THE MASS PARAMETER IN THE GENERATOR COORDINATE METHOD

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Abstract: The collective kinetic energy for the fission mode is discussed in terms of the generator coordinate method. A comparison of the GCM mass formula with the cranking result and the result of the adiabatic time-dependent Hartree–Fock theory is established and the zero-point energies obtained in the GCM are examined in some detail. A numerical pilot study on the basis of a two-center shell model with pairing serves as an illustration of the general discussion.

1. Introduction

The description of collective phenomena in microscopic terms has been a challenge in the development of theoretical nuclear physics. There are essentially two microscopic approaches in use. On one side, we have time-dependent methods such as the cranking model¹⁾ and the adiabatic time-dependent Hartree–Fock (ATDHF) theory^{2,3)}. These lead to a classical collective hamiltonian, for which a requantization procedure is required. The reason for the partial loss of quantal aspects in ATDHF is the restriction to determinantal wave functions and the consequent non-linearity of the theory. On the other side, we have as a time-independent approach the generator coordinate method (GCM)⁴⁾ which leads to a quantal collective hamiltonian. In the GCM the superposition principle of quantum mechanics is incorporated and requantization is not needed.

In recent years the GCM has been the subject of renewed interest, in particular for the study of large amplitude collective motion (vibrations of soft nuclei, fission, heavy ion collisions)^{5–9)}. In the present paper we intend to investigate the collective mass parameter of the fission process in the context of the GCM.

Our knowledge of dynamical aspects of the fission process has greatly increased with the calculation of potential barriers with the aid of the shell correction method, but a comparable understanding of the mass parameter is still lacking. The cranking prescription is the only microscopic method that has been used so far for the calculation of mass parameters in fission¹⁰⁾, but a number of inconsistencies^{11,12)} have been discussed in connection with this approximation.

Notwithstanding the fact that the ATDHF theory does not lead directly to a quantal, collective picture, there is evidence that it provides a reasonable description

of collective masses. The correct translational mass is obtained on the basis of galilean invariance. The situation is more involved for vibration and fission modes as the calculation of the fully self-consistent inertial parameters presents a formidable task. In addition, experimental information about the mass parameter is for that case only indirect. One usually restricts the discussion to mass parameters obtained in low-order iterations²⁾ or to the Inglis cranking formula, which involves further approximations.

The full benefit of the GCM formulation can not be utilized for systems with a large number of particles. The normal approach applied in this situation is the gaussian overlap approximation (GOA). We will rely on this approximation and then face the task of establishing a relation between the GCM mass obtained in this fashion with the result obtained in ATDHF.

A detailed comparison of the inertial parameter in the GCM and the ATDHF is presented in sect. 2. We examine the general structure of the GCM mass and compare it to the cranking formula. The conclusion is: the single-particle limit of the GCM mass cannot exceed the cranking value. The general expressions for the ATDHF and the GCM masses can be compared at the minimum point of the potential energy. At this point the GCM mass cannot exceed the ATDHF value, in conformity with the result obtained in the single-particle picture. An upper limit for the difference between the two masses is explicitly given.

In sect. 3 we investigate the kinetic and potential zero-point energies (ZPE), which arise naturally in the GCM formulation. Evaluating the kinetic ZPE either with the GCM mass or with the ATDHF mass and comparing it with the potential ZPE, we conclude that the potential ZPE should not be disregarded.

Finally in sect. 4 we present a numerical pilot study for the calculation of the GCM mass parameter and kinetic ZPE for the fission process on the basis of a simple two-center shell-model (TCSM) hamiltonian plus pairing in the BCS approximation. We investigate the difference between the cranking and GCM masses, as well as the effects of the residual interaction, which remains after the transformation to quasi-particles, on the GCM mass. Although these residual contributions are not found to be very important for the situation considered, they enlarge the difference between the cranking and GCM results. The GCM kinetic ZPE is calculated with and without the effect of residual forces and it is compared to the cranking kinetic ZPE and to the potential ZPE.

2. The GCM mass parameter

2.1. DERIVATION OF THE GCM MASS PARAMETER

The GCM ansatz for an eigenstate of a system described by a many-body hamiltonian H relies on the specification of a collective subspace $\{|q\rangle\}$, which takes account of the physical situation by a suitable parametrization. Subjecting the linear

superposition of states

$$|\psi\rangle = \int dq f(q)|q\rangle \quad (1)$$

to the time-independent variational procedure, one obtains the so-called Griffin–Hill–Wheeler equation

$$\int dq' (\langle q|H|q'\rangle - E\langle q|q'\rangle)f(q') = 0. \quad (2)$$

For simplicity we consider only one real parameter q , which describes the “deformation” of the system.

For large systems a direct numerical solution of the integral eq. (2) is not feasible, but in this case the GOA

$$\langle q|q'\rangle = \exp\left[-\frac{1}{2}\langle q|P^2|q\rangle(q-q')^2\right], \quad P \equiv i\frac{\partial}{\partial q}, \quad (3)$$

is supposed to provide an adequate description and offers the distinct advantage of further analytical treatment. The GOA corresponds to the adiabaticity assumption of ATHDF: both are valid for systems with a large number of particles, which present a well-developed collective behaviour.

