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GENERATOR COORDINATE CALCULATIONS

OF GIANT RESONANCES WITH SKYRME'S INTERACTION

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# Abstract

Skyrme's interaction is shown to lead to significant simplifications in generator coordinate calculations. As an illustration giant resonances are calculated using pure oscillator wave functions. We present results for monopole, dipole and quadrupole isoscalar and isovector modes using two different Skyrme forces SIII and SIV. A good agreement with available experimental data is obtained.

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#### I - INTRODUCTION

In the past few years the Skyrme interaction [1] has proved to be a very useful tool for investigating ground state properties of nuclei in the Hartree-Fock approximation. Indeed, because of its computational simplicity, it has allowed calculations which would become prohibitive with other interactions, e.g. deformation properties of heavy nuclei including their fission barriers [2].

The purpose of the present paper is to demonstrate that the Skyrne force also leads to significant simplifications in generator coordinate calculations and to generalize some preliminary results which have already been reported elsewhere [29]. In particular we show in section II that the energy kernel occuring in the Hill-Wheeler equation can be constructed from a local energy functional involving one-body densities only. As an illustration we consider in section III the calculation of giant resonances, for which the Skyrme force is expected to be an appropriate effective interaction [3,4]. Using pure harmonic oscillator wave functions we are able to obtain analytic expressions for the energy and overlap kernels in the case of isoscalar and isovector monopole, dipole and guadrupole vibrations. In section IV our numerical method for solving the Hill-Wheeler equation is presented while section V discusses the corrections arising from the center-of-mass motion. In Section VI we consider the evaluation of energy weighted sum rules and in section VII we present numerical results for two different Skyrme torons SIII and SIV [5] whose parameters are listed in Table 1. Finally a summary of our main conclusions is given in section VIII.

#### II - EXPRESSION OF THE ENERGY KERNEL WITH THE SKYRME INTERACTION

In this paper we shall work with a set of Slater determinants depending on one or two generator coordinates a, i.e.  $\dagger(a)$  or  $\dagger(a,\beta)$ . We shall restrict our description to spin saturated N=Z nuclei and we shall neglect spin-orbit and Coulomb forces. The Slater determinants  $\dagger(a)$  are products of proton and neutron Slater determinants  $\dagger_n(a)$ ,  $\dagger_p(a)$ . Each orbital  $\varphi_{\lambda n}(\hat{\tau}_{p})(\varphi_{\lambda p}(\hat{\tau}_{p}))$  in  $\dagger_n(a)$  ( $\mathring{\varphi}_p(a)$ ) is occupied by two neutrons (protons) with spin up or down. A straighforward calculation (see for example the appendix of Ref.6)) shows that with the Skyrme interaction one obtains

$$\langle \psi(\alpha) | \tilde{H}[\psi(\alpha^{\dagger}) \rangle = \langle \psi(\alpha) | \psi(\alpha^{\dagger}) \rangle \int d^{3}\mathbf{r} \cdot H(\vec{r})$$
 (1)

where  $\langle \psi | \alpha \rangle \langle \phi | \alpha \rangle \langle \hat{\mu} | \psi | \alpha \rangle \rangle$  are respectively the overlap kernel  $\mathcal{N}^{2}$   $\langle \alpha, \alpha \rangle$  and the hamiltonian kernel  $\mathcal{H}^{2}$   $\langle \alpha, \alpha \rangle$  of the Hill-Wheeler equation and  $H(\hat{r})$  is a functionnal given by

$$\begin{split} ii(\hat{r}) &= \frac{h^2}{2m} (x_n + x_p) + \frac{t_2}{4} ((1 - x_0) (\mu_n^2 + \rho_p^2) + 2(2 + x_0) \rho_n \rho_p) \\ &+ \frac{t_1}{3} (\mu_n^2 \rho_p + \rho_n \rho_p^2) + \frac{t_4 + 3t_2}{8} (\rho_n T_n + \tilde{J}_n^2 + \rho_p T_p + \tilde{J}_p^2) \end{split}$$
(2)  
$$&+ \frac{t_1 - t_2}{4} (\rho_n T_p + \rho_p T_n + 2\tilde{J}_n \tilde{J}_p) + \frac{3(t_1 - t_2)}{32} (\tilde{V} \rho_n^2 + \tilde{V} \rho_p^2) \\ &+ \frac{3t_1 - t_2}{8} (\tilde{V} \rho_n - \tilde{V} \rho_p) \end{split}$$

The coefficients  $t_0$ ,  $t_1$ ,  $t_2$ ,  $t_3$  and  $x_0$  are the parameters of the Skyrme force. The densities  $\rho_n$ ,  $\rho_p$ , the kinetic energy densities  $T_n$ ,  $T_p$ , and the current densities  $j_n j_n$ , are defined by

$$\begin{split} \mu_{\mathbf{n}}(\mathbf{\dot{r}}) &= 2 \sum_{\lambda_{||}=1}^{\lambda/4} \left(\mathbf{N}_{\mathbf{n}}^{-1}\right)_{\mu\lambda} \varphi_{\lambda\mathbf{n}}^{\mathbf{\hat{r}}}(\mathbf{\dot{r}}_{\mu}) \varphi_{\mu\mathbf{n}}(\mathbf{\dot{r}}_{\mu}^{*}) \\ \Psi_{\mathbf{n}}(\mathbf{\dot{r}}) &= 2 \sum_{\lambda_{||}=1}^{\lambda/4} \left(\mathbf{N}_{\mathbf{n}}^{-1}\right)_{\mu\lambda} \quad \vec{\nabla} \varphi_{\lambda\mathbf{n}}(\mathbf{\dot{r}}_{\mu}) \cdot \vec{\nabla} \varphi_{\mu\mathbf{n}}(\mathbf{\dot{r}}_{\mu}^{*}) \end{split}$$
(3)

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$$\vec{j}_{n}(\vec{r}) = \sum_{\lambda\mu=1}^{N/4} (N_{n}^{-1})_{\mu\lambda} \langle \varphi_{\lambda n}^{\star}(\vec{r}\mu) \vec{v} \varphi_{\mu n}(r\mu') - \langle \vec{v} \varphi_{\lambda n}^{\star}(\vec{r}\mu) \rangle \varphi_{\mu n}(\vec{r}\mu') \rangle$$

where A is the mass number of the nucleus and the neutron overlap matrix  $(N_n)_{\pm u}$  is defined by

$$(N_n)_{\lambda\mu} = \int \varphi^{\dagger}_{\lambda n}(\vec{r}_{\mu}) \varphi_{\mu n}(\vec{r}_{\mu'}) d^3r \qquad (4)$$

Similar equations hold for the densities  $\rho_p$ ,  $T_p$ ,  $J_p$  and the matrix  $N_p$ . The determinant of the overlap matrix is equal to the total overlap kernel

$$\mathcal{N}^{\circ}(\alpha, \alpha') = (\det N_n \det N_p)^2$$
 (5)

The exponent 2 appears because each orbital is occupied by two particles with opposite spins . For isoscalar modes we have  $\varphi_{\lambda p}(\vec{r}\mu) \neq \varphi_{\lambda n}(\vec{r}\mu)$  which implies  $\psi^{\alpha} \rho_{n} + \rho_{p}^{-\alpha} \rho_{n}$  and similar relations for T and  $\vec{j}$  and

$$H(\hat{r}) = \frac{\hbar^2}{2m} + \frac{3}{8} t_{c\nu}^2 + \frac{1}{16} (3t_1 + 5t_2) (\rho T + \frac{1}{2}) + \frac{1}{64} (9t_1 - 5t_2) (\bar{\nabla}\rho)^2 \quad (6)$$
$$+ \frac{1}{16} t_2 \rho^2$$

III - CALCULATION OF GIANT RESONANCES WITH OSCILLATOR WAVE FUNCTIONS

### A) Evaluation of the densities $\rho$ , T and $\frac{1}{2}$

In this paragraph we shall only consider neutron densities. Proton densities are trivially obtained by interchanging, indices n and p. The Slater determinant  $\Phi_n(\alpha)$  contains the lowest eigenstates of a spherical or axially deformed oscillator well not necessarily centered at the origin. The occupied states are defined by

$$2n_{\mu} + |\Lambda| + n_{\mu} \leq N \tag{7}$$

with  $n_{r}{}^{,\Lambda}$  and  $n_{g}$  being the usual asymptotic quantum numbers (7). The number N is 0 for  ${}^{4}\mathrm{He}$ , 1 for  ${}^{16}\mathrm{O}$  and 2 for  ${}^{40}\mathrm{Ca.}$ 

## a) Monopole and guadrupole modes

To describe monopole and guadrupole modes we choose the generator coordinates to be the oscillator parameters  $\gamma_z = \frac{m\omega_z}{h}$  and  $\gamma_I = \frac{-1}{h}$  where  $\omega_z$  and  $\omega_I$  are oscillator frequencies along the z-axis and in the xy plane.

