed, this function is peaked at $\lambda$ and due to the power of the denominator of Eq. 44 decreases very rapidly so that only few levels give important coefficients. For a valid BCS solution, a relative weak value of $\Delta$ gives significant coefficient $c_{\nu\nu}$. For example, we give in Fig. 3 (bottom and top) the coefficients $c_{\nu\nu}$ (black stars) and the square of the matrix elements $|\langle \nu| \frac{\partial V}{\partial \beta_i}|\nu \rangle|^2$ (black squares) for the neutron contributions of the same two isotopes as before and the same deformation. First of course, we especially can check that these coefficients are important near the Fermi level ($41^{th}$ and $35^{th}$ level). We have thus computed the four major neutron contributions of the energy levels and we have found 97% and 82% respectively for $N = 82$ and $N = 70$ cases. These contributions are not only due to the strongest values of the coefficients $c_{\nu\nu}$ but also to the "corresponding" matrix elements (see Eq. 43). We also can see very clearly the shell structure of the squared matrix elements which is the same for these two cases (because the deformation and hence the spectrum are the same in the both cases). An other remark is that the maxima of the matrix elements are situated at the levels $N^015, 25, 41, 65$ which correspond to the nucleon numbers $30, 50, 82, 130$ which are magic or nearly magic, but these numbers are obtained for a weak deformed shape of the nucleus, whereas in the binding energy they match the spherical shape. Moreover these maxima are immediately preceded or followed by small values. Thus the shell structure of the matrix elements appears less regular than the one of the energy levels. As we can see, the shell structure is "contained" not only in the level density but also in the matrix elements. Thus the mass parameters are characterized by a complex "dual" shell structure.

At last, as a special case, we must point out the very strong values of the coefficients (i.e., the stars) in Fig. 3 bottom involving very large the mass parameters at $\beta = 0.2$. This very exceptional situation arises in the so called one crossing levels (see Ref. (11) and (12)) near the Fermi energy. This will be analyzed in the next subsection.

E. Effects of the crossing levels on the diagonal part

In Fig. 4 we have plotted the energy levels for different values of the deformation parameter $\beta$ ($\gamma$ being fixed to 0). The BCS Fermi level is indicated by a star. This level is situated in the middle of a gap constituted by the last filled and the first unfilled levels. As $\beta$ increases, these two levels approach little by little each other. From the first ($\beta = 0$) and up to the fourth deformation ($\beta = 0.2$), the Fermi level lies always in the middle of a gap corresponding to the neutron magic number $N = 82$. In these locations, the level density is so small with respect to the pairing strength so that it (i.e., the level density) is not able to insure a valid (non-trivial) BCS solution. Therefore, due to the weakness of $\Delta$, the diagonal term of Eq. (37) does not contribute at all to the mass parameters. In these situations, the mass parameters are very small ($\sim 25\hbar^2 MEV^{-1}$ in our case). However, for the deformation $\beta = 0.2$, the two levels become very close to the Fermi level. It occurs in the immediate vicinity of the Fermi level a crossing levels. This happens inside a gap and gives rise to two very strong coefficients. Moreover, the corresponding values of the squared matrix elements are also important, giving practically all the contribution to the mass parameters. This phenomenon is characteristic of a phase transition (compare with Fig. 3 bottom). The remaining cases ($\beta$ beyond 0.25) can be considered as "normal cases". They correspond to values about $c_{\nu\nu} \approx 0.1 - 0.2$. 

\hspace{1cm} 11
F. Some other important precisions

We have focused our discussion around the mass parameter $D_{\beta\beta}$, but similar studies will lead to analog general conclusions (seen above) for the two other mass parameters $D_{\gamma\gamma}$ and $D_{\beta\gamma}$. However, we will make further useful remarks. For the quadrupole deformation $(\beta, \gamma)$, we write the detailed form for the three mass parameters (naturally, once more without the derivatives):

$$D_{\beta\beta} = 2\hbar^2 \sum \sum c_{\nu\mu} \langle \nu | \frac{\partial V}{\partial \beta} | \mu \rangle^2$$  \hspace{2cm} (45)