With the GOA, the integral eq. (2) is transformed into a second-order differential equation of the form of a collective Schrödinger equation, in which the mass parameter and the potential energy can be identified. We only quote the final result as the derivation can be found in standard references ¹³⁾

$$H_C g(q) = E g(q), \quad (4)$$

with

$$H_C = \frac{1}{2} P M_{\text{GCM}}^{-1}(q) P + V(q), \quad (4a)$$

$$M_{\text{GCM}}^{-1}(q) = \frac{\langle\{P, \{\bar{H}, P\}\rangle}{4\langle P^2 \rangle^2}, \quad \bar{H} = H - \langle H \rangle, \quad (4b)$$

$$V(q) = \langle H \rangle - \frac{\langle P^2 \rangle}{2M_{\text{GCM}}(q)} - \frac{1}{8\langle P^2 \rangle} \frac{d^2}{dq^2} \langle H \rangle. \quad (4c)$$

All expectation values are to be taken with respect to the generating states $|q\rangle$. The inverse mass parameter is proportional to a double anticommutator and the potential energy includes, beyond the classical term $\langle H \rangle$, the kinetic and potential ZPE's. It is assumed that $\langle P^2 \rangle$ is a constant but corrections due to the q -dependence of $\langle P^2 \rangle$ can be considered ¹⁴⁾.

The collective wave function $g(q)$ is related to the weight function of the GCM ansatz by

$$g(q) = \left(\frac{2\pi}{\langle P^2 \rangle}\right)^{1/4} \exp\left(-\frac{1}{4\langle P^2 \rangle} P^2\right) f(q). \quad (4d)$$

It is normalized to unity, so that $|g(q)|^2$ can be interpreted as a probability density. By contrast, the formulation presented in ref. ⁵⁾ considers a differential equation for $f(q)$ and identifies the collective mass parameter on this basis. The GCM mass parameter obtained in this fashion turns out to be too small.

In order to stress possible similarities with the ATDHF formulation we present an alternative derivation of the GCM mass formula based on a complex parametrization of the trial states. A time-even many-body state $|q\rangle$, usually assumed to be a Slater determinant or a state of the HFB type, can be written as a Taylor series with respect to a reference state $|0\rangle$:

$$|q\rangle = \sum_n \frac{1}{n!} (P^n |q\rangle)_{q=0} (-iq)^n \equiv e^{-iqP} |0\rangle. \quad (5)$$

The collective path is specified by the collective momentum operator P :

$$|q + \delta q\rangle = (1 - i \delta q P) |q\rangle.$$

In order to obtain a path along Slater determinants (or HFB) states, P is required to be a one-body operator. It can be restricted to have only a particle-hole component, as particle-particle and hole-hole components merely lead to a change of phase. For real values of the collective coordinate q and for hermitean, time-odd operators P , the transformation (5) preserves the norm and the time-reversal parity: the state $|q\rangle$ will be normalized and time-even, if the reference state $|0\rangle$ has these properties.

This is in contrast to the statement, that a time-dependent state representing a dynamical situation must develop a time-odd component. There are basically two possibilities of satisfying this requirement with the ansatz (5):

- (i) One performs a second transformation

$$|qp\rangle = e^{ipQ} |q\rangle, \quad (6)$$

where p is real and Q a time-even, hermitean operator. This transformation is the basis of the ATDHF theory ^{2,3)}.

- (ii) One allows q to become complex

$$|qq'\rangle = e^{-i(q+iq')P} |0\rangle = e^{q'P} |q\rangle. \quad (7)$$

This procedure corresponds to the time-dependent GCM method ¹⁵⁾. The transformation (7) is, in contrast to the transformation (6), not unitary and renormalization is required.

Evaluating the expectation value of the microscopic hamiltonian up to second order in p with the ansatz (6) one obtains

$$\mathcal{H}_{\text{ATDHF}}(q, p) = \langle qp | H | qp \rangle = \langle q | H | q \rangle + \frac{1}{2} p^2 \langle q | [Q, [H, Q]] | q \rangle. \quad (8)$$

The expectation value of the operator P is

$$\langle qp | P | qp \rangle = -ip \langle q | [Q, P] | q \rangle = p. \quad (9)$$

The parameter p can, in view of the weak commutation relation imposed on Q and P , be identified with the collective momentum.

On the other hand, one obtains with the transformation (7) up to second order in q'

$$\begin{aligned}\mathcal{H}_{\text{GCM}}(q, q') &= \frac{\langle qq'|H|qq'\rangle}{\langle qq'|qq'\rangle} = \frac{\langle q|H|q\rangle + \frac{1}{2}q'^2\langle q|\{P, \{H, P\}\}|q\rangle}{1 + 2q'^2\langle q|P^2|q\rangle} \\ &= \langle q|H|q\rangle + \frac{1}{2}q'^2\langle q|\{P, \{\bar{H}, P\}\}|q\rangle.\end{aligned}\quad (10)$$

The expectation value of the operator P is in this case

$$\frac{\langle qq'|P|qq'\rangle}{\langle qq'|qq'\rangle} = 2q'\langle q|P^2|q\rangle = p, \quad (11)$$

indicating that the imaginary part of the collective variable times the factor $2\langle P^2\rangle$ is to be identified with the collective momentum. Using (11) in (10) one obtains for the classical collective hamiltonian in the GCM

$$\mathcal{H}_{\text{GCM}}(q, q') = \mathcal{H}_{\text{GCM}}(q, p) = \langle q|H|q\rangle + \frac{p^2}{2} \frac{\langle q|\{P, \{\bar{H}, P\}\}|q\rangle}{4\langle q|P^2|q\rangle^2}, \quad (12)$$

which differs from the classical limit of (4a–c) by the absence of ZPE's. In agreement with eq. (4b), the mass parameter

$$M_{\text{GCM}}^{-1}(q) = \frac{\partial^2}{\partial p^2} \mathcal{H}_{\text{GCM}}(q, p) = \frac{\langle q|\{P, \{\bar{H}, P\}\}|q\rangle}{4\langle q|P^2|q\rangle^2}$$

can be extracted. The truncation of the GCM representation of the classical collective hamiltonian is justified, if the imaginary part of the complex generator coordinate is small:

$$|q'| \ll 1$$

or, with (11),

$$|p| \ll 2\langle P^2\rangle. \quad (13)$$

This condition (adiabatic condition) can be supposed to hold for systems with a sufficiently large number of particles.