To evaluate the densities (3) corresponding to the individual wave functions  $\varphi_{\lambda n}(\gamma_z, \gamma_1, \vec{r})$  and  $\varphi_{\lambda n}(\gamma_z, \gamma_1, \vec{r})$  it is convenient to note that the following relations hold

$$\varphi_{\lambda n}^{\star}(\bar{\gamma}_{z}, \gamma_{1}, \vec{r}) = e^{\tilde{\lambda}_{n}(\hat{r})} \sum_{\nu=1}^{\lambda/4} (L_{n})_{\lambda \nu} \varphi_{\nu n}^{\star}(\tilde{\gamma}_{z}, \tilde{\gamma}_{1}, \vec{r})$$
(8)

$$\varphi_{\mu n}(\gamma'_{z},\gamma'_{1},\vec{r}) = e^{-\chi_{n}(\vec{r})} \sum_{\nu=1}^{A/4} (M_{n})_{\kappa \mu} \varphi_{\kappa n}(\vec{\gamma}_{z},\vec{\gamma}_{1},\vec{r})$$
(9)

where  $\lambda_{11} = \frac{1}{4} (\gamma_{2} - \gamma_{2}^{t}) z^{2} + \frac{1}{4} (\gamma_{1} - \gamma_{1}^{t}) (x^{2} + y^{2})$  (10)

and 
$$\overline{\gamma}_{g} = \frac{1}{2} (\gamma_{g} + \gamma_{g}^{\dagger}) , \quad \overline{\gamma}_{L} = \frac{1}{2} (\gamma_{L} + \gamma_{L}^{\prime})$$
 (11)

In eqs (8) and (9)  $L_n$  and  $M_n$  are two triangular matrices. Their coefficients are respectively functions of  $\frac{Y_z}{\overline{\gamma}_z}$ ,  $\frac{Y_1}{\overline{\gamma}_1}$  and  $\frac{Y_z}{\overline{\gamma}_z}$ ,  $\frac{Y_1'}{\overline{\gamma}_1}$ .

As a consequence of Eqs (8-9) we find that the one body operator

$$\sum_{\rho_{n}}^{n} \langle \vec{z} \vec{z}^{*} \rangle = 2 \sum_{\lambda \mu = 1}^{A/4} (N_{n}^{-1})_{\mu \lambda} \varphi_{\lambda n}^{\sharp} (\gamma_{z}, \gamma_{\perp}, \vec{z}) \varphi_{\mu n} (\gamma_{z}^{*}, \gamma_{\perp}^{*}, \vec{z}^{*})$$
(12)

which thanks to the definition of N<sub> $\lambda\mu$ </sub> satisfies the relations  $Tr \tilde{\rho}_n^{-2A/2}$  and  $\tilde{\rho}_n^2 = \tilde{\rho}_n$  (but not  $\tilde{\rho}_n^+ = \tilde{\Omega}_n^2$  can be related to the density matrix

$$\hat{\rho}_{on}(\vec{x}\vec{x}') = 2 \sum_{\lambda=1}^{A/4} \varphi_{\lambda n}^{a}(\vec{\gamma}_{z},\vec{\gamma}_{\perp},\vec{z}) \varphi_{\lambda n}(\vec{\gamma}_{z},\vec{\gamma}_{\perp},\vec{z}')$$
(13)

by

$$\hat{\rho}_{n}(\vec{r}\vec{r}') = \sum_{n}^{n} (\vec{r}) \quad \hat{\rho}_{nn}(\vec{r}\vec{r}') = \sum_{n}^{n} (\vec{r}) \quad (14)$$

The densities (3) are then immediately obtained from equation (14)

$$\rho_{n}(\vec{x}) = \rho_{on}(\vec{x}) \qquad T_{n}(\vec{x}) = T_{on}(\vec{x}) - \rho_{on}(\vec{x})(\vec{v}_{X_{n}})^{2}$$

$$\vec{J}_{n}(\vec{x}) = -\rho_{on}(\vec{x})\vec{v}_{X_{n}}(\vec{x}) \qquad (15)$$

Here  $\rho_{\rm OR}$  and  $T_{\rm OR}$  are the density and kinetic energy density constructed from the density matrix  $\hat{\rho}_{\rm OR}(\vec{r},\vec{r}\,')$ .

## β) dipole mode

The generator coordinate is now the distance  $z_n$  of the center of the harmonic potential generating the set  $\{\varphi_{\lambda n}\}$  to the origin. We shall consider motion along the z axis (unit vector  $\vec{k}$ ). We then have

$$\varphi_{\lambda p}(\mathbf{z}, \mathbf{r}) = \varphi_{\lambda p}(\mathbf{0}, \mathbf{r} - \mathbf{z} \mathbf{k})$$
(16)

We also choose the wave functions  $\varphi_{\lambda n}(0, \hat{\mathbf{r}})$  to be eigenvectors of a spherical oscillator potential whose parameter  $\gamma$  minimizes the total binding energy. In analogy with the definition (11) we introduce

$$\vec{z}_{n} = \frac{1}{2} (z_{n} + z_{n}')$$
 (17)

When one expresses the wave functions  $\{\varphi_{\lambda n}(\mathbf{z}_n, \dot{\mathbf{r}})\}$  and  $\{\varphi_{\lambda n}(\mathbf{z}_n', \dot{\mathbf{r}})\}$ in terms of the set  $\{\varphi_{\lambda n}(\overline{\mathbf{z}}_n, \dot{\mathbf{r}})\}$  one obtains expressions identical to (8) and (9) with

$$\chi_{\mathbf{n}}(\vec{\mathbf{r}}) = \frac{1}{2} \sqrt{\gamma} \left( \mathbf{z}_{\mathbf{n}} - \mathbf{z}_{\mathbf{n}}' \right) \vec{\mathbf{r}} \cdot \vec{\mathbf{k}}$$
(1B)

Equations (14) and (15) can also be shown to hold provided  $\tilde{\rho}_{on}(\vec{r},\vec{r}')$  is defined as

$$\tilde{\vec{p}}_{on}(\vec{z},\vec{r}^{\dagger}) = 2 \sum_{\lambda=1}^{A/4} \varphi_{\lambda n}^{\sharp}(\vec{z}_{n},\vec{z}) \varphi_{\lambda n}(\vec{z}_{n},\vec{r}^{\dagger}) \qquad (19)$$

### B) Explicit expressions of the overlap and energy kernels

## c) monopole and quadrupole modes

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The relations (15) show that the quantities  $\rho_n T_n + j_n^2$ ,  $\rho_p T_p + j_p^2$  are respectively equal to  $\rho_{on} T_{on}, \rho_{op} T_{op}$ . Furthermore for isoscalar modes  $\rho T + j^2 = \rho_0 T_0$  and the quantity fH(r) defined in (6) is

$$(H(\mathbf{r})d^{3}\mathbf{r} = E(\overline{\gamma}_{z},\overline{\gamma}_{\perp}) - \frac{\hbar^{2}}{2m} f_{p_{0}} (\nabla_{\chi})^{2} d^{3}\mathbf{r}$$
(20a)

where

$$E(\bar{\gamma}_{z},\bar{\gamma}_{1}) = \int \left[\frac{\hbar^{2}}{2m}T_{0} + \frac{3}{8}t_{0}\rho_{0} + \frac{1}{16}(3t_{1}+5t_{2})\rho_{0}T_{0} + \frac{1}{64}(9t_{1}-5t_{2})(\bar{\nabla}\rho_{0})^{2} + \frac{1}{16}t_{3}\rho_{0}^{3}\right]d^{4}r$$
(20b)

The quantity  $E(\overline{Y}_{z}, \overline{Y}_{1})$  is just the expectation value of the Skyrme hamiltonian for the Slater determinant containing the wave functions  $\varphi_{\lambda}(\overline{Y}_{z}, \overline{Y}_{1}, \vec{r})$  and depends only on the arithmetic mean of genetor coordinates. Thus the only term in (20a) depending on the difference of the generator coordinates arises from the kinetic energy.

In order to include isovector modes we need to consider four generator coordinates  $\gamma_{zn}$ ,  $\gamma_{zp}$ ,  $\gamma_{in}$ ,  $\gamma_{ip}$ . In this case the quantity  $(\rho_n T_p + \rho_p T_n + 2 \tilde{J}_n \tilde{J}_p)$  is still a function of  $\chi_n$  and  $\chi_p$  and the part of H depending on  $(\gamma_{zn} - \gamma'_{zn})$ ,  $(\gamma_{zp} - \gamma'_{zp})$  and  $(\gamma_{in} - \gamma'_{in})$ ,  $(\gamma_{ip} - \gamma'_{ip})$  will be a function of the Skyrme-parameter combination  $(t_i + t_2)$ .