$$D_{\gamma\gamma} = 2\hbar^2 \sum \sum c_{\nu\mu} \langle \nu | \frac{\partial V}{\partial \gamma} | \mu \rangle^2$$  \hspace{2cm} (46)

$$D_{\beta\gamma} = 2\hbar^2 \sum \sum c_{\nu\mu} \langle \nu | \frac{\partial V}{\partial \beta} | \mu \rangle \langle \mu | \frac{\partial V}{\partial \gamma} | \nu \rangle$$  \hspace{2cm} (47)

with $c_{\nu\mu}$ given by Eq. (40).

It is easy to compare these three quantities. First it is to be noted that they have the same coefficient so that the only difference will come from the matrix elements. The latter have not a definite sign in such a way that the third mass parameters will be the result of the sum of positive as well as negative terms. It will be thus necessary smaller than the two first mass parameters for which we have only positive contributions. Moreover, it is found numerically that $D_{\beta\beta}$ is generally larger than $D_{\gamma\gamma}$. This can also be easily explained by the fact that the single-particle potential is generally more sensitive to the $\beta$ degree of freedom than the $\gamma$’s one, especially for the region the Barium isotopes. In other words for the quadrupole deformations and a Woods-Saxon potential we have,

$$\frac{\partial V}{\partial \beta} \gg \frac{\partial V}{\partial \gamma}$$  \hspace{2cm} (48)
FIG. 4: Energy levels for $^{136}_{54}Xe_{82}$ at different deformations; For small deformations due to the spherical symmetry there is a high degeneracy; For this reason it seems that there are less levels at $\beta = 0$ and approximately for the nearest deformations. The fermi level is indicated by a star; Due to the neutron magic number $N = 82$, it is situated in the center of an important energy gap (between the 41$^{th}$ and the 42$^{nd}$ level); Note that the gap reduces gradually as $\beta$ increases from the spherical shape; For the four first levels there is no BCS solution and the mass parameters are small; For $\beta = 0.2$, we obtain a crossing level which contributes strongly to the mass parameters through the diagonal part; Compare these comments with the results of fig(1-bottom).

Although the present work is devoted exclusively to the mass parameters, we would like to add an important remark concerning the moments of inertia. Indeed, these quantities can also be evaluated with the help of the cranking approximation including pairing correlations.\(^{(49)}\):

$$3_k(\beta, \gamma) = 2\hbar^2 \sum_\nu \sum_\mu \frac{(u_\nu v_\mu - u_\mu v_\nu)^2}{E_\nu + E_\mu} |\langle \mu | j_k | \nu \rangle|^2$$

(49)

Because the latter looks like to the one of the mass parameter (of course without the derivatives), it is tempting to conclude that the behaviour of these two quantities will in principle be the same. However, it is well known that unlike the mass parameters, the behaviour of the moments of inertia is always found as a smooth function of particle-number. It depends mainly on the deformation of the nucleus. This means that contrarily to the mass parameters, there are no shell effects in the moments of inertia. From our previous study, it is easy to interpret this difference.

First, this is due partly to the lower power of the denominator of Eq. \(^{(49)}\), but the main reason is that there is no diagonal contribution ($\nu = \mu$) to this sum because the "coefficient" vanishes when $\nu = \mu$. Remembering that the shells effects come almost exclusively from the diagonal part of the total contribution, we can conclude here that they will be necessary quasi absent in the moments of inertia.

VII. COMPARISON BETWEEN THE BOTH FORMULAE THROUGH THE EXPERIMENTAL COLLECTIVE LEVELS

We have also solved numerically the generalized Bohr Hamiltonian with the help of the numerical fortran code of Ref. \(^{[17]}\). The six inertial functions have been calculated of course via the two versions of the cranking formula and the potential energy of deformation with the Strutinsky method. The two types of calculation are compared to
FIG. 5: Collective levels deduced numerically (see text) from the generalized Bohr Hamiltonian including the seven inertial functions (three mass parameters, three moments of inertia, and the potential energy of the deformation). Two typical cases with and without phase transition are considered.