2.2. COMPARISON WITH THE INGLIS FORMULA

The inverse GCM mass parameter can be decomposed into two parts

$$M_{\text{GCM}}^{-1}(q) = \frac{\langle P\bar{H}P\rangle}{2\langle P^2\rangle^2} + \frac{\langle \bar{H}P^2\rangle}{2\langle P^2\rangle^2}. \quad (14)$$

The first term is proportional to an excitation energy due to the “translation” of

the state in collective space, the second term is proportional to the correlation coefficient of the operators H and P^2 :

$$\langle \bar{H}P^2 \rangle = \langle \bar{H}\bar{P}^2 \rangle = \langle (H - \langle H \rangle)(P^2 - \langle P^2 \rangle) \rangle.$$

The correlation contribution is related to the energy spread of the generating states. An upper limit of this quantity can be readily established using the Schwartz inequality

$$|\langle \bar{H}P^2 \rangle|^2 = |\langle \bar{H}\bar{P}^2 \rangle|^2 \leq \langle \bar{H}^2 \rangle \langle \bar{P}^2{}^2 \rangle$$

and the relations (valid in the GOA)

$$\begin{aligned} \langle P^4 \rangle &= 3\langle P^2 \rangle^2, \\ \langle \bar{P}^2{}^2 \rangle &= \langle P^4 \rangle - \langle P^2 \rangle^2 = 2\langle P^2 \rangle^2. \end{aligned}$$

One arrives at

$$\left| \frac{\langle \bar{H}P^2 \rangle}{2\langle P^2 \rangle^2} \right| \leq \left(\frac{\langle \bar{H}^2 \rangle}{2\langle P^2 \rangle^2} \right)^{1/2}. \quad (15)$$

If P is a generator of symmetries of the hamiltonian

$$[P, H] = 0$$

the excitation term is equal to the correlation term and one recovers the well-known Peierls–Yoccoz formula ¹⁶⁾

$$M_{\text{GCM}}^{-1}(q) = \frac{\langle P\bar{H}P \rangle}{\langle P^2 \rangle^2} = \frac{\langle \bar{H}P^2 \rangle}{\langle P^2 \rangle^2} = M_{\text{PY}}^{-1}(q), \quad (16)$$

which is valid for translations and rotations.

For other collective modes, such as vibrations or fission, the equality of the two contributions does not hold. One expects the excitation term to dominate over the correlation term if the energy spread is small, i.e. if the generating state is a reasonable approximation of an eigenstate of H .

We first compare the GCM result with the Inglis cranking approximation, which incorporates a single-particle shell-model picture. In the case of vibrations or fission the shell-model hamiltonian and consequently the corresponding eigenvalues and eigenstates depend explicitly on the collective parameter

$$H_{\text{SM}}|n, q\rangle = e_n(q)|n, q\rangle.$$

The corresponding mass parameter is ¹¹⁾

$$M_{\text{C}}(q) = 2 \sum_n \frac{|\langle n, q|P|0, q\rangle|^2}{e_n(q) - e_0(q)} = 2\langle 0, q|P\bar{H}_{\text{SM}}^{-1}P|0, q\rangle$$

or, with the identification $|q\rangle \equiv |0, q\rangle$,

$$= 2\langle q|P\bar{H}_{\text{SM}}^{-1}P|q\rangle. \quad (17)$$

If one uses a corresponding approximation for the calculation of the GCM mass parameter for vibration and fission, i.e. if one replaces in eq. (14) the “true” hamiltonian H by an effective shell-model hamiltonian H_{SM} , one finds that the correlation contribution vanishes. The remaining excitation contribution

$$M_{\text{E}}^{-1}(q) = \frac{\langle q | P \bar{H}_{\text{SM}} P | q \rangle}{2 \langle P^2 \rangle^2} \quad (18)$$

can be compared directly to the cranking result (17). With the aid of Schwartz’s inequality one finds

$$M_{\text{E}}^{-1}(q) M_{\text{C}}(q) = \frac{\langle P \bar{H}_{\text{SM}} P \rangle \langle P \bar{H}_{\text{SM}}^{-1} P \rangle}{\langle P^2 \rangle^2} \geq \frac{|\langle P \bar{H}_{\text{SM}} \bar{H}_{\text{SM}}^{-1} P \rangle|^2}{\langle P^2 \rangle^2} = 1$$

and therefore

$$M_{\text{E}}(q) \leq M_{\text{C}}(q). \quad (19)$$

The shell-model approximation of the GCM mass can not be larger than the cranking mass. The equality is obtained if $P|q\rangle$ is an eigenstate of the shell-model hamiltonian.

In terms of the shell-model moments

$$m_k(F) = \sum_n |\langle m | F | 0 \rangle|^2 (e_n - e_0)^k, \quad k = 0, \pm 1, \dots \quad (20)$$

the cranking and the appropriate GCM expressions take the form

$$M_{\text{C}} = 2m_{-1}(P), \quad (21)$$

$$M_{\text{E}} = \frac{2(m_0(P))^2}{m_1(P)} \quad (22)$$

and the inequality (19) can be written as

$$m_1(P) m_{-1}(P) \geq (m_0(P))^2. \quad (23)$$

2.3. COMPARISON WITH THE ATDHF RESULT

In the discussion of ATDHF we will use the formalism of Villars based on state vectors²⁾ rather than the closely related formalism of Baranger and Veneroni in terms of the density matrix³⁾.

