VARIATIONAL APPROACH TO THE NUCLEAR COLLECTIVE MOTION (*)

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ABSTRACT — A new method for obtaining a classical collective hamiltonian is presented. The starting point is the many-body hamiltonian and the derivation is based on the variational principle of quantum mechanics. The force and mass parameters are determined without ambiguity by the single particle energies and by some matrix elements of the two-body interaction. The theory is applied to the dipole state of $^{16}0$. Our results, which have been obtained by a simple calculation, compare favourably with results obtained by the diagonalisation of the R. P. A. matrix, but the present method is valid even when the groundstate of the nucleus can not be represented by a single Slater determinant.

RÉSUMÉ — On présente une dérivation de l'hamiltonien collectif fondée sur le principe variationel dependent du temp de la mécanique quantique. La théorie developée est apliquée à l'étude de l'état dipolaire de $^{16}0$. Les résultats, obtenus par un calcul très simple, peuvent être comparés favorablement avec les résultats de la diagonalisation de la matrice de la R. P. A. La présente méthode est valable même quand l'état nucléaire fondamentale ne peut pas être représenté par un seul determinant de Slater.

1. *INTRODUCTION*

The collective behaviour of nuclei may be understood from two different starting points. The first one is based on a phenomenological collective hamiltonian (1) which governs the motion of a small number of collective variables, but contains unspecified parameters, to be

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determined experimentally. This approach leads to a relatively simple calculational scheme, but, since it is phenomenological, it contains arbitrary features. The second starting point for the description of collective states is based on the consideration of the exact many-body hamiltonian. This approach gives rise to the so called microscopic theory (2) of the collective motion, is more powerful, more fundamental, but is also harder to carry out in practice. Therefore it would be convenient to eliminate the arbitrariness from the collective hamiltonian used in the first approach by determining its parameters, not phenomenologically but from first principles. As it has recently been remarked by BELYAEV (3), who has investigated already this question, one would obtain in this way a method having the advantages, but not the drawbacks, of the two previously mentioned methods. Actually, the problem of determining the parameters of the collective hamiltonian on a more or less fundamental basis is not new, since it has been treated in the past by several authors (4). We will consider again the same problem, but from a different point of view, which is related to the time-dependent Hartree-Fock derivation of the Random Phase Approximation (R. P. A.). We will derive the equations of motion for the collective variables — and, therefore, the collective hamiltonian — by a rather simple procedure, based directly on the time dependent variational principle of quantum mechanics.

2. *THE COLLECTIVE HAMILTONIAN*

The exact hamiltonian of a N-body system, having two-body interactions between the particles, is of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2M} + \sum_{i<j=1}^{N} v_{ij} \quad . \tag{1}$$

Since in general it is practically impossible to diagonalise a hamiltonian of this kind, it is convenient to describe the states of the system to which it corresponds by means of an independent particle wave functions Φ. These model wave functions $\Phi = \Phi(\zeta)$ contain a number of real parameters ζ, corresponding to the size and deformation of the potential well with the help of which the single particle wave functions have been determined, or refering to the distance between the centers of the wells for protons and neutrons, etc. We may assume, without loss of generality, that the values $\zeta = 0$ of

the parameters minimize the expectation value of the hamiltonian,

$$\left[\frac{\partial}{\partial \zeta} < \Phi(\zeta) \mid H \mid \Phi(\zeta) >\right]_{\zeta=0} = 0 . \tag{2}$$

Then, the wave function $\Phi_o = \Phi(0)$ will represent the groundstate. It may be remarked that, since the wave functions $\Phi(\zeta)$ are (usually) real, for real ζ, the minimum of the expectation value of the hamiltonian will be obtained for $\zeta = 0$, even if one allows the parameters ζ to become complex.

In order to describe the excited states of our system we may use the time dependent variational principle (we consider $\hbar/2\pi = 1$),

$$-i\,[\,<\delta\Phi \mid \dot{\Phi}> - <\dot{\Phi} \mid \delta\Phi>\,] + \delta <\Phi \mid H \mid \Phi> = 0, \tag{3}$$

but now we must allow the parameters ζ to become complex,

$$\zeta = \xi + i\,\eta\ , \tag{4}$$

so that the norm of the wave functions is not preserved. Considering $\Phi(\zeta)$ to be real and normalized to unity for real ζ, we have, indeed,

$$<\Phi(\zeta) \mid \Phi(\zeta)> = <\Phi_o \mid \Phi_o> - \frac{1}{2}(\zeta^* - \zeta)^2 <\partial\Phi/\partial\xi \mid \partial\Phi/\partial\xi> + \ldots . \tag{5}$$

The wave function Φ must, therefore, be multiplied by a complex normalising factor. Instead of eq. (3), we obtain in this way the following equation (5)

$$-\frac{i}{2}\left[\delta\frac{<\Phi \mid \dot{\Phi}> - <\dot{\Phi} \mid \Phi>}{<\Phi \mid \Phi>} + \frac{d}{dt}\,\frac{<\delta\Phi \mid \Phi> - <\Phi \mid \delta\Phi>}{<\Phi \mid \Phi>}\right] + \\ + \delta\,\frac{<\Phi \mid H \mid \Phi>}{<\Phi \mid \Phi>} = 0 . \tag{6}$$