The experimental levels. For this task we chose two Barium isotopes. This choice is justified by the fact that the magic nuclei \( ^{138}\text{Ba} \) undergoes the phase transition near the spherical shape whereas for the other (non-magic) nuclei \( ^{132}\text{Ba} \) there is not the case.

The formula without derivatives is called as the "new" formula whereas the other is called the "old" formula. The experimental low lying collective levels are denoted by "exp". From the figure it is clear that for the phase transition (\( ^{138}\text{Ba} \)) the both formulae give very different results. The advantage of the new version of the formula is clear because the old version gives a completely absurd result. In the other case the difference is much more less important but the theoretical "new" and "old" formulae do not give identical spectra.

VIII. CONCLUSION

The cranking formula of the mass parameters is widely used in the study of the dynamics of the nucleus. However, its applications are not free from ambiguities and contradictions. The aim of this paper is to convince that these problems are inherent to a spurious presence of the so-called derivatives in the formula. Therefore, by means of a simple "proved assertion" based on a number of pertinent arguments (see text), it is simply recommended to remove these derivatives. It turns out that the cranking formula without derivatives is no more subject to the cited problems and becomes simpler to interpret. Let us re-examine some advantages:

i) The "new" formula reduces in a naturally way to that of the unpaired system when \( \Delta = 0 \) whereas the old version leads to an inextricable paradox.

ii) The problem of the unphysical large values of the mass (singularity) and thereby unphysical collective spectra disappears.

iii) The shell effects are physically no more "masked" or "perturbed" by the derivatives.

iv) The formula becomes more transparent and a number a features have been highlighted in this paper. For example, the shell effects are not only connected to the level density as it is usually claimed, but also to the matrix elements which have also their proper shell structure. Thus, the shell effects appear to be governed by a "dual" shell structure. Therefore, examining the mass parameters only through the level density, as it is usually done, is surely insufficient to explain the results.
We hope that this work will help the reader to a better understanding of the mass parameters and will encourage further investigations in this direction.

Appendix A: The cranking formula in the independent-particle model

The cranking formula for the mass parameters is given by Eq. (2). If we want to apply the cranking formula in the framework of the independent-particle model, we assume that the excited states are simply one particle-one hole excitations. We proceed to the following replacements:

\[ |O\rangle \rightarrow |\text{core}\rangle \quad \text{and} \quad |M\rangle \rightarrow a^+_k a^-_k |\text{core}\rangle \quad \text{where} \quad |\text{core}\rangle = \prod_{n<\lambda} a^+_n |0\rangle \]

is the ground state or the core of the independent-particle model. In this expression, |0\rangle is the "real" vacuum and \( a^+_n \) is the creation operator of a real particle in the state \( n \).

In the second quantization formalism, we can write:

\[ \partial /\partial \beta = \sum_{\nu,\mu} \langle \nu | \partial /\partial \beta | \mu \rangle a^+_\nu a^-_\mu \]

We choose |\mu\rangle as the eigenfunctions of the single particle hamiltonian \( H_{\text{sp}} |\mu\rangle = \epsilon_\mu |\mu\rangle \). The \( \epsilon_\mu \) are then the associated eigenenergies.

The matrix element entering in the cranking formula reads then:

\[ \langle M | \partial /\partial \beta | O \rangle = \langle \text{core} | a^+_{k<\lambda} a^-_{l>\lambda} \sum_{\nu,\mu} \langle \nu | \partial /\partial \beta | \mu \rangle a^+_\nu a^-_\mu | \text{core} \rangle \]

It is clear that the only non-vanishing matrix elements imply that: \( \mu = k \) and \( \nu = l \).