In appendix A we present details of the calculation of /H(r) d'r for coupled isoscalar and isovector monopole modes. The value of E( $\gamma, \gamma$ ) (Eq.(20b)) is obtained from Eq.A4° by setting  $\gamma'=\gamma$ . To obtain  $E(\gamma_{z}, \gamma_{1})$  we notice that deformation of the harmonic oscillator wave functions correspond to the scale transformations

$$x^{2} + x^{2} \frac{Y}{Y_{1}}$$
,  $y^{2} + y^{2} \frac{Y}{Y_{1}}$ ,  $z^{2} + z^{2} \frac{Y}{Z_{2}}$ , (21)

with the "volume conservation" condition

$$\gamma_{\perp}^{2} \gamma_{z} = \gamma^{3} \qquad (22)$$

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We then obtain

$$E(\gamma_{z},\gamma_{\perp}) = \frac{\hbar^{2}}{2m} \frac{2}{3} c_{1} (\gamma_{z}+2\gamma_{\perp}) + t_{0} \frac{3}{2(2\pi)^{3/2}} d_{0} (\gamma_{z}\gamma_{\perp}^{2})^{3/2}$$

$$+ \left\{ (3t_{1}+5t_{2}) \frac{\hbar_{0}}{24(2\pi)^{3/2}} + (5t_{1}-5t_{2}) \frac{g_{0}}{4B(2\pi)^{3/2}} \right\} (\gamma_{z}\gamma_{\perp}^{2})^{1/2} (\gamma_{z}+2\gamma_{\perp})$$
(23)

$$\div t_3 \xrightarrow{4j_0} \gamma_z \gamma_{\perp}^2$$

The values of the coefficients  $c_1, d_0, h_0, g_0$  and  $j_0$  are given in Table 8 for the three magic nuclei <sup>4</sup>He, <sup>16</sup>O and <sup>40</sup>Ca. We finally note that

$$\frac{\hbar^2}{2m} \int \rho_{OR} (\overline{\nabla}\chi_R)^2 d^3 x = \frac{\hbar^2}{2m} \frac{c_1}{3} \left( \frac{(\gamma_z - \gamma_z^*)^2}{4\overline{\gamma}_z} + 2 \frac{(\gamma_1 - \gamma_1^*)^2}{4\overline{\gamma}_1} \right)$$
(24)

At this point we still need the value of the overlap kernel. Using formulae (8) and (9) one notices that

$$\left(N_{n}^{\prime}\right)_{\lambda \mu} = \left(L_{n}^{\prime}, M_{n}^{\prime}\right)_{\lambda \mu}$$
(25)

Since  $L_n$  and  $M_n$  are triangular matrices their determinants are equal to the products of their diagonal elements

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$$(L_{n})_{\lambda\lambda}^{2} = \left(\frac{\gamma_{z}}{\overline{\gamma}_{z}}\right)^{n_{z}+\frac{1}{2}} \left(\frac{\gamma_{1}}{\overline{\gamma}_{1}}\right)^{2n_{z}+\lfloor\lambda\lfloor+1]} , \qquad (M_{n})_{\lambda\lambda}^{2} = \left(\frac{\gamma_{z}}{\overline{\gamma}_{z}}\right)^{n_{z}+\frac{1}{2}} \left(\frac{\gamma_{1}}{\overline{\gamma}_{1}}\right)^{2n_{z}+\lfloor\lambda\rfloor+1}$$

$$(26)$$

In equation (26)  $n_g$ ,  $n_{\chi}$  and  $|\Lambda|$  are the asymptotic quantum numbers of the state  $\lambda$ . We thus find

$$(\det N_{\eta})^{2} = \left(\frac{\gamma_{\underline{z}}}{\overline{\gamma}_{\underline{z}}^{2}}\right)^{D} \left(\frac{\gamma_{\underline{i}}}{\overline{\gamma}_{\underline{j}}^{2}}\right)^{2D}$$
(27)

with D=1 for  ${}^{4}$ He ,6 for  ${}^{16}$ O and 20 for  ${}^{40}$ Ca.

β) <u>dipole\_mode</u>

Using the same procedure as in the above subsection and setting  $z_n \neq z_p = z$  in Eq. 16 and its analog for protons we obtain for the isoscalar dipole mode (translation) from Eq.6

$$fH(x)d^{3}x = g(y,y) - \frac{\hbar^{2}}{2m}\frac{A}{4} - y(z-z^{*})^{2}$$
(28)

where  $E(\gamma,\gamma)$  is defined by eq.(23). The calculation for the isovector dipole mode, which corresponds to  $z_n = -z_p = z$  in Eq.16, is still straighforward but more tedious. Details and results are given in appendix B. Noticing that

$$(L_n)_{\lambda\lambda} = \exp\left(-\frac{3}{8}\gamma(z-z^*)^2\right) \qquad (M_n)_{\lambda\lambda} = \exp\left(-\frac{1}{8}\gamma(z-z^*)^2\right) \qquad (29)$$

for all  $\lambda$  we find for the neutron overlap kernel

det N<sub>n</sub> = exp 
$$(-\frac{h}{8}\gamma(z-z')^2)$$
 (30)

IV - SOLUTION OF THE HILL-WHEELER EQUATION

equation

As usual we replace the Hill-Wheeler integral

$$f\left(\mathcal{H}\left(\alpha,\alpha^{\dagger}\right)-\mathbf{B}\right)\left(\mathbf{A}^{\dagger}\left(\alpha,\alpha^{\dagger}\right)\right)f\left(\mathbf{A}^{\dagger}\right)=0$$
(31)

where a stands for one or two generator coordinates, by a matrix generalized eigenvalue problem

$$h \sum_{j=1}^{n} (\mathcal{U}(\alpha_{1},\alpha_{j}) - E \mathcal{V}(\alpha_{1},\alpha_{j}))f(\alpha_{j}) = 0 \qquad (32)$$

The quantity h is the step of the (regular) mesh  $\{a_{\underline{i}}\}$  while n is the number of points of the mesh. In our calculation n was choosen equal to 143<sup>#</sup>. This value is large enough to ensure the stability of all the observables under consideration (energies, root mean square radii, quadrupole moments, transitions rates) against any change of the mesh.

For the monopole modes we use a regular mesh in  $\gamma_n$  and  $\gamma_p$ . The isoscalar monopole mode is obtained by choosing identical values of  $\gamma_n$  and  $\gamma_p$ . For the quadrupole mode we define

 $q = \frac{\gamma_1}{\gamma_2} \quad \text{and} \quad \gamma^3 = (\gamma_2 \gamma_1^2) \quad (33)$ 

For a pure quadrupole mode  $\gamma$  is fixed. For coupled monopole and quadrupole modes q and  $\gamma$  are two independent generator coordinates. We have used a regular mesh in the quantity  $(q-1)^{\gamma}(1+q)$ .

For dipole modes the generator coordinates are  $z_n$  and  $z_p$  i.e the distances of the centers of mass of the neutron and protons densities from the origin. The isovector mode corresponds to opposite values of  $z_n$  and  $z_p$  ( $z_n^{=-}z_p^{\exists z}$ ).

\*Such a large number of mesh points is necessary to describe accurately the weight functions graphed on Figures 5 and 6. However a smaller number of mesh points e.g. 15 is sufficient to obtain energies and radii with 4 significant figures.

The solution of the generalized eigenvalue problem (32) cannot be achieved by a direct inversion of the matrix  $\mathscr{N}^{2}(\alpha_{1},\alpha_{4})$  [28].

Indeed when the mesh  $\{\alpha_i\}$  is dense the matrix  $\mathcal{N}^{(\alpha_i,\alpha_j)}$  is nearly singular. To bypass this difficulty we diagonalize the hermitian matrix  $\mathcal{N}^{(\alpha)}$  and eliminate all the eigenvectors of  $\mathcal{N}^{(\alpha)}$  with eigenvalues lower than a small positive number  $\varepsilon$ . In the subspace spanned by the remaining eigenvectors we construct and diagonalize the operator  $\mathcal{N}^{-1/2}\mathcal{A}$ .  $\mathcal{O}^{(\alpha)-1/2}$ . This prescription amounts to substracting from the original variational space all the vectors with a zero (or nearly zero) norm. It can be shown that the solutions of this restricted eigenvalue problem are stable with respect to small perturbations of the matrix [8]. In particular the results presented hereafter do not depend on the value of the quantity  $\varepsilon$  which in our calculations was  $10^{-3}$ .