A simple calculation leads to the following results

$$-\frac{i}{2}\left[\delta\frac{<\Phi \mid \dot{\Phi}> - <\dot{\Phi} \mid \Phi>}{<\Phi \mid \Phi>} + \frac{d}{dt}\,\frac{<\delta\Phi \mid \Phi> - <\Phi \mid \delta\Phi>}{<\Phi \mid \Phi>}\right] = \\ = 2\,\mathrm{M}\,(\delta\xi\,\dot{\eta} - \delta\eta\,\dot{\xi}) \tag{7}$$

$$\frac{<\Phi \mid H \mid \Phi>}{<\Phi \mid \Phi>} = E_o + N\,\xi^2 + P\,\eta^2 + \ldots \tag{8}$$

with

$$E_o = <\Phi_o \mid H \mid \Phi_o> \tag{9}$$

$$M = <\partial\Phi / \partial\xi \mid \partial\Phi / \partial_\xi >_{\zeta=0} \tag{10}$$

$$N = \frac{1}{2}\left[\frac{\partial^2}{\partial\xi^2}<\Phi \mid H \mid \Phi>\right]_{\zeta=0} \tag{11}$$

$$P = 2 <\partial\Phi / \partial\xi \mid H \mid \partial\Phi / \partial\xi>_{\zeta=0} - 2\,E_o\,M - N \tag{12}$$

With the help of eq. (6) we arrive finally at the equations of motion for one collective variable, in the limit of small oscillations,

$$M\,\dot{\eta} + N\,\xi = 0\ , \tag{13}$$

$$M\,\dot{\xi} - P\,\eta = 0\ . \tag{14}$$

The case of several collective variables may also be obtained as a straight forward generalisation of these equations but, for simplicity, we do not consider that situation now. By eliminating η we finally have

$$\frac{M^2}{P}\,\ddot{\xi} + N\,\xi = 0\ , \tag{15}$$

so that the frequency of the collective oscillations, which can be interpreted as the excitation energy of the collective state, is given by

$$\omega_o = \frac{\sqrt{P\,N}}{M}\cdot \tag{16}$$

We are now able to write down the classical collective hamiltonian H_c, corresponding to eq. (15),

$$H_c = \frac{1}{2}\frac{\mathrm{P}}{\mathrm{M}^2}\,\not{p}_\xi^2 + \frac{1}{2}\,\mathrm{N}\,\xi^2, \tag{17}$$

where $\not{p}_\xi$ denotes the momentum conjugated with the variable ξ and is given by

$$\not{p}_\xi = \frac{\mathrm{M}^2}{\mathrm{P}}\,\dot{\xi} = \mathrm{M}\,\eta\,. \tag{18}$$

We obtain in this way a simple interpretation of the imaginary part of ζ.

If Φ_o is a SLATER determinant of orthonormalized single particle wave functions and if $\Phi(\xi)$ may be written in the form

$$\Phi(\xi) = exp\left[i\,\xi \sum_{i=1}^{N} \varkappa_i\right]\Phi_o\,, \tag{19}$$

where $\varkappa$ represents an hermitian operator, then we may rewrite eqs. (9) — (12) as follows

$$\mathrm{E}_o = \sum_i < i \mid \frac{\not{p}^2}{2\,M} \mid i > + \sum_{i<j} < ij \mid v \mid ij > \tag{20}$$

$$\mathrm{M} = \sum_{i\,m} < i \mid \varkappa \mid m > < m \mid \varkappa \mid i > \tag{21}$$

$$\mathrm{N} = -\frac{1}{2}\left[\sum_i < i \mid [\varkappa, [\varkappa, \frac{\not{p}^2}{2M}]] \mid i > \right.$$

$$\left. + \sum_{i<j} < ij \mid [\,(\varkappa_1 + \varkappa_2), [\,(\varkappa_1 + \varkappa_2), v_{12}\,]\,] \mid ij > \right], \tag{22}$$

$$\mathrm{P} = 2\Big\{\sum_{i\,m\,n} < i \mid \varkappa \mid m > \Big[< m \mid \frac{\not{p}^2}{2M} \mid n > + \sum_k < mk \mid v_{12} \mid nk > \Big] < n \mid \varkappa \mid i >$$

$$- \sum_{i\,j\,m} < m \mid \varkappa \mid i > \Big[< i \mid \frac{\not{p}^2}{2M} \mid j > + \sum_k < ik \mid v_{12} \mid jk > \Big] < j \mid \varkappa \mid m >$$

$$+ \sum_{i\,m\,j\,n} < i \mid \varkappa \mid m > < mj \mid v_{12} \mid in > < n \mid \varkappa \mid j > \Big\} - \mathrm{N}\,. \tag{23}$$

We use the letters i, j, k, etc., to denote occupied single particle states and the lecters m, n, etc., to denote unoccuppied states, and by the kets $| a\ b >$ we mean normalized antissymmetric two-body wave functions.