Assuming that in the independent-particle model the energy of the nucleus amounts simply to the one of its nucleons we will have \( E_M - E_O = \epsilon_l - \epsilon_k \), therefore the cranking formula becomes:

\[ D_{ij} \{ \beta_1, .., \beta_n \} = 2\hbar^2 \sum_{l>\lambda, k<\lambda} \frac{\langle k | \frac{\partial}{\partial \beta_l} | l \rangle \langle l | \frac{\partial}{\partial \beta_k} | k \rangle}{\epsilon_l - \epsilon_k} \quad (A1) \]

Appendix B: The cranking formula with pairing correlations

The BCS theory gives the ground state and two-quasiparticle excited states for a paired system as follows

\[ |\text{BCS}\rangle = \prod_{k>\lambda}(u_k + v_k a^+_k a^-_k)|0\rangle, \]

\[ a^+_\nu a^-_\mu |\text{BCS}\rangle = a^+_\nu a^-_\mu \prod_{k\neq \nu,\mu}(u_k + v_k a^+_k a^-_k)|0\rangle \quad \text{for} \quad \nu \neq \mu, \quad \text{and} \quad a^+_\nu a^-_\mu |\text{BCS}\rangle = (-u_\nu + u_\mu a^+_\nu a^-_\nu) \prod_{k\neq \nu}(u_k + v_k a^+_k a^-_k)|0\rangle \]

where \((u_k, v_k)\) are the usual probability amplitudes of the pairs of particles in the mutual time-reversed states |k\rangle, |−k\rangle.

Starting again from the cranking formula (2), we have to evaluate the matrix elements \( \langle M | \partial /\partial \beta | O \rangle \). Then, we will replace the state |O\rangle by the BCS state. The excited states |M\rangle are supposed to be two quasiparticle excitations states \( |M\rangle = a^+_\nu a^-_\mu |\text{BCS}\rangle \).

Expressing the operator \( \partial /\partial \beta \) in the second quantization formalism and keeping in mind however that the differential operator acts not only on the wave functions of the BCS state but also on the occupations probabilities \( u_k, v_k \), we have to consider two types of differentiation:

\[ \frac{\partial}{\partial \beta} = \left( \frac{\partial}{\partial \beta} \right)_{\text{wave func}} + \left( \frac{\partial}{\partial \beta} \right)_{\text{occup.prob}} \]

We must therefore to evaluate successively two types of matrix elements

1. Calculation of the first type of matrix elements

We have in second quantization representation:

\[ \left( \frac{\partial}{\partial \beta} \right)_{\text{wave func}} = \sum_{\nu,\mu} \langle \nu | \frac{\partial}{\partial \beta} | \mu \rangle a^+_\nu a^-_\mu \]

Applying this operator on the paired system we find:

\[ \left( \frac{\partial}{\partial \beta} \right)_{\text{wave func}} |\text{BCS}\rangle = \sum_{\nu,\mu} \langle \nu | \frac{\partial}{\partial \beta} | \mu \rangle a^+_\nu a^-_\mu |\text{BCS}\rangle \]

Two excited quasiparticle states of an even-even nucleus are obtained by breaking one pair of correlated particles so that we must take \( \nu \neq \mu \). (It is easy to verify that this correspond to the first type of the excited states given above).

Using the inverse of the Bogoliubov-Valatin transformation:

\[ a^-_\nu = u_\nu a^-_\nu - v_\nu a^+_\nu, \quad a^-_\mu = u_\mu a^-_\mu + v_\mu a^+_\mu \]
We considered here only the states with two quasiparticle (for the even-even nuclei). We calculate then the first type of matrix elements:

\[ I_1 = \langle M^\ast | \sum_{\nu,\mu \neq \nu} \langle \nu | \frac{\partial}{\partial \beta_{l}} | \mu \rangle \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle \]

The above form of the formula suggests that the excited states must be of the form \( |M\rangle = \alpha_{\nu}^+ \alpha_{l}^+ |BCS\rangle = |k, l\rangle \).