As a consequence of the non-orthogonality of the G.C.M. basis the Hill-Wheeler functions f are not orthogonal and their discussion becomes rather involved [28]. Furthermore they are not stable against any change in the mesh. For this reason we have calculated the set of orthonormal functions  $\{g_i\}$  which are obtained from  $\{f_i\}$  by

 $g_i = \mathcal{K}^{1/2} f_i \qquad (34)$ 

and are numerically stable.

In eq. (34)  $f_1$  is a vector and  $\mathcal{N}^{p\,1/2}$  a matrix satisfying

Nº 1/2 = N

The index i just labels the different solutions of the Hill-Wheeler equation. In section VII of this paper we shall discuss the behavior of these functions. It should be noted that the functions g are the natural quantities to consider when trying to replace the integral Hill-Wheeler problem by a Schrödinger-like equation [9,10].

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V - CORRECTIONS

Center of mass (C.M.) effects are known to be important for light nuclei. A standard way to correct for them is to subtract from the total energy average value of the operator  $\dot{P}^2/2mA$  where  $\dot{P}$  is the total momentum of the system i.e. to make the substitution  $\hat{H} + \hat{H} - P^2/2mA$  in the left hand side of Eq.1. This prescription seems to be rather accurate as far as energy levels are concerned but less satisfactory for properties involving nuclear wave functions e.g. form factors (21) . In our calculations we substracted only the one-body part of  $\frac{1}{2}^2/2mA$ . For the nucleus <sup>4</sup>He this approximation is exact since the two-body term vanishes identically. For the heavier nuclei 160 and 40 ca for which C.M. effects are smaller we have checked that C.M. corrections affect neither correlations nor energy differences between the ground state and the first excited states. From a technical point of view the correction of C.M. motion will not change the formal expression of (H(r)d<sup>3</sup>r (23, 28, A3, B2). One needs only to replace the coefficients  $c_1$  by  $c_2 = c_1 (A-1)/A$ , where A is the mass of the nucleus.

Our calculations do not include angular momentum projection effects. As was found in the calculations of Reference 13 these effects are negligible for energies of quadrupole modes in 0xygen-16 and calcium-40, but may be sizeable in helium-4 [21].

## VI - ENERGY WEIGHTED SUM RULES (E.W.S.R.)

In appendix D we show that energy weighted sum rules must be saturated in the present generator coordinate calculations. In this section we recall some results which have been obtained and discussed in Refs.4,11). Although the Skyrme interaction is velocity depan-

dent it can be shown that the formal expressions for isoscalar monopole and quadrupole E.W.S.R. are identical to those corresponding to local two-body interactions.

For a given reference ground state |0> we have for the monopole sum ruleEMS

EMS = 
$$\langle 0 | \frac{1}{2} (\hat{r}^2 | \hat{r}^2 | ] | 0 \rangle = \frac{\hbar^2}{2m} 4 \langle 0 | \hat{r}^2 | 0 \rangle$$
 (35)

where  $\hat{r}^{z}$  is the one body operator  $\sum_{\underline{i}} x_{\underline{i}}^{2} + y_{\underline{i}}^{2} + z_{\underline{i}}^{2}$ . For the quadrupole isoscalar mode the E.W.S.R. is

$$LQS = \langle 0|\frac{1}{2} \{\hat{Q}_{1}\hat{H}\hat{Q}_{1}\} \} |0\rangle \approx \frac{\hbar^{2}}{2m} 4 (2\langle 0|\hat{r}^{2}|0\rangle + \langle 0|\hat{Q}|0\rangle)$$
(36)

where Q is the quadrupole operator  $\hat{Q} = \frac{1}{4} 2z_{1}^{2} - x_{1}^{2} - y_{1}^{2}$ .

In the isovector case the interaction appears in the EMSR through its neutron-proton exchange part. The monopole isovector sum rule (corresponding to the one body operator  $\frac{\tau}{2} \tau_1^2 \tau_1$  where  $\tau_1=1$  for neutrons and -1 for protons) calculated with the Skyrme interaction is

$$EMV = \langle 0 | \frac{L}{2} [ \sum_{i} r_{i}^{2} \tau_{i} | \hat{H}_{i} \sum_{i} r_{i}^{2} \tau_{i} | ] | 0 \rangle = \frac{1}{2}$$

$$4 \left( \frac{h^{2}}{2m} \langle 0 | \hat{r}^{2} | 0 \rangle + \frac{1}{2} (t_{1} + t_{2}) \langle 0 | \frac{1}{2} \sum_{ij} (1 - \tau_{i} \tau_{j}) r_{i}^{2} \delta(\hat{r}_{i} - \hat{r}_{j}) | 0 \rangle \right) \quad (37)$$

The dipole isovector sum rule corresponding to the operator  $\sum_{i} z_i \tau_i$  is

If one chooses (0> to be the generator coordinate ground state the evaluation of EMV and EDV will involve the calculation of

$$\langle \phi(\alpha) | \frac{1}{2} \sum_{ij} (1 - \tau_i \tau_j) r_i^2 \delta(\vec{r}_i - \vec{r}_j) | \phi(\alpha') \rangle = \mathcal{H}(\alpha, \alpha') 2 \int r^2 \rho_n \rho_p d^2 r \quad (39)$$

and

$$\langle \phi(\alpha) | \frac{1}{2} \sum_{ij} (1 - \tau_i \tau_j) \delta(\vec{x}_i - \vec{x}_j) | \phi(\alpha') \rangle = \mathcal{H}^0(\alpha, \alpha') - 2 \int \rho_n \rho_p d^3 r \quad (40)$$

where  $\rho_n$  and  $\rho_n$  are defined in (3).

VII - RESULTS FROM THE GENERATOR COORDINATE METHOD (G.C.M)

## A) Isoscalar modes

a) monopole mode

In Table 2 we give the eigenvalues of Eq. 32 for the first monopole states of the nuclei  ${}^{4}\text{He}$ ,  ${}^{16}\text{O}$  and  ${}^{40}\text{Ca}$ . We have also included the variational binding energy  $\text{E}_{v}$  of a pure Slater determinant of oscillator wave functions as well as the difference  $\text{E}_{1}-\text{E}_{0}=\Delta\text{E}_{1}$ .

From Table 2 one can see that except from the case of <sup>4</sup>He the eigenvalues  $E_0$  of the lowest generator coordinate state are very close to the variational values  $E_v$ . We shall return later to the special case of <sup>4</sup>He. The differences  $\Delta E_1$  give the monopole excitation energy. The small difference between the SIII and SIV predictions is correlated with the incompressibility modulus in nuclear matter which is 356 MeV for the first interaction and 325 MeV for the second. One can also calculate directly the incompressibility modulus K in <sup>16</sup>O and <sup>40</sup>Ca. For a nucleus with mass number A described by a Slater determinant of oscillator wave functions we define K as

$$K = \frac{4\gamma^2}{A} \frac{d^2 E(\gamma_* \gamma)}{d\gamma^2} \gamma = \gamma_0$$
(41)

In this expression the notation is that of equation (20) and  $\gamma_0$  is the variational value of the oscillator parameter  $\gamma$ . Using equation (20) one finds for <sup>16</sup>O a value of K equal to 200 MeV for SIII and 182 MeV for SIV. From these numbers one can easily verify that  $\Delta E_1$ is proportional to  $\sqrt{K}$  as is the case for the hydrodynamics model [12]. For <sup>40</sup>Ca values of K are 231 MeV for SIII and 210 MeV for SIV. As expected they lie between the values for <sup>16</sup>O and those for nuclear matter. As compared to other theoretical approaches [13-18] our monopole excitations energies are generally larger

by 4 to 10 MeV due to the rather larger incompressibility associated with the Skyrme interaction. That the Skyrme interaction and not the G.C.M. treatment is responsible for this difference is demonstrated by the evaluation of the same guantity by the R.P.A. method. Indeed using the same Skyrme forces the authors of Refs. 4,11,14. obtain very similar results. We should also mention that recent experiments [19] suggest that an important fraction of the isoscalar monopole strength may be located near 20 MeV in calcium-40, which is considerably lower than our predictions.

The calculation of E.W.S.R. shows that the first monopole state of  ${}^{16}O$  and  ${}^{40}Ca$  exhausts more than 90% of the sum rule. This seems to be a typical feature of the generator coordinate method [13]. In the case of  ${}^{4}$ He the first excited state exhaust only 45%. The rest is presumably associated with transitions to the continuum. Such transitions are not included in our variational space. Furthermore they cannot be computed accurately with our discretization metiod. In fig.1 we have notothed as a function of the

parameter  $\gamma$  the diagonal part of the energy kernel of <sup>16</sup>O. When  $\gamma=0$  the nucleus has an infinite radius and the corresponding energy is zero. Due to the kinetic repulsion the energy first becomes positive. When the nuclear forces become important they overcome the kinetic energy increase. After the equilibrium point the short distance nuclear repulsion starts predominating and the energy tends to infinity as the nuclear radius decreases.