For comparison of the GCM mass parameter with the ATDHF result we note that the mass parameter extracted from eq. (8),

$$M_{\text{ATDHF}}^{-1}(q) = \langle q | [Q, [H, Q]] | q \rangle, \quad (24)$$

can be written in matrix form as

$$= (Q^* - Q) S \begin{pmatrix} Q \\ -Q^* \end{pmatrix} = (Q^* \quad Q) \mathcal{M}^{-1} \begin{pmatrix} Q \\ Q^* \end{pmatrix}$$

$$\mathcal{M}^{-1} = \eta S \eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix}.$$

The operator Q and the states $|q\rangle$ should satisfy the ATDHF equations. One of these equations is a CHF (constrained Hartree-Fock) equation where Q is the constraining operator. The other can be written in the form

$$-iM_{\text{ATDHF}}^{-1}(q) \begin{pmatrix} P \\ -P^* \end{pmatrix} = \mathcal{M}^{-1} \begin{pmatrix} Q \\ Q^* \end{pmatrix}.$$

Using the weak commutation between Q and P we obtain from there the following expression for the ATDHF mass

$$M_{\text{ATDHF}}(q) = \begin{pmatrix} P^* & P \end{pmatrix} S^{-1} \begin{pmatrix} P \\ P^* \end{pmatrix}. \quad (25)$$

The expressions (24) and (25) are equivalent for self-consistent solutions, i.e. for optimized states $|q\rangle$ and operators Q and P .

The mass parameter (4b) of the GCM formulation can be written in matrix form as

$$M_{\text{GCM}}^{-1}(q) = \frac{1}{4\langle P^2 \rangle^2} \begin{pmatrix} P^* & P \end{pmatrix} S \begin{pmatrix} P \\ P^* \end{pmatrix} = \frac{1}{4\langle P^2 \rangle^2} \begin{pmatrix} P^* & -P \end{pmatrix} \mathcal{M}^{-1} \begin{pmatrix} P \\ -P^* \end{pmatrix}. \quad (26)$$

The excitation term is determined by the submatrix A , while the correlation term depends on the submatrix B of S .

From the following theorem about quadratic forms¹⁷⁾

$$(x, x)^2 \leq (x, Sx)(x, S^{-1}x) \leq \frac{1}{4} \frac{(\mu_1 + \mu_N)^2}{\mu_1 \mu_N} (x, x)^2, \quad (27)$$

which holds for any positive definite hermitean matrix S , which has μ_1 and μ_N respectively as the highest and the lowest eigenvalues, and from (25) and (26) we conclude that

$$1 \leq M_{\text{GCM}}^{-1}(q_{\text{st}}) M_{\text{ATDHF}}(q_{\text{st}}) \leq \frac{1}{4} \frac{(\mu_1 + \mu_N)^2}{\mu_1 \mu_N}, \quad (28)$$

where q_{st} labels the static point, for which the stability matrix S is positive definite. The first inequality in (27) is a trivial consequence of the Schwartz inequality and the second is a formulation of the so-called Kantorovich inequality.

The first inequality in (28)

$$M_{\text{GCM}}(q_{\text{st}}) \leq M_{\text{ATDHF}}(q_{\text{st}}) \quad (29)$$

is similar to the inequality (19) of the single-particle picture (note however that

(19) is valid for all the deformations, while (29) is restricted to $q = q_{\text{st}}$. The fact that the GCM mass can not exceed the ATDHF mass, at the static point, has been indicated before in a different fashion¹⁸⁾. Equality is obtained if the column vector formed with the particle-hole matrix elements of P is an eigenvector of S .

An intuitive way to convince oneself of the validity of (29) is to observe that the eq. (25) follows from a variational principle to determine the best time-odd part of the ansatz wave function (6), whereas in the time-dependent GCM there is no such variational procedure. The classical GCM energy (12) has therefore the ATDHF energy (8) as a lower bound and the GCM mass has the ATDHF mass as an upper bound, for $q = q_{\text{st}}$.

The second inequality in (28)

$$\left| \frac{M_{\text{ATDHF}} - M_{\text{GCM}}}{M_{\text{ATDHF}}} \right|_{q=q_{\text{st}}} \leq \left(\frac{\mu_1 - \mu_N}{\mu_1 + \mu_N} \right)^2 \quad (30)$$

establishes a maximal value for the difference between the ATDHF and the GCM masses. It has also a correspondent in the single-particle picture, in which the matrix S is diagonal, its matrix elements being the particle-hole excitation energies. We can write for all q 's

$$\left| \frac{M_C - M_E}{M_C} \right|_q \leq \left(\frac{e_1 - e_N}{e_1 + e_N - 2e_0} \right)^2. \quad (31)$$

For the point $q = q_{\text{st}}$ sum rules expressions for the ATDHF mass are feasible but this is not the case for the GCM mass. Since we aim for a unified view of the various expressions for the adiabatic mass parameter at the static point, we will express the ATDHF result in terms of RPA moments.

With F , a one-body hermitean operator, the sum rules can be cast in the following form¹³⁾

$$(F^* \quad F)(\eta S)^k \eta \begin{pmatrix} F \\ F^* \end{pmatrix} = 2m_k(F), \quad k = \pm 1, \pm 3, \dots, \quad (32a)$$

with the RPA moments

$$m_k(F) = \sum_n |\langle n | F | 0 \rangle|^2 (E_n - E_0)^k. \quad (32b)$$

The moments satisfy the inequalities

$$m_{k+2}(F)m_k(F) \geq (m_{k+1}(F))^2, \quad k = 0, \pm 1, \pm 2, \dots, \quad (32c)$$

under the condition that we are at the minimum point of the potential energy, for which S is positive definite and the RPA frequencies are real.