We obtain then:

\[ I_1 = \langle BCS | \alpha_{-l} \alpha_{k} \sum_{\nu,\mu \neq \nu} \langle \nu | \frac{\partial}{\partial \beta_{l}} | \mu \rangle \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle \]

\[ = \sum_{\nu,\mu \neq \nu} \langle \nu | \frac{\partial}{\partial \beta_{l}} | \mu \rangle \alpha_{\nu} \alpha_{\mu}^+ | BCS \langle \alpha_{-l} \alpha_{k} | BCS \rangle \]

\[ = \langle \nu | \frac{\partial}{\partial \beta_{l}} \rangle \prod_{\nu,\mu \neq \nu} \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle \]

We use the following usual Fermions anticommutation relations:

\[ \{ \alpha_k, \alpha^+_l \} = 0 \]

Thus the quantity between brakets gives:

\[ \langle BCS | \alpha_{-l} \alpha_{k} \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle = \langle BCS | \alpha_{-l} \delta_{\nu k} \alpha_{k} \alpha_{\mu}^+ | BCS \rangle \]

and consequently:

\[ \langle \nu | \frac{\partial}{\partial \beta_{l}} \rangle \Rightarrow \prod_{\nu,\mu \neq \nu} \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle = \delta_{\nu k} \delta_{\mu l} \]

\[ \langle \nu | \frac{\partial}{\partial \beta_{l}} \rangle \prod_{\nu,\mu \neq \nu} \alpha_{\nu} \alpha_{\mu}^+ | BCS \rangle = |k, l\rangle \]

The only non vanishing possibility is given by \( k = l \) otherwise the result cancels for \( k \neq l \).

Noting that if \( T \) is the time-reversal conjugation operator

\[ \langle -k | \frac{\partial}{\partial \beta_{l}} | -l \rangle = \langle k | T^+ \frac{\partial}{\partial \beta_{l}} T | l \rangle = \langle k | T^{-1} \frac{\partial}{\partial \beta_{l}} T | l \rangle \]

and assuming that \( \frac{\partial}{\partial \beta_{l}} \) is time-even, we get:

\[ \langle -k | \frac{\partial}{\partial \beta_{l}} | -l \rangle = \langle k | \frac{\partial}{\partial \beta_{l}} | l \rangle \]

Moreover, using the well-known property

\[ u_{-l} = u_{l} \]

we obtain finally:

\[ I_1 = \langle k, l | \left( \frac{\partial}{\partial \beta_{l}} \right)_{\text{wave func}} | BCS \rangle = (u_k v_l + u_l v_k) \langle k | \frac{\partial}{\partial \beta_{l}} | l \rangle (1 - \delta_{k,l}) \]  

(B1)

2. Calculation of the second type of matrix elements

Differentiating the BCS state, we obtain:

\[ \left( \frac{\partial}{\partial \beta_{l}} \right)_{\text{occup.prob}} | BCS \rangle = \sum_{\tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) \prod_{k \neq \tau} \alpha_{k \tau} \alpha_{l \tau}^+ | 0 \rangle \]

This corresponds to the second type of the excited states given above because for the pair in the state \( \tau \) we have a linear combination of the vacuum state with a state of two particles in conjugate states. The excited states will be necessarily here, of the following form:

\[ |M\rangle = \alpha_{\nu}^+ \alpha_{\mu}^+ |BCS\rangle = |m, -m\rangle \]

We have therefore to calculate:

\[ I_2 = \langle BCS | \alpha_{-m \tau} \alpha_{m \tau} \sum_{\tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) \prod_{k \neq \tau} \alpha_{k \tau} \alpha_{l \tau}^+ | 0 \rangle \]

It is simple to show that:

\[ \prod_{k \neq \tau} \alpha_{k \tau} \alpha_{l \tau}^+ | 0 \rangle = (u_{\tau} + v_{\tau} a_{\tau}^+ a_{\tau}^{-1})^{-1} | BCS \rangle \]

then

\[ I_2 = \langle BCS | \alpha_{-m \tau} \alpha_{m \tau} \sum_{\tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) (u_{\tau} + v_{\tau} a_{\tau}^+ a_{\tau}^{-1})^{-1} | BCS \rangle \]

The case \( m \neq \tau \) leads to the cancellation of \( I_2 \). The only non vanishing possibility is given by \( \tau = m \).

\[ I_2 = \langle BCS | \alpha_{-m \tau} \alpha_{m \tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) (u_{m} + v_{m} a_{m}^+ a_{m}^{-1})^{-1} | BCS \rangle \]