In the same figure we have reported the functions g of the three first G.C.M. states of <sup>16</sup>0. The ground state function has the usual bell-shape and the g corresponding to the first and second states are very close to the first and second derivatives respectively of the ground state g function. This result is reminiscent of the well known scaling method which describes the monopole vibration as  $\frac{\partial}{\partial \gamma} = \Phi_0(\vec{x_1}...\vec{x_n}) \Big|_{\gamma=1}^{\gamma=1}$  where  $\Phi_0$  is the ground state wave function [20].

In figure 2 we have presented the functions  $g_0$  of the three magic nuclei  ${}^{4}\text{He}$ ,  ${}^{16}\text{O}$ ,  ${}^{40}\text{Ca}$ . One notices that the width of  $g_0$  decreases with increasing values of  $\mathbb{P}$ . The vertical bars indicate the values of the oscillator parameter  $\gamma_0$  which minimizes the energy. The maximum of  $g_0$  occurs for  ${}^{40}\text{Ca}$  and  ${}^{16}\text{O}$  at about  $\gamma_0$ . On

the contrary that of the  ${}^{4}$ He curve is noticeably shifted from  $\gamma_{0}$ . This leads to a 0.2 fm decrease of the root mean square radius associated with the inclusion of the G.C.M. correlations.

This can also be seen in fig.3 where we have plotted the charge density of He<sup>4</sup> and its form factors. The form factor of the oscillator density  $(\gamma=\gamma_{0})$  is a straight line while that of the G.C.M. ground state exhibits addp (in agreement with experimental data). However the second maximum of the G.C.M. form factor is not high enough as compared to experiment. In the same figure we have plotted the results obtained by a complete Hartree-Fock (H.F.) calculation. At low momentum transfer the H.F. form factor is very close to the oscillator form factor. The dip appearing in the H.F. curve occurs at a too small momentum transfer .

The G.C.M. and oscillator densities of <sup>16</sup>0 and <sup>40</sup>Ca have been found to be very close and the small differences between them do not lead to any significant effect on electron-scattering differentiat cross sections.

# β) translation (dipole) mode

Let  $|\vec{R}\rangle$  be the state deduced from the oscillator ground state  $|0\rangle$  by a translation  $\vec{R}$ . Within the pushing model the energy  $E_k^*$  of the nucleus moving with a velocity  $\dot{v} = \frac{\hbar \vec{k}}{m}$  is

 $E_{\vec{k}} = \frac{\int e^{i\vec{k}\vec{k}} \langle \vec{k} | \hat{H} | 0 \rangle d^{3}r}{\int e^{i\vec{k}\vec{k}} \langle \vec{k} | 0 \rangle d^{3}r}$ (42)

The evaluation of  $\langle \vec{R} | H | 0 \rangle$  and  $\langle \vec{R} | 0 \rangle$  is trivially obtained from Equations 28 and 30 by replacing  $(z-z')^2$  by  $R^2$ .

\*It is not clear that one can draw definite conclusions in the case of <sup>4</sup>He since an exact treatment of center of mass motion would presumably affect noticeably the G.C.M. results for the form factor [21].

Notice that equation (42) involves the hamiltonien  $\hat{H}$  and not  $\hat{H}-P^{2}/2mA$ .

Using equations (1), (28) and (30) one immediately obtains

$$E_{k}^{+} = E(\gamma, \gamma) - \frac{\hbar^{2}}{2m} \frac{3 \Upsilon}{2} + \frac{\hbar^{2}}{2mA} k^{2}$$
(43)

The first term on the right-hand side of (43) is just the oscillator energy. The second term is the center of mass energy of the oscillator state  $<0|\frac{p^2}{2mA}|_{0>}$ . The third term which is the only one depending on  $\stackrel{*}{}$  is the kinetic energy. One sees that the translational mass is correct. This result is due to the fact that we use a harmonic oscillator Slater determinant to describe the nucleus.

y) Quadrupole mode

In the figure 4 we present the ground state wave function g, of the three magic nuclei  ${}^{4}\text{Ke}$ ,  ${}^{16}\text{O}$ ,  ${}^{40}\text{Ca}$  plotted as a function of the dimensionless quantity  $q=\gamma_{I}/\gamma_{z}$ . It is seen that the width of  $q_{i}$  decreases with the mass of the nucleus.

In Table 3 we give the results of a calculation with SIII for coupled monopole and quadrupole modes. The comparison with the results of the G.C.M. calculation of monopole mode alone shows that the ground state correlation energy of 160 and 40 ca is not much increased by the inclusion of the quadrupole degree of freedom. For these two nuclei the energy of the second excited state of the coupled Hill-Wheeler problem is close to that of the breathing mode (Table 2). One is then led to identify the second excited state with the giant monopole resonance. This is confirmed by the consideration of its quadrupole moment which is nearly zero and by the contributions to the E.W.S.R. reported in the columns EMS and EGS. This state nearly exhausts the monopole sum rule ( 9135 MeV fm<sup>4</sup> for  $^{16}$ O and 38267 MeV fm<sup>4</sup> for <sup>40</sup>Ca) and does not contribute to the quadrupole sum rule. (18288 MeV fm<sup>4</sup> for <sup>16</sup>O and 76576 for <sup>40</sup>Ca). The first excited state which exhausts more than 90% of this latter E.W.S.R. can thus be identified as the quadrupole mode,

In figure 5 we show a contour plot of the three first functions g solutions of the coupled calculation for  ${}^{40}$ Ca. The ground state function g, loods like a bell shaped surface centered around the optimal values ( $\gamma_0 = .258 \text{ fm}^{-2}, q=1$ ). From the two lower graphs the quadrupole and monopole character of the first and second excited state is evident.

The results of Table 3 indicate that in <sup>4</sup>He there exists some mixing of the monopole and quadrupole vibrations. The quadrupole degree of freedom has induced a decrease of 1.6 MeV of the energy of the ground state obtained with the inclusion of monopole correlations only (Table 2). On the other hand the first excited state, although it exhausts an important fraction of the quadrupole sum rule (2470 MeV fm<sup>4</sup>), contributes also in a non negligible way to the monopole sum rule (1234 MeV fm<sup>4</sup>). Therefore the two excited states whose energies are rather close do not have a definite monopole or quadrupole character. It would then be interesting to see if a treatment including projection of total angular momentum would not change these results.

In Table 4 we give the energies of the giant quadrupole resonance calculated with SIII and SIV and the curvatures  $K_Q=1/A \ d^2 \ E \ (\gamma_0 q^{-2/3}, \gamma_0 q^{1/3})/dq^2|_{q=1}$ . The lower energies obtained with SIII are seen to be associated with lower values of the curvature.

It is now very likely that the set of observed resonances [22,23] with energies following the empirical law  $E=60 A^{-1/3}$  have an isoscalar quadrupole character. It should be noted that this law is very close to the estimate  $\cdots$  solar and Mottelson [24] for the same resonances. Before comparing our results to experimental data one must not forget that our calculated quadrupole resonances exhaust almost completely the E.W.S.R.. Therefore it should be more suitable to compare the G.C.M. energies to the center of gravity of the experimental E.W.S.R[25]. However the available data do not allow yet a precise determination of this center of gravity. If one assumes as a first approximation that it corresponds to the energy of the resonance, the experimental data agree better with the results obtained with SIII.

#### B) Isovector modes

# a) Monopola mode

The results of a G.C.M. calculation with interaction SIII of coupled monopole isoscalar and isovector modes are given in Table 5 and figure 6. The contributions to the isoscalar (EMS) and isovector (EMV) sum rule show clearly that the excited state have a pure T=0 or T=1 character. The isoscalar mode is as expected the lowest. This is also visible on the drawings of figure 6 which display the contour plots of the three first solutions of the Hill-Wheeler problem. The comparison with results of Table 2 also shows that the monopole isovector degree of freedom does not affect much the ground state. Because of the proton-neutron exchange part of the interaction the T=1 E.W.S.R. is larger than the T=0 E.W.S.R.. The enhancement factor can be written as (1+x) with x equal to .12 im <sup>4</sup>He .21 in <sup>16</sup>O and .25 in <sup>40</sup>Ca. Finally we compare in Table 6 the resonance energies of the T=1 modes calculated with SIII and SIV.