For the ATDHF mass two specific relations to RPA moments can be established. First, we apply the normal energy-weighted sum rule directly to (24) and obtain

$$M_{\text{ATDHF}}(q_{\text{st}}) = \frac{1}{2m_1(Q)}. \quad (33)$$

On the other hand, the application of the inverse energy-weighted sum rule to (25) gives

$$M_{\text{ATDHF}}(q_{\text{st}}) = 2m_{-1}(P). \quad (34)$$

This expression has the same structure as the cranking formula (21) but differs from it in the use of a CHF procedure instead of a shell model for the path and the RPA for the matrix elements and energies instead of the uncorrelated picture. It is equal to the so-called constrained RPA mass¹⁹⁾.

For self-consistent solutions (33) is identical to (34):

$$m_1(Q)m_{-1}(P) = \frac{1}{4}. \quad (35)$$

For non self-consistent solutions (33) differs from (34). In an ATDHF calculation one starts with a local operator Q_0 (the quadrupole operator, for quadrupole motion and fission), which is inserted as a constraint in the CHF equation. One obtains as first approximation to the full ATDHF problem the hydrodynamical irrotational mass

$$M_{\text{ATDHF}}^{(0)}(q_{\text{st}}) = \left[(Q_0^* \quad -Q_0) S \begin{pmatrix} Q_0 \\ -Q_0^* \end{pmatrix} \right]^{-1} = \frac{1}{2m_1(Q_0)} \quad (36)$$

and the self-consistent cranking mass

$$M_{\text{ATDHF}}^{(1)}(q_{\text{st}}) = (P_0^* \quad P_0) S^{-1} \begin{pmatrix} P_0 \\ P_0^* \end{pmatrix} = 2m_{-1}(P_0), \quad (37)$$

where P_0 is the momentum conjugate to Q_0 . Expressions (36) and (37) may be called respectively the zero- and first-order iterations for the ATDHF mass²⁾. In the literature [see for instance ref.¹⁸⁾], the name of ATDHF mass is also used for expression (37), although no optimized path is considered.

With the inequality¹⁷⁾

$$|(x, y)|^2 \leq (x, Sx)(y, S^{-1}y), \quad (38)$$

which holds for any positive definite hermitean matrix S , the weak commutation between Q_0 and P_0 , and eqs. (36) and (37) we conclude that

$$M_{\text{ATDHF}}^{(0)}(q_{\text{st}}) \leq M_{\text{ATDHF}}^{(1)}(q_{\text{st}}). \quad (39)$$

The hydrodynamical mass can not exceed the self-consistent cranking mass at the static point. The inequality (39) can be rewritten as

$$m_1(Q_0)m_{-1}(P_0) \geq \frac{1}{4}, \quad (40)$$

which resembles an energy-weighted uncertainty relation. We see from (35) that the self-consistent solutions of ATDHF minimize this uncertainty.

The usual Heisenberg uncertainty relation can be written as

$$m_0(Q)m_0(P) \geq \frac{1}{4}. \quad (41)$$

Equality occurs for the so-called coherent states. It was pointed out in ref. ⁷⁾ that for the coherent states the mass expressions (4b) and (24) agree. We show here that at the static point the association of ATDHF solutions with coherent states requires exact exhaustion of sum rules in Q and P by one excited state.

We note finally that the expression (37) can be reformulated in terms of moments of the operator Q_0 . Using the fact that the RPA states involved in (37) are approximate eigenstates of the operator $H - \lambda Q_0$ for the minimum point $\lambda = d/dq\langle H \rangle = 0$, one obtains

$$\begin{aligned} M_{\text{ATDHF}}^{(1)}(\lambda = 0) &= 2m_{-1} \left(i \frac{\partial}{\partial \lambda} \right) = 2 \sum_n \frac{\left| \langle n | \frac{\partial}{\partial \lambda} | 0 \rangle \right|^2}{E_n - E_0} \\ &= 2 \sum_n \frac{|\langle n | Q_0 | 0 \rangle|^2}{(E_n - E_0)^3} = 2m_{-3}(Q_0). \end{aligned}$$

Considering that the coordinate q corresponds to the expectation value of the operator Q_0 , one finds with the aid of the dielectric theorem

$$m_{-1}(Q) = \frac{1}{2} \frac{\partial^2}{\partial \lambda^2} \langle H \rangle \Big|_{\lambda=0} = \frac{1}{2} \frac{\partial}{\partial \lambda} \langle Q \rangle \Big|_{\lambda=0}$$

the final form

$$M_{\text{ATDHF}}^{(1)}(q_{\text{st}}) = M_{\text{ATDHF}}^{(1)}(\lambda = 0) \left(\frac{\partial \lambda}{\partial q} \right)^2 \Big|_{\lambda=0} = \frac{m_{-3}(Q_0)}{2(m_{-1}(Q_0))^2}. \quad (42)$$

The expression (42) can be compared in a straightforward fashion with (36) using the sum rules inequalities (32c) and the result agrees with (39). The order of magnitude of the difference between the two ATDHF iterations was investigated in ref. ²⁰⁾ using Skyrme forces.

The inequality (29) is valid for any parametrization of the states, and the states need not to be optimized. Thus the GCM mass, with CHF states using the constraint Q_0 , cannot exceed the self-consistent cranking mass (37) at the static point. But a direct analytical comparison of the GCM mass with the hydrodynamical irrotational mass seems not feasible and the difference between the two should be investigated in cases of practical interest.

3. GCM kinetic and potential zero-point energies

The necessity for ZPE corrections of the collective potential has been discussed widely in the literature on fission and heavy ion reactions ⁶⁻⁹⁾. Kinetic as well as potential ZPE's arise naturally in the GOA limit of the GCM [see eq. (4c)].

Usually, only the kinetic ZPE with the cranking mass is treated. This part of the ZPE provides the link between the static and dynamical aspects of all types of

collective motion. For translations and rotations the potential ZPE vanishes, but for other collective modes such as vibrations and fission it does exist and its order of magnitude should be investigated. In the following we give a general interpretation of the total ZPE and point out that the potential part is certainly of relevance for vibrational modes at the minimum point of the potential, assuming for the generating states CHF solutions of a many-body hamiltonian H .