Using the inverse transformation of Bogoliubov-Valatin by "selecting" only two quasiparticle states

\[ I_2 = \langle BCS | \alpha_{-m \tau} \alpha_{m \tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) (u_{m} + v_{m} a_{m}^+ a_{m}^{-1})^{-1} | BCS \rangle \]

Making an expansion to first order in \( \alpha_{\tau}^+ \alpha_{m}^+ \) of the inverse operator of the above formula (other terms containing more than two quasiparticle excitations are of course neglected)

\[ (u_{m} + v_{m} a_{m}^+ a_{m}^{-1})^{-1} = u_{m}^{-1} (1 + v_{m} a_{m}^+ a_{m}^{-1})^{-1} = u_{m}^{-1} (1 - v_{m} a_{m}^+ a_{m}^{-1}) \]

Replacing this quantity in \( I_2 \)

\[ I_2 = \langle BCS | \alpha_{-m \tau} \alpha_{m \tau} \left( \frac{\partial u_{l \tau}}{\partial \beta_{l}} + \frac{\partial v_{l \tau}}{\partial \beta_{l}} \right) (u_{m}^{-1} (1 - v_{m} a_{m}^+ a_{m}^{-1}) | BCS \rangle \]

Again taking again into account only two quasiparticle excitations,
The two matrix elements which can be cast as follows:

\[ \sum_{\beta} \partial H / \partial \beta \] 

knowing that the normalization condition is:

\[ u_m^2 + v_m^2 = 1 \]

we find by differentiation

\[ 2u_m \frac{\partial u_m}{\partial \beta} + 2v_m \frac{\partial v_m}{\partial \beta} = 0 \]

combining these two relations, we obtain in \( I_2 \):

\[ I_2 = \frac{1}{v_m} \frac{\partial u_m}{\partial \beta} \]

then, the second term reads:

\[ I_2 = \langle m, -m | \left( \frac{\partial}{\partial \beta} \right)_{\text{prob}} | BCS \rangle = - \frac{1}{v_m} \frac{\partial u_m}{\partial \beta}, \]

which can be cast as follows:

\[ I_2 = \langle k, -l | \left( \frac{\partial}{\partial \beta_i} \right)_{\text{prob}} | BCS \rangle = \frac{1}{v_k} \frac{\partial u_k}{\partial \beta_i} \delta_{kl} \quad (B2) \]

The two matrix elements \( I_1 \) and \( I_2 \) corresponding to the two cases \( k \neq l \) and \( k = l \) are now known. Reassembling the two parts \( I_1 \) and \( I_2 \) in the only one formula, we get:

\[ \langle M | \frac{\partial}{\partial \beta} | O \rangle = I_1 + I_2 = \langle k, -l | \left( \frac{\partial}{\partial \beta} \right)_{\text{BCS}} | k \rangle \frac{\partial}{\partial \beta} | l \rangle - \frac{1}{v_k} \frac{\partial u_k}{\partial \beta_i} \delta_{kl} \]

Replacing this quantity in the cranking formula, noting that the crossed terms \( (I_1 I_2 \text{ and } I_2 I_1) \) cancel in the product and knowing that \( E_M - E_O = E_k + E_l \) (see subsec [III] we find:

\[ D_{ij} \{ \beta_1, ..., \beta_n \} = 2\hbar^2 \sum_{k,l} \frac{(u_k v_l + u_l v_k)^2}{E_k + E_l} \langle l | \frac{\partial}{\partial \beta_i} | k \rangle \langle k | \frac{\partial}{\partial \beta_j} | l \rangle (1 - \delta_{k,l}) + 2\hbar^2 \sum_k \frac{1}{2E_k} \frac{1}{v_k} \frac{\partial u_k}{\partial \beta_i} \frac{\partial u_k}{\partial \beta_j} \quad (B3) \]

The first term of the r.h.s of the formula is the so-called non-diagonal term, whereas the second is the diagonal one.