## B) Dipole mode

In the lower part of figure 7 we have reported as a function of the half-distance between the centers of gravity of neutron and proton densities the diagonal part of the energy kernel. It looks like a parabola. However for larger distances ±z an inflexion point appears and when z goes to plus or minus infinity the energy reaches a constant value which is the total energy of the nucleus minus the proton-neutron interaction energy.

The upper part of the figure 7 shows the functions  $g_0$  of the three first solutions of the G.C.M. problem in  ${}^{40}$ Ca. The ground state function  $g_0$  is an even function of z while  $g_1$  is odd. We find that the first excited state exhausts nearly all the dipole sum rule in the three magic nuclei. This sum rule (105 MeV fm<sup>2</sup> in  ${}^{4}$ He, 441 MeV fm<sup>2</sup> in  ${}^{16}$ O and 1133 MeV fm<sup>2</sup> in  ${}^{40}$ Ca) is larger than the Thomas-Reiche-Kuhn value [26]. The enhancement factor is 1.24 in  ${}^{4}$ He, 1.33 in  ${}^{16}$ O and 1.37 in  ${}^{40}$ Ca. For interaction SIII these results

compars reasonably well with those obtained by summing all the experimental contributions to the E.W.S.R. up to 30 or 40 MeV. For interaction SIV the enhancement factors are 1.8 for  ${}^{4}$ He, for  ${}^{16}$ O, and for  ${}^{40}$ Ca.

In figure 8 we show the ground state functions g: of the three magic nuclei. Here also the width decreases with increasing values of A.

Finally in Table 7 we give the energies of the two first solutions of the Hill-Wheeler equation. The comparison with the oscillator energies (Table 2) shows that the dipole correlations do not affect much the ground state energy. Since our calculated resonances exhaust completely the sum rules the discussion already made concerning the comparison with experimental data in the T=0 quadrupole case also applies here. The measurement of the contributions to E.W.S.R. up to 30 MeV seems to show that the center of gravity of the contributions is about 21-22 MeV for  $^{40}$ Ca and 24-25 MeV for  $^{16}$ o (27-23). The differences (E<sub>1</sub>-E<sub>0</sub>) obtained with SIII agree with these numbers.

In table 7 we also give the dipole curvature  $K_z = \frac{1}{A} = \frac{3^2 E}{3 (z_n - z_p)^2}$  calculated for the two interactions SIII and SIV. As

it was expected this quantity decreases with 1/A. Indeed in nuclear matter it should vanish. It is also seen that the different results obtained with SIII and SIV for the giant dipole resonance energies are not compatible with the simple irrotational formula  $2h/K_{\pi}/mA$ .

#### VIII - SUMMARY AN: CONCLUSIONS

The structure of the Hill-Wheeler equation has been investigated in the case of the Skyrme force. We have shown in particular that a simple formula involving one-body densities only can be derived for the Hamiltonian kernel. From this formula analytic expressions have been obtained in the case of monopole, dipole and quadrupole modes calculated with oscillator wave functions.

Numerical results have been presented in helium-4, oxygen-16 and calcium-40 using two different Skyrme interactions SIII and SIV. Except for the case of helium, it has been found that the coupling to collective modes does not affect the properties of the nuclear ground state, namely its density distribution and its binding energy. We have also found that the Hill-Wheeler weightfunctions become narrower with increasing mass number, in heavy nuclei.

It has been shown that the Skyrme interaction SIII provides a good agreement with available experimental data concerning isovector dipole and isoscalar quadrupole resonances. For isoscalar monopole modes our predictions are somewhat higher that those of other theoretical approaches. This difference has been attributed to the rather high nuclear incompressibility obtained with the Skyrme force.

One systematic feature of our calculations is that the collective strength is always nearly exhausted by one single state. This means that in our model, giant resonances are well described by a multipole operator acting on the ground state wave function.

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#### Appendix A

Hamiltonian kernel for coupled isoscalar and isovector monopole modes

We denote by  $2\rho(\gamma, \hat{r})$  the mass distribution obtained by filling oscillator states with a parameter  $\gamma = m\omega/\hbar$ and by  $2T(\gamma, \hat{r})$  the corresponding kinetic energy density. With these notations we define the following quantities

$$\begin{aligned} \mathbf{c}_{1} &= \mathbf{y} \int \rho\left(\mathbf{y}, \vec{\mathbf{z}}\right) \mathbf{x}^{2} \mathbf{d}^{3} \mathbf{r} = \frac{1}{\mathbf{y}} \int \left[ \left(\mathbf{y}, \vec{\mathbf{z}}\right) \mathbf{u}^{1} \mathbf{x} \right] - \int \rho\left(\mathbf{y}, \mathbf{z}_{1} \mathbf{y}, \mathbf{x}^{1}, \mathbf{z}\right) \mathbf{d}^{2} \mathbf{x} \\ \mathbf{B}_{1}\left(\mathbf{y}, \mathbf{y}^{1}\right) &= \int \rho\left(\mathbf{y}, \vec{\mathbf{z}}\right) \rho\left(\mathbf{y}^{1}, \vec{\mathbf{z}}\right) \mathbf{x}^{2} \mathbf{d}^{3} \mathbf{x} \\ &= \mathbf{B}_{2}\left(\mathbf{y}, \mathbf{y}^{1}\right) \approx \int \rho^{2}\left(\mathbf{y}, \vec{\mathbf{z}}\right) \rho\left(\mathbf{y}^{1}, \vec{\mathbf{z}}\right) \mathbf{d}^{3} \mathbf{x} \end{aligned}$$

$$\begin{aligned} & (\mathbf{A}\mathbf{1}) \\ \mathbf{B}_{3}\left(\mathbf{y}, \mathbf{y}^{1}\right) &= \int \vec{\nabla} \rho\left(\mathbf{y}, \vec{\mathbf{z}}\right) \cdot \vec{\nabla} \rho\left(\mathbf{y}^{1}, \vec{\mathbf{z}}\right) \mathbf{d}^{3} \mathbf{x} \\ &= \mathbf{E}_{4}\left(\mathbf{y}, \mathbf{y}^{1}\right) = \int \left(\rho\left(\mathbf{y}, \vec{\mathbf{z}}\right) \mathbf{T}\left(\mathbf{y}^{1}, \mathbf{z}\right) + \rho\left(\mathbf{y}^{1}, \vec{\mathbf{z}}\right) \mathbf{T}\left(\mathbf{y}, \vec{\mathbf{z$$

The functions B are algebraic functions of y and y' namely

$$B_{0}(\gamma,\gamma^{1}) = \gamma_{0}^{3/2} (d_{0}+d_{1}x+d_{2}x^{2})$$

$$B_{1}(\gamma,\gamma^{1}) = \gamma_{0}^{3/2} (e_{0}+e_{1}x+e_{2}x_{2})/2(\gamma+\gamma^{1})$$

$$B_{2}(\gamma,\gamma^{1}) = \frac{1}{\pi^{3}} \left(\frac{\gamma^{2}\gamma^{1}}{2\gamma+\gamma^{1}}\right)^{3/2} (f_{0}+f_{1}u^{2}+f_{2}uv+f_{3}v^{2}+f_{6}u^{2}v^{2}+f_{5}u^{4}+f_{6}u^{6}v^{2})$$

$$B_{3}(\gamma,\gamma^{1}) = 2\pi - \gamma_{0}^{5/2} (g_{0} + g_{1}x + g_{2}x^{2})$$

$$B_{4}(\gamma,\gamma^{1}) = (\gamma+\gamma^{1}) - \gamma_{0}^{3/2} (h_{0}+h_{1}x+h_{2}x^{2}+h_{3}x^{3})/2$$
(A2)

where  $\gamma_0=2\gamma\gamma'/\pi(\gamma+\gamma')$ ,  $x=(\gamma-\gamma')^2/(\gamma+\gamma')^2$ ,  $u=\gamma/(2\gamma+\gamma')$  and  $v=\gamma'/(2\gamma+\gamma')$ . The coefficients c, d, e, f, g and h are given in Table 8 for helium-4, oxygen-16 and calcium-40.