As the kinetic ZPE is proportional to a double anticommutator

$$E_{\text{KZPE}}^{\text{GCM}}(q) = \frac{\langle P^2 \rangle}{2M_{\text{GCM}}(q)} = \frac{1}{4\langle P^2 \rangle} (\langle P\bar{H}P \rangle + \langle \bar{H}P^2 \rangle) \quad (43)$$

and the potential ZPE is proportional to a double commutator

$$E_{\text{PZPE}}(q) = \frac{1}{8\langle P^2 \rangle} \frac{d^2}{dq^2} \langle H \rangle = \frac{1}{4\langle P^2 \rangle} (\langle P\bar{H}P \rangle - \langle \bar{H}P^2 \rangle) \quad (44)$$

(note that H in eq. (44) can not be replaced by a q -dependent shell-model hamiltonian) the total ZPE is simply one half of the excitation energy

$$E_{\text{ZPE}}(q) = E_{\text{KZPE}}^{\text{GCM}}(q) + E_{\text{PZPE}}(q) = \frac{1}{2} \frac{\langle P\bar{H}P \rangle}{\langle P^2 \rangle}. \quad (45)$$

This result, which has been obtained without reference to a small amplitude limit, is a generalization of the corresponding statement for the quantum-mechanical harmonic oscillator.

The difference between the two GCM ZPE's is one half of the "correlation energy"

$$E_{\text{KZPE}}^{\text{GCM}}(q) - E_{\text{PZPE}}(q) = \frac{1}{2} \frac{\langle \bar{H}P^2 \rangle}{\langle P^2 \rangle}. \quad (46)$$

The kinetic ZPE is larger (lower) than the potential ZPE for a positive (negative) correlation coefficient of H and P^2 . As we do not expect the correlation to be very large we can conclude approximate equipartition of the ZPE in kinetic and potential parts within the GCM framework (at least for $q = q_{\text{st}}$).

We can also consider the kinetic ZPE where the GCM mass is replaced by the ATDHF mass. In this case the interpretation given above for the total ZPE is not valid but a relation can be found, under certain conditions, between the two ZPE terms. Introducing RPA states instead of the HF states envisaged before, one obtains for $q = q_{\text{st}}$:

$$E_{\text{KZPE}}^{\text{ATDHF}}(q_{\text{st}}) = \frac{m_0(P)}{4m_{-1}(P)}, \quad (47)$$

$$E_{\text{PZPE}}(q_{\text{st}}) = \frac{m_1(P)}{4m_0(P)}, \quad (48)$$

which can be compared directly using (32c)

$$E_{\text{KZPE}}^{\text{ATDHF}}(q_{\text{st}}) \leq E_{\text{PZPE}}(q_{\text{st}}). \quad (49)$$

The potential ZPE is not smaller than the ATDHF kinetic ZPE. Equipartition occurs in the case of exhaustion of the strength of P in a single excited state.

4. Calculation of the GCM mass parameter and ZPE's in a model for fission

In the GCM we have a certain amount of freedom in the choice of the trial states and hence the selection of a suitable collective subspace. Shell-model states offer themselves because of their simplicity. For an initial, numerical investigation of the statements outlined in sects. 2 and 3 we investigate a TCSM²¹⁾ augmented by a residual pairing interaction

$$H = H_{\text{TCSM}} + V_{\text{P}}, \quad (50)$$

$$H_{\text{TCSM}} = \sum_{i>0} \varepsilon_i(z_0)(a_i^+ a_i + a_{-i}^+ a_{-i}), \quad (50a)$$

$$V_{\text{P}} = -G \sum_{i,j>0} a_j^+ a_{-j}^+ a_{-i} a_i, \quad (50b)$$

where z_0 is half the distance between the two oscillator wells. The TCSM is often invoked for the description of fission processes, since it incorporates the correct asymptotic limit. We will restrict ourselves to a simple symmetric version, without deformation of the fragments and no rounding at the barrier cusp. Furthermore the $l \cdot s$ and l^2 terms are replaced by $l_z s_z$ and l_z^2 . The constants are the same as those of ref.²¹⁾. Volume conservation is used for the determination of the oscillator frequency as a function of z_0 starting with $\hbar\omega(z_0=0) = 41A^{-1/3}$ MeV.

With the Bogolyubov-Valatin transformation we obtain from (50) the quasi-particle hamiltonian

$$H = H_{\text{TCSM(QP)}} + V_{\text{res}}. \quad (51)$$

Apart from an additive constant, the part conserving the number of quasi-particles is

$$H_{\text{TCSM(QP)}} = \sum_{i>0} E_i(z_0)(\alpha_i^+ \alpha_i + \beta_i^+ \beta_i), \quad (51a)$$

$$E_i(z_0) = [(\varepsilon_i(z_0) - \lambda)^2 + \Delta^2]^{1/2},$$

while the remainder,

$$V_{\text{res}} = H_{40} + H_{22} + H_{31}, \quad (51b)$$

contains terms with four-quasi-particle, two-quasi-particle and three-quasi-particle creation operators, respectively.