Appendix C: Another version of the cranking formula

Let be \( H \) some nuclear hamiltonian and \( |O⟩, |M⟩ \) its ground and excited state: noting that:

\[ \langle M | \left( \frac{\partial}{\partial \beta} \right)_{\text{wave func}} | O \rangle = (E_M - E_O) \langle M | \left( \frac{\partial}{\partial \beta} \right)_{\text{wave func}} | O \rangle \]

since the commutator gives:

\[ \left[ H, (\partial / \partial \beta_i)_{\text{wave func}} \right] = -\partial H / \partial \beta_i \]

the cranking formula becomes:

\[ D_{ij} \{ \beta_1, ..., \beta_n \} = 2\hbar^2 \sum_{M \neq O} \frac{\langle O | (\partial / \partial \beta_i) | M \rangle \langle M | (\partial / \partial \beta_j) | O \rangle}{(E_M - E_O)^2} + 2\hbar^2 \sum_{M \neq O} \frac{\langle O | (\partial / \partial \beta_i)_{\text{occup.prob}} | M \rangle \langle M | (\partial / \partial \beta_j)_{\text{occup.prob}} | O \rangle}{(E_M - E_O)^2} \]

where \( (\partial / \partial \beta_i)_{\text{wave func}} \) and \( (\partial / \partial \beta_i)_{\text{occup.prob}} \) have already defined in the appendix [III]

In the independent-particle approximation, we have in the second quantization representation:

\[ \partial H / \partial \beta_i = \sum_{\mu} \langle \nu | \partial H_{sp} / \partial \beta_i | \mu \rangle a^+_\mu a^\mu \]

After similar calculations than the ones performed in the appendix [III] we find

\[ I_1 = \langle k, -l | (\partial / \partial \beta_i)_{\text{wave func}} | BCS \rangle = -(u_k v_l + u_l v_k) \langle k | \partial H_{sp} / \partial \beta_i | l \rangle \quad k \neq l \]

therefore, the first part of the r.h.s of the above formula reads (the second remains unchanged):

\[ 2\hbar^2 \sum_{M \neq O} \frac{\langle O | (\partial / \partial \beta_i)_{\text{wave}} | M \rangle \langle M | (\partial / \partial \beta_j)_{\text{wave}} | O \rangle}{(E_M - E_O)^2} = 2\hbar^2 \sum_{k,l} \frac{(u_k v_l + u_l v_k)^2}{(E_k + E_l)^3} \langle l | \partial H_{sp} / \partial \beta_j | k \rangle \langle k | \partial H_{sp} / \partial \beta_j | l \rangle (1 - \delta_{k,l}) \]

Then we obtain for the cranking formula:

\[ D_{ij} \{ \beta_1, ..., \beta_n \} = 2\hbar^2 \sum_{k,l} \frac{(u_k v_l + u_l v_k)^2}{(E_k + E_l)^3} \langle l | \partial H_{sp} / \partial \beta_j | k \rangle \langle k | \partial H_{sp} / \partial \beta_j | l \rangle (1 - \delta_{k,l}) + 2\hbar^2 \sum_k \frac{1}{2E_k} \frac{1}{v_k} \frac{\partial u_k}{\partial \beta_i} \frac{\partial u_k}{\partial \beta_j} \quad (C1) \]