In the case of coupled isoscalar and isovector monopole modes the two generator coordinates are the oscillator parameters  $\gamma_n$  and  $\gamma_p$  of the neutron and proton distributions. Denoting by  $|\gamma_n\gamma_p^{>}$  the corresponding Slater determinant we have from equations 2, 10, 15 and Al

$$\langle \gamma_{\mathbf{n}} \gamma_{\mathbf{p}} | \mathbf{H} | \gamma_{\mathbf{n}}^{\dagger} \gamma_{\mathbf{p}}^{\dagger} \rangle \langle \gamma_{\mathbf{n}} \gamma_{\mathbf{p}} | \gamma_{\mathbf{n}}^{\dagger} \gamma_{\mathbf{p}}^{\dagger} \rangle = \mathbf{E} (\overline{\gamma}_{\mathbf{n}}, \overline{\gamma}_{\mathbf{p}}) - \frac{\hbar^{2}}{2m} \mathbf{c}_{1} (\delta_{\mathbf{n}}^{2} / \overline{\gamma}_{\mathbf{n}} + \delta_{\mathbf{p}}^{2} / \overline{\gamma}_{\mathbf{p}})$$

$$- \frac{t_{1} + t_{2}}{4} (\delta_{\mathbf{n}}^{-} \delta_{\mathbf{p}}^{-})^{2} \mathbf{B}_{1} (\overline{\gamma}_{\mathbf{n}}, \overline{\gamma}_{\mathbf{p}}) , \qquad (A3)$$

where  $\delta_n = \gamma_n - \gamma_n'$ ,  $\delta_p = \gamma_p - \gamma_p'$ ,  $2\widetilde{\gamma}_n = \gamma_n + \gamma_n'$  and  $2\widetilde{\gamma}_p = \gamma_p + \gamma_p'$ . The function  $E(\widetilde{\gamma}_n, \widetilde{\gamma}_p)$  is the expectation value  $\langle \widetilde{\gamma}_n, \widetilde{\gamma}_p | \mathbf{H} | \widetilde{\gamma}_n, \widetilde{\gamma}_p \rangle$ . From the definitions Al this function is

$$\begin{split} \mathbf{E}(\mathbf{\gamma},\mathbf{\gamma}^{*}) &= \frac{\hbar^{2}}{2m} \, \mathbf{G}_{1}\left(\mathbf{\gamma}+\mathbf{\gamma}^{*}\right) + \frac{\mathbf{t}_{d}}{4}\left(1-\mathbf{x}_{0}\right) \left(\mathbf{B}_{0}\left(\mathbf{\gamma},\mathbf{\gamma}\right)+\mathbf{B}_{0}\left(\mathbf{\gamma}^{*},\mathbf{\gamma}^{*}\right)\right) + 2\left(2+\mathbf{x}_{0}\right) \mathbf{B}_{0}\left(\mathbf{\gamma},\mathbf{\gamma}^{*}\right)\right) \\ &+ \frac{\mathbf{t}_{2}\left(\mathbf{B}_{2}\left(\mathbf{\gamma},\mathbf{\gamma}^{*}\right)+\mathbf{B}_{2}\left(\mathbf{\gamma}^{*},\mathbf{\gamma}\right)\right) + \frac{\mathbf{t}_{1}+3\mathbf{t}_{2}}{16}\left(\mathbf{B}_{n}\left(\mathbf{\gamma},\mathbf{\gamma}\right)+\mathbf{B}_{n}\left(\mathbf{\gamma}^{*},\mathbf{\gamma}^{*}\right)\right) + \frac{\mathbf{t}_{1}+\mathbf{t}_{1}}{4} \, \mathbf{B}_{n}\left(\mathbf{\gamma},\mathbf{\gamma}^{*}\right) \\ &+ \frac{3\left(\mathbf{t}_{1}-\mathbf{t}_{2}\right)}{32}\left(\mathbf{B}_{2}\left(\mathbf{\gamma},\mathbf{\gamma}\right)+\mathbf{B}_{0}\left(\mathbf{\gamma}^{*},\mathbf{\gamma}^{*}\right)\right) + \frac{3\mathbf{t}_{1}-\mathbf{t}_{2}}{8} \, \mathbf{B}_{3}\left(\mathbf{\gamma},\mathbf{\gamma}^{*}\right) \end{split} \tag{A4}$$

The expression of the overlap kernel is given by equation 27.

## Appendix B

# Hamiltonian kernel for dipole modes

Let us denote by  $2p(z, \dot{r})$  and  $2T(z, \dot{r})$  the total mass and kinetic energy densities obtained by filling oscillator states with a parameter  $\gamma=m\omega/\hbar$  centered at (0,0,z). We define

$$D_{0}(z) = \int \rho(z, \vec{r}) \rho(-z, \vec{r}) d^{3}r \qquad D_{1}(z) = \int \rho^{2}(z, \vec{r}) \rho(-z, \vec{r}) d^{3}r$$
(B1)
$$D_{2}(z) = \int \vec{\nabla} \rho(z, \vec{r}) \cdot \vec{\nabla} \rho(-z, \vec{r}) d^{3}r \qquad D_{3}(z) = \int (\rho(z, \vec{r}) \uparrow (-z, \vec{r}) + \rho(-z, \vec{r}) \intercal(z, \vec{r})) d^{3}r$$

For dipole modes the generator coordinate is taken to be the distance 2z between the centres of the neutron and proton distributions. Denoting by  $|z\rangle$  the corresponding Slater determinant we obtain from equations 2, 15, 18 and Bl

$$\langle z | H | z' \rangle \langle z/z' \rangle = E(\overline{z}) - \frac{\lambda}{4} \frac{\hbar^2}{2m} \gamma^2 \delta^2 - \frac{t_1 + t_2}{4} \gamma^2 \delta^2 D_0(\overline{z})$$
(B2)

where  $2\overline{z}=z+z^{\prime}$ ,  $\delta=z-z^{\prime}$ ,  $E(\overline{z})=\langle \overline{z} \mid H \mid \overline{z} \rangle$  and where A is the mass of the nucleus. From equations 15 and Bi the function E is found to be

$$E(z) = 2 \frac{h^2}{2m} c_1 \gamma + \frac{t_2}{2} (1-x_0) D_0(0) + \frac{t_0}{2} (2+x_0) D_0(z) + \frac{t_3}{2} D_1(z) + \frac{t_1+3t_2}{8} D_3(0) + \frac{t_1+t_2}{2} D_3(z) + \frac{3(t_1-t_2)}{16} D_2(0) + \frac{3t_1-t_3}{8} D_2(z)$$
(B3)

where  $c_1$  is given in Table 9. Simple analytic expressions for the functions B, which can be derived in a straightforward but tedious way, are given in reference 30.

#### Appendix C

27.

## Energy weighted sum rules and the generator coordinate method

Let us first prove a preliminary statement.

Let S be a Hilbert subspace and  $\{|m\rangle\}$  a set of eigenvectors (with eigenvalues  $E_m$ ) of the projection of the hamiltonian  $\hat{H}_i$  on S,  $|0\rangle$  being the ground state in S. Let  $\hat{O}$  be an operator such that  $\tilde{O}|0\rangle$  belongs to S then one has the relation

$$\frac{1}{2} < 0 | [\hat{0}, [\hat{H}, \hat{0}] ] | 0 \rangle = \sum_{m} (E_{m} \sim E_{0}) | \langle m | \hat{0} | 0 \rangle |^{2}$$
(D1)

In other words the E.W.S.R. corresponding to  $\hat{O}$  is exhausted in the subspace S. Indeed

$$\frac{1}{2} <0 |[\hat{0},[\hat{H},\hat{0}]]|0> = <0 |\hat{0}|\hat{H}|\hat{0}|0> -\frac{1}{2} <0 |\hat{0}|\hat{0}|\hat{H}|0> -\frac{1}{2} <0 |\hat{H}|\hat{0}|\hat{0}|0>$$

By definition the states { | m>} verify

$$\langle \mathbf{n} | \hat{H} | \mathbf{n} \rangle = \mathbf{E}_{\mathbf{n}} \delta_{\mathbf{n}\mathbf{n}}$$
 (D2)

Using this property and the fact that  $\hat{O}|O\rangle$  belongs to S one obtains

and

$$\frac{1}{2} (<0|\hat{0} \ \hat{0} \ \hat{H}|0> \ \ <0|\hat{H} \ \hat{0} \ \hat{0}|0>) = \sum_{m} E_{0} ||^{2} Q.E.D.$$

When S is the G.C.M. space spanned by a set of wave functions {|a>} the G.C.M. ground state |0> is a linear combination of states |a>. Therefore proving that  $\hat{O}|a>$  belongs to S will prove that  $\hat{O}|0>$  also belongs to S.