The BCS ground state of the hamiltonian (51a) is the obvious choice for the generating states

$$|q\rangle \equiv |z_0\rangle = \prod_{i>0} (u_i + v_i a_i^+ a_{-i}^+) | \rangle, \quad (52)$$

with

$$\begin{pmatrix} u_i \\ v_i \end{pmatrix} = \frac{1}{\sqrt{2}} \left(1 \pm \frac{\varepsilon_i - \lambda}{E_i} \right)^{1/2}.$$

The effect of the operator P on the states (52) can be expressed by ²²⁾

$$P|z_0\rangle = \sum_{j,k>0} i P_{jk}(z_0) a_j^+ \beta_k^+ |z_0\rangle \quad (53)$$

with

$$P_{jk}(z_0) = -\langle k | \frac{\partial H_{\text{TCSM}}}{\partial z_0} | j \rangle \frac{u_j v_k + u_k v_j}{E_j + E_k}, \quad j \neq k, \quad (54a)$$

$$P_{jj}(z_0) = -\frac{\Delta}{2E_i^2} \left(\langle j | \frac{\partial H_{\text{TCSM}}}{\partial z_0} | j \rangle - \frac{\partial \lambda}{\partial z_0} - \frac{\varepsilon_i - \lambda}{\Delta} \frac{\partial \Delta}{\partial z_0} \right). \quad (54b)$$

The effect of the residual interaction (51b), which remains after the transformation to quasi-particles, on the GCM mass is twofold. It modifies the excitation term (it is expected to be lowered) and it contributes to the correlation term. The correction to the excitation energy is due to H_{22} ; the correlation term is determined by H_{40} . A straightforward calculation leads to

$$\begin{aligned} \langle P \bar{H} P \rangle &= \sum_{j,k>0} P_{jk}^2 (E_j + E_k) - G \sum_{j,k>0} P_{jj} P_{kk} [(u_j u_k)^2 + (v_j v_k)^2] \\ &\quad - 2G \sum_{j,k>0} P_{jk}^2 u_j v_j u_k v_k, \\ \langle \bar{H} P^2 \rangle &= -4G \sum_{j,k>0} (P_{jj} P_{kk} - P_{kj} P_{jk}) [(u_j v_k)^2 + (u_k v_j)^2]. \end{aligned}$$

In the actual calculation we consider a system with $Z = 92$, $A = 236$. Such a system should be sufficiently heavy to insure the validity of the GOA [in ref. ⁶⁾ it has been shown directly that the overlap of BCS states constructed on the basis of the TCSM can be well represented by the GOA if the number of particles is larger than $A \approx 40$].

We have chosen the BCS parameters according to the formalism of ref. ²²⁾. The pairing strength is

$$G = [\bar{g}(\bar{\lambda}) \log(2\Omega/\bar{\Delta})]^{-1}$$

and the number of levels on either side of the Fermi state is

$$n = 2\bar{g}(\bar{\lambda})\Omega,$$

where $\Omega = 8 \text{ MeV}$, $\bar{\Delta} = 12 A^{-1/2} \text{ MeV}$ and $\bar{g}(\bar{\lambda})$ is the smooth pair density calculated at the Fermi energy. The values of $\bar{g}(\bar{\lambda})$ for neutrons and protons have been computed following the Strutinsky prescription, at the point $z_0 = 2 \text{ fm}$, giving the parameters:

$$G_n = \frac{20.61}{A}, \quad n_n = 60,$$

$$G_p = \frac{28.63}{A}, \quad n_p = 44.$$

The resulting pairing gap for neutrons and protons as a function of z_0 is shown in fig. 1. The neutron pairing gap goes to zero for large values of z_0 because there is a neutron shell closure for the model situation considered.

Fig. 1. The pairing gap for neutrons and protons as a function of the coordinate z_0 .

In fig. 2, we illustrate the excitation and correlation contributions to the inverse mass parameter according to eq. (14). The first contribution is clearly dominant. The excitation term is lowered slightly with respect to the pure shell-model value by the residual interaction (51b). For large separations both the excitation and the correlation contributions approach approximately constant values.

In fig. 3, we compare the GCM and the cranking masses. Both curves display a similar shell structure, but the GCM one is smoother. The minimum values of the two masses occur for the point $z_0 = 2 \text{ fm}$, which corresponds approximately to the minimum of the potential energy (this result was checked up by summation of the energies of the occupied single-particle states of H_{TCSM}). Just before the scission point $z_0 = 5.9 \text{ fm}$ there is a pronounced peak. For asymptotic separations the masses approach a value somewhat larger than the reduced mass $M_{z_0 z_0} = 236 m_p$, due to

Fig. 2. Excitation and correlation contributions to the GCM mass as a function of the coordinate z_0 .

the nonrealistic character of the model used. We remark that the coordinate z_0 of the TCSM can not be identified directly with the actual separation R of the centre of mass of the two nuclei, except for the asymptotic region. For smaller distances a suitable relation between R and z_0 could be established²³⁾.

For the present model [as for the Lipkin model²⁴⁾] the GCM mass is always smaller than the cranking mass. The difference amounts to 25% of the cranking mass, on the average, but can attain 48% (this maximal deviation occurs for the

Fig. 3. The mass parameter in the GCM in comparison with the cranking result, as a function of the coordinate z_0 .

static point). The GCM mass calculated without the effect of the residual force (42b) is already lower than the cranking result, in agreement with the inequality (19). In the single-particle picture the difference between the GCM and the cranking masses is, on the average, 20% and its particular values are in agreement with the inequality (31). The residual correction to the excitation energy and the correlation have opposite sign. The second is positive and as it is larger in magnitude leads to the decrease of the GCM mass.

Fig. 4. Zero-point energies: the kinetic ZPE in the GCM, with (—) and without (— · —) residual forces, and in the cranking model (---), as a function of the coordinate z_0 .