Appendix D: Final version of the cranking formula

\[ \sum_{k} \frac{1}{2E_k} \frac{1}{v_k} \frac{\partial u_k}{\partial \beta_i} \frac{\partial u_k}{\partial \beta_j} \]
meet in the above formula can be further clarified. Recalling that:
\[ u_k = \frac{1}{\sqrt{2}} \left( 1 + \frac{e_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{1/2} \]
and
\[ v_k = \frac{1}{\sqrt{2}} \left( 1 - \frac{e_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{1/2} \]
where \( \varepsilon_k = \epsilon_k - \lambda \) is the single-particle energy with respect to the Fermi level and assuming for the moment that the deformation dependence appears through \( \epsilon_k, \Delta, \) and \( \lambda, \) we have to evaluate \( \frac{\partial u_k}{\partial \beta_k} = \frac{\partial u_k}{\partial \epsilon_k} \frac{\partial \epsilon_k}{\partial \beta_k} + \frac{\partial u_k}{\partial \Delta} \frac{\partial \Delta}{\partial \beta_k} + \frac{\partial u_k}{\partial \lambda} \frac{\partial \lambda}{\partial \beta_k}. \) Thus, a simple differentiation of \( u_k \) with respect to \( \beta_k \) leads to:
\[ \frac{\partial u_k}{\partial \beta_k} = \frac{1}{2^{1/2}} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{-1/2} \left[ \frac{\partial \varepsilon_k}{\partial \beta_k} \left( \varepsilon_k^2 + \Delta^2 \right)^{-1/2} - \varepsilon_k \left( \varepsilon_k^2 + \Delta^2 \right)^{-3/2} \left( \varepsilon_k \frac{\partial \varepsilon_k}{\partial \beta_k} + \Delta \frac{\partial \Delta}{\partial \beta_k} \right) \right] \]
multiplying by \( u_k^{-1} \) and simplifying we get:
\[ v_k^{-1} \frac{\partial u_k}{\partial \beta_k} = \frac{1}{2^{1/2}} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{-1/2} \left\{ \Delta \frac{\partial \varepsilon_k}{\partial \beta_k} - \varepsilon_k \frac{\partial \Delta}{\partial \beta_k} \right\} \]
using \( \varepsilon_k = \varepsilon_k - \lambda \), we obtain:
\[ v_k^{-1} \frac{\partial u_k}{\partial \beta_k} = \frac{1}{2^{1/2}} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{-1/2} \left\{ \Delta \frac{\partial \varepsilon_k}{\partial \beta_k} - \varepsilon_k \frac{\partial \Delta}{\partial \beta_k} - (\varepsilon_k - \lambda) \frac{\partial \lambda}{\partial \beta_k} \right\} \]
Moreover, noting that:
\[ \frac{\partial u_k}{\partial \beta_k} = \langle k | \frac{\partial H_{sp}}{\partial \beta_k} | k \rangle \]
we find:
\[ v_k^{-1} \frac{\partial u_k}{\partial \beta_k} = \frac{1}{2^{1/2}} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} \right)^{-1/2} \left\{ \Delta \langle k | \frac{\partial H_{sp}}{\partial \beta_k} | k \rangle - \Delta \frac{\partial \lambda}{\partial \beta_k} - (\varepsilon_k - \lambda) \frac{\partial \lambda}{\partial \beta_k} \right\} \]
the quasiparticle energy is \( E_k = (\varepsilon_k^2 + \Delta^2)^{1/2} \) so that:
\[ v_k^{-1} \frac{\partial u_k}{\partial \beta_k} = \frac{1}{2 E_k} \left\{ \Delta \langle k | \frac{\partial H_{sp}}{\partial \beta_k} | k \rangle - \Delta \frac{\partial \lambda}{\partial \beta_k} - (\varepsilon_k - \lambda) \frac{\partial \lambda}{\partial \beta_k} \right\} \]
putting:
\[ R_k^i = - \langle k | \frac{\partial H_{sp}}{\partial \beta_k} | i \rangle + \frac{\partial \lambda}{\partial \beta_k} + \frac{i(\varepsilon_k - \lambda)}{\Delta} \frac{\partial \Delta}{\partial \beta_k} \]
the product of the similar terms gives finally:
\[ I_2 = \sum_k \frac{1}{2 E_k} \frac{1}{v_k} \frac{1}{u_k} \frac{1}{u_k} = \sum_k \frac{1}{2 E_k} \frac{\Delta R_k^i}{2 E_k} \frac{R_k^i}{2 E_k} \]
The cranking formula of the mass parameters becomes therefore:
\[ D_{ij} \{ \beta_1, \ldots, \beta_n \} = 2h^2 \sum_{k,j} \frac{(u_k u_l + u_l u_k)^2}{(E_k + E_l)^3} \left| l \right| \frac{\partial H_{sp}}{\partial \beta_i} \left| k \right| \frac{\partial H_{sp}}{\partial \beta_j} \left| l \right| (1 - \delta_{k,l}) + 2h^2 \sum_k \frac{\Delta^2}{8 E_k} R_k^i R_k^j \]