When { | a> } is the set of Slater determinants

 $\Psi(\gamma_z, \gamma_{\perp})$  containing the <u>lowest</u> oscillator wave functions  $\varphi_1(\gamma_z, \gamma_{\perp}, \vec{r})$  $(1 \le i \le A)$  and  $\hat{0}$  the one-body operator  $(\sum_{i=1}^{2} z_i^2)$  one has

$$\begin{pmatrix} \hat{\Gamma} \\ i=1 \end{pmatrix} \begin{pmatrix} \hat{\tau}_{z} \\ i \end{pmatrix} \Phi(\gamma_{z}, \gamma_{\perp}) = -\frac{d}{d\gamma_{z}^{i}} \Phi(\gamma_{z}^{i}, \gamma_{\perp}) \begin{pmatrix} \gamma_{z}^{i} \\ \gamma_{z}^{i} \end{pmatrix} \begin{pmatrix} \gamma_{z}^{i} \\ \gamma_{z}^{i} \end{pmatrix} (D3)$$

A similar property implying derivatives with respect to  $\gamma_{\perp}$  holds for the operator  $\sum_{i=1}^{A} (\chi_{1}^{2} + \gamma_{1}^{2})$ . This proves that within the space spanned i=1 by the functions  $\varphi(\gamma_{2}, \gamma_{\perp})$  the monopole and quadrupole isoscalar sum rule are exhausted. Mutatis mutandis a similar proof holds for the isovector monopole and quadrupole sum rules.

When  $|\alpha\rangle$  is the set of Slater determinant  $\Psi(z_0)$ containing the <u>lowest</u> oscillator wave functions  $\Psi_1(\gamma,\gamma,\vec{r}-z_0\vec{k})$  $(\Psi_1(\gamma,\gamma,\vec{r}+z_0\vec{k}))$  for neutrons (protons) and  $\hat{O}$  the one-body operator.  $\hat{A}$ ( $\sum_{i=1}^{L} z_i \tau_i$ )  $(\tau_i = 1$  for neutrons, -1 for protons) one has i=1 $\begin{pmatrix} \hat{E} & z_i \tau_i \\ z_i \tau_i \end{pmatrix} \Phi(z_0) = \frac{1}{2\gamma} \frac{d}{dz_0} \Phi(z_0) \Big|_{z_0=z_0} \Phi(z_0)$  (D4)

This relation proves that in the space spanned by  $\Phi(z_0)$  the dipole isovector sum rule is exhausted.

# Table Captions

Table 1	Parameters of the SKyrme interactions SIII and SIV. Notations and units are those of Ref.5
Table 2	Energies of the three first solutions of the Hill-Wheeler equation for isoscalar monopole modes. The minimum $E_v$ of the energy calculated with oscillator w.f. is also shown
Table 3	Results of a G.C.M. treatment of coupled isoscalar monopole and quadrupole modes (SIII)
Table 4	Energies $E_Q$ of the giant isoscalar quadrupole resonance. The values of the isoscalar quadrupole incompressibility $K_Q$ (see text) are also shown
Table 5	Results of a G.C.M. treatment of coupled isoscalar and isovector monopole modes (SIII)
Table 6	Energies in MeV of the giant isovector monopole resonance
Table 7	Energies in MeV of the two first solutions of the Hill-Wheeler equation for isovector dipole modes. The values of the isovector dipole incompressibility $K_z$ in MeV fm <sup>-2</sup> (see text) are also shown.
Table 8	Numerical values of the coefficients $c, d, e, f, g, h$ and $i$ occuring in Eqs. 42 and 23

Table 1

	t,	t,	t2	t,	×e	W
\$I <b>I</b> I	-1128.75	395.0	-95.0	14000.0	.0.45	120.0
SIV	-1205.6	765.0	35.0	5000.0	0.05	150.0

# Table 2

		4 <sub>He</sub>	16 <sub>0</sub>	40 <sub>Ca</sub>
	e <sub>v</sub>	-26.40	-139.16	-402.5
	Eo	-32.93	-140.32	-403.26
SIII	Bı	~ 5.35	-108.65	-374.86
	E2	-	- 81.75	-346.97
	ΔΕ,	27,58	31.67	28.4
	E <sub>v</sub>	-26.72	-138.82	-403,88
	R <sup>6</sup>	-32.04	-139.66	-404.42
SIV	E	~ 5.69	-109.42	-377.2
	Ē2	-	- 83.67	-350.64
	ΔΒ,	26.35	30.24	27.22

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		E Mev	AE MeV	r fm	Q fm <sup>2</sup>	EMS MeVfm <sup>4</sup>	EQS MeVfm <sup>4</sup>
	٥	-35.58	-	1.69	4	-	
4 <sub>ile</sub>	1	- 8.06	27.52	2.39	18.5	108.7	916.8
	2	- 6.39	29.19	2.67	-9.4	312.1	343.7
1 <sup>6</sup> 0	0	-140.41	-	2.62	0.2	-	-
	1	-118.38	22.03	2.73	13.1	4.2	17012.2
	2	-107.58	32.83	2.90	0.1	7467.1	17.0
	0	-403.41	-	3,40	0.6	-	-
<sup>40</sup> са	1	-386.01	17.4	3.43	14.6	0.1	73300.8
	2	-375.50	27.9	3.47	2.6	36249.1	2.3

Table 4

	16		40 <sub>Ca</sub>		
	EQ MeV	K <sub>Q MeV</sub>	EQ MeV	K <sub>Q MeV</sub>	
SIII	22.03	4.67	17.40	4,60	
SIV	25.59	6.68	22.06	6.69	

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Table 5

		E MeV	ΔE	r fm	EMS MeVfm <sup>4</sup>	emv Mevfm <sup>4</sup>
	0	~33.83	-	1.78	-	-
.4 He	ł	- 5.02	28.8	3.00	220.7	0.0
•	2	'- 4.18	29.65	2.98	0.0	347.3
;	0	-141.03	-	2.61	-	-
۱۰ <sub>۵</sub>	i	,-109.19	31.84	2.81	8239.8	0.0
I	2	-100.38	40.65	2.73	0.0	10352.3
	0	-104.08	-	3,40	-	-
40 Ca	ı	-375.59	28 <b>.5</b> Ú	3.48	37641.1	0.0
	2	- 168 - 18	\$5.4	3.44	0.0	47642.3

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Table 6

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	1.6	40 <sub>Ca</sub>
sitt	40.65	35,90
STV	43.49	41.09

Table 7

		<sup>4</sup> Ke	16 <sub>0</sub>	40 <sub>Ca</sub>
SIII	E <sub>0</sub>	-27.64	-139.89	-402.99
	E.	- 0.63	-115.59	-382.99
	ĸz	3.8	2.64	1.74
SIV	E <sub>9</sub>	-26.86	-138.86	-403,88
	E 1	- 0.24	-112.57	-382.71
	K <sub>z</sub>	3.03	2.04	1.32

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	C1	de	d.	da	eq	<b>6</b> 1	81	fo	f1	f2	fı.
<sup>4</sup> He	3	4	0	0	12	0	0	в	0	0	0
<sup>16</sup> 0	18	31	-15	0	177	-105	0	32	120	240	0
40 <sub>Ca</sub>	60	19 <u>45</u> 16	<u>645</u> 8	. <u>945</u> 16	157 <u>97</u> 16	<u>9135</u> 16	<u>10395</u> 16	125	750	0	575
	f,	fs	f <sub>6</sub>	go .	gı	g2	h,	hı	h2	h1	je
4 <sub>8e</sub>	0	0	0	12	0	0	6	6	0,	o	1
<sup>16</sup> 0	840	0	0	57	-105	0	249 2	0	- <u>105</u> 2	0	<u>116</u> 9
40 <sub>Ca</sub>	0	4725	135135	<u>2595</u> 16	<u>- 4095</u> 8	<u>10395</u> 16	<u>23715</u> 32	<u>7035</u> 32	<u>7875</u> 32	1 <u>0395</u> 32	<u>2060</u> 27

# Figure Captions

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Figure 1	Weight-functions g for the first three G.C.M. states of oxygen-15 in the case of monopole vibra- tions. The diagonal part of the energy kernel is also indicated by the dot- dot- dashed line (SIII).
Figure 2	Ground-state weight-functions $g_0$ for monopole vibra- tions in helium-4, oxygen-16 and calcium-40 (SIII).
∀igure 3	Density and form factor of helium-4 calculated with harmonic oscillator wave-functions (H.D.), with the Hartree-Fock method (H.F.) and with the generator coordinate method (G.C.). Experimental data are taken from reference 27 (SIII).
Pigure 4	Ground state weight-functions $g_0$ for quadrupole isoscalar vibrations in helium-40, oxygen-16 and calcium-40 (SIII).
Figure 5	Contour plot of the first three weight-functions g for coupled isoscalar monopole and quadrupole vibrations in calcium-40 (SIII).
Figure ó	Contour plot of the first three weight-functions g for coupled isoscalar and isovector monopole vibra- tions in oxygen-16 (SIII).
Figure 7 '	Weight-functions g for the first three G.C.M. Ftates of calcium-40 in the case of dipole vibrations. The diagonal part of the energy kernel is also indicated by the dot- dot- dashed curve (SIII).
Figure 8	Ground state weight functions g, for dipole vibra- tions in helium-4, oxygen-16 and calcium-40 (SIII).





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Fig.3





Fig.5



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Fig.7



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