In fig. 4, we represent the GCM kinetic ZPE calculated with and without the effect of residual forces. For comparison we also show the kinetic ZPE using the cranking approximation for the mass. The difference between the GCM and the cranking kinetic ZPE is the same as the difference between the respective masses. The GCM kinetic ZPE without residual forces is larger than the cranking kinetic ZPE as already pointed out in ref. ⁶), in a numerical calculation for the lighter system $Z = 52$, $A = 112$, and the residual forces considered here enlarge the difference. The potential ZPE has been calculated at the static point through a simple numerical differentiation of the BCS ground state energy:

$$U = \sum_{i>0} (2v_i^2 \epsilon_i - Gv_i^4) - \frac{\Delta^2}{G} + E_{\text{Coul}},$$

with E_{Coul} being the Coulomb energy which we have evaluated classically. One obtains the value $E_{\text{PZPE}}(z_0 = 2 \text{ fm}) = 8. \text{ MeV}$, which is by far larger than the kinetic ZPE for the same mode. The discrepancy is exaggerated in relation to a more realistic scheme envisaged in sect. 3 because our model hamiltonian depends explicitly on the collective coordinate.

5. Conclusions

The discussion of the collective motion of a many-body system is usually split into three main parts:

- (i) The definition of the significant degrees of freedom.
- (ii) The extraction of a collective hamiltonian.
- (iii) The quantum-mechanical calculation of the dynamical behaviour of the system in the collective coordinates.

The approach to the first task is either based on phenomenological considerations (e.g. via the specification of a suitable shell model) or on variational techniques as CHF or ATDHF.

In this contribution we have concentrated on the second task, in particular on the question of finding an acceptable representation for the collective kinetic energy of the fission process. The basis of our discussion was the GCM in the GOA. We were able to show in general that:

(a) The GCM mass, evaluated with shell-model states and a shell-model hamiltonian, can not exceed the Inglis cranking formula.

(b) The GCM mass, evaluated with appropriate CHF states and a many-body hamiltonian, cannot exceed the ATDHF result at the static point of the potential energy. An upper limit for the difference between the two masses can be indicated.

We also discussed the question of ZPE's, concluding that the potential ZPE can not be neglected for vibration and fission modes.

In a first numerical application statement (a) has been checked in detail and the effect of including a simple two-body force was investigated. A next step would be the calculation of the GCM mass on the basis of the same shell-model generating states, but using a more complete microscopic hamiltonian.

In ref. ¹²⁾ it has been shown that the cranking mass with the inclusion of pairing in the BCS formalism appears to be too small by a factor of 2 to account for the experimental information about the vibrational energies. From our study we conclude that the GCM mass with the same approximations is even slightly lower than the cranking mass. Therefore either the approximations currently used in the calculation of adiabatic mass parameters are not adequate [e.g. see ref. ¹⁹⁾] or the assumption of adiabaticity of the vibrational motion should be questioned.

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References

- 1) D.R. Inglis, Phys. Rev. **96** (1954) 1059 and **103** (1956) 1786
- 2) F. Villars, Proc. Int. Conf. Nucl. on self-consistent fields, Trieste, 1975, ed. G. Ripka and M. Porneuf (North-Holland, Amsterdam, 1975) p. 3;
F. Villars, Nucl. Phys. **A285** (1977) 269

- 3) M. Baranger and M. Veneroni, *Ann. of Phys.* **114** (1978) 123
- 4) D.L. Hill and J.A. Wheeler, *Phys. Rev.* **89** (1953) 1102;
J.J. Griffin and J.A. Wheeler, *Phys. Rev.* **108** (1957) 311
- 5) P.K. Haff and L. Wilets, *Phys. Rev.* **C7** (1973) 951 and **C10** (1974) 353
- 6) P.G. Reinhard, *Nucl. Phys.* **A261** (1976) 291
- 7) K. Goeke and P.G. Reinhard, *Ann. of Phys.* **124** (1980) 249
- 8) J.F. Berger and D. Cogne, *Nucl. Phys.* **A333** (1980) 302
- 9) J.N. Urbano, K. Goeke and P.G. Reinhard, *Nucl. Phys.* **A370** (1981) 329
- 10) A. Sobiczewski, *Sov. Journ. Part. Nucl.* **10** (1979) 466
- 11) D.J. Rowe, *Nuclear collective motion* (Methuen, London, 1970) p. 125
- 12) J. Dudek, W. Dudek, E. Ruchowski and J. Salewski, *Z. Phys.* **A294** (1980) 341
- 13) P. Ring and P. Schuck, *The nuclear many-body problem* (Springer, New York, 1980) pp. 424 and 330
- 14) M.H. Caldeira and J.M. Domingos, *Progr. Theor. Phys.* **61** (1979) 1342
- 15) A. Alves *et al.*, *Progr. Theor. Phys.* **58** (1977) 223
- 16) R. Peierls and J. Yoccoz, *Proc. Phys. Soc.* **A70** (1957) 381;
J. Yoccoz, *Proc. Phys. Soc.* **A70** (1957) 388
- 17) R. Bellman and E.F. Beckenbach, *Inequalities* (Springer, Berlin, 1971), p. 69
- 18) K. Goeke, A.M. Lane and J. Martorell, *Nucl. Phys.* **A296** (1978) 109
- 19) M.K. Pal, O. Zawischa and J. Speth, *Z. Phys.* **A272** (1975) 387
- 20) M. Giannoni and P. Quentin, *Phys. Rev.* **C21** (1980) 2060 and 2076
- 21) P. Holzer, U. Mosel and W. Greiner, *Nucl. Phys.* **A138** (1969) 241;
D. Scharnweber, W. Greiner and U. Mosel, *Nucl. Phys.* **A164** (1971) 257
- 22) M. Brack *et al.*, *Rev. Mod. Phys.* **44** (1972) 320
T. Lederberger and H.-C. Pauli, *Nucl. Phys.* **A207** (1973) 1
- 23) P. Lichtner, D. Drechsel, J. Maruhn and W. Greiner, *Phys. Rev. Lett.* **28** (1972) 829
- 24) G. Holzwarth, *Nucl. Phys.* **A207** (1973) 545