We end this section by noting that eqs. (13) and (14), governing the time evolution of the collective variable, might also have been derived, together with eqs. (20) — (23), from the THOULESS variational principle (2) for the R. P. A.. Nevertheless, in some sense, the present method is more general than the R. P. A., because it might be applied even if the groundstate could not be represented by a single Slater determinant (for instance, if the groundstate is the result of a superposition of two Slater determinants).

3. *TRANSITION PROBABILITIES*

We will study now the effect of an external time dependent field $W(t)$. In order to investigate the evolution of our system in the presence of this perturbation, we add to the previously calculated expectation value of the hamiltonian H (eq. (8)), the linear terms in ζ of the expectation value of $W(t)$,

$$\frac{< \Phi \mid W(t) \mid \Phi >}{< \Phi \mid \Phi >} = \mathrm{W}^{(0)}(t) + 2\,\xi\,\mathrm{W}^{(1)}(t) \tag{24}$$

with

$$\mathrm{W}^{(0)}(t) = < \Phi_o \mid W(t) \mid \Phi_o > , \tag{25}$$

$$\mathrm{W}^{(1)}(t) = < \partial\,\Phi \,/\, \partial\,\xi \mid W(t) \mid \Phi >_{\zeta=0} . \tag{26}$$

Now we have, with the help of the variational principle expressed by eq. (6),

$$\mathrm{M}\,\dot{\eta} + \mathrm{N}\,\xi + \mathrm{W}^{(1)}(t) = 0 , \tag{27}$$

$$\mathrm{M}^{\cdot} - \mathrm{P}\,\eta = 0 . \tag{28}$$

Although it is very easy to integrate this system as it stands, it is convenient to make the transformation

$$\zeta = \xi + i\,\eta , \tag{29}$$

$$\zeta^* = \xi - i\,\eta , \tag{30}$$

in order to establish the connection with the usual R. P. A. result (2). The equations for the variables ζ, ζ^* may be cast into the matrix form

$$i\,\mathrm{M}\begin{pmatrix} \dot{\zeta} \\ -\dot{\zeta}^* \end{pmatrix} - \begin{pmatrix} \frac{1}{2}(\mathrm{N}+\mathrm{P}) & \frac{1}{2}(\mathrm{N}-\mathrm{P}) \\ \frac{1}{2}(\mathrm{N}-\mathrm{P}) & \frac{1}{2}(\mathrm{N}+\mathrm{P}) \end{pmatrix}\begin{pmatrix} \zeta \\ \zeta^* \end{pmatrix} = \mathrm{W}^{(1)}(t)\begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{31}$$

We start by considering the eigenvalue problem,

$$\mathrm{M}\,\omega\begin{pmatrix} x \\ -y \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(\mathrm{N}+\mathrm{P}) & \frac{1}{2}(\mathrm{N}-\mathrm{P}) \\ \frac{1}{2}(\mathrm{N}-\mathrm{P}) & \frac{1}{2}(\mathrm{N}+\mathrm{P}) \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}. \tag{32}$$

The solutions of this problem are the following

$$\begin{pmatrix} x_{+1} \\ y_{+1} \end{pmatrix} = \frac{1}{2}(\mathrm{N}\,\mathrm{P})^{-\frac{1}{4}}\begin{pmatrix} \sqrt{\mathrm{N}}+\sqrt{\mathrm{P}} \\ \sqrt{\mathrm{N}}-\sqrt{\mathrm{P}} \end{pmatrix},\quad \omega_{+1} = \omega_o \tag{33}$$

$$\begin{pmatrix} x_{-1} \\ y_{-1} \end{pmatrix} = \frac{1}{2}(\mathrm{N}\,\mathrm{P})^{-\frac{1}{4}}\begin{pmatrix} \sqrt{\mathrm{N}}-\sqrt{\mathrm{P}} \\ \sqrt{\mathrm{N}}+\sqrt{\mathrm{P}} \end{pmatrix},\quad \omega_{-1} = -\omega_o \tag{34}$$

These eigenvectors satisfy the following normalisation condition

$$(x_\lambda \quad -y_\lambda)\begin{pmatrix} x_\gamma \\ y_\gamma \end{pmatrix} = \frac{\omega_\gamma}{|\,\omega_\gamma\,|}\,\delta_{\lambda\gamma}. \tag{35}$$

In order to solve eq. (31) we expand the vector $(\zeta \;\; \zeta^*)$ in the basis of the eigenvectors of eq. (32)

$$\begin{pmatrix} \zeta(t) \\ \zeta^*(t) \end{pmatrix} = \sum_\lambda c_\lambda(t)\begin{pmatrix} x_\lambda \\ y_\lambda \end{pmatrix} e^{-i\omega_\lambda t} \tag{36}$$

Then, eqs. (31) and (35) lead to the following equation for the quantities $c_\lambda(t)$,

$$i\,\mathrm{M}\,\dot{c}_\lambda = \lambda\,(x_\lambda + y_\lambda)\,\mathrm{W}^{(1)}(t)\,e^{i\omega_\lambda t} = \lambda\,(\mathrm{N}/\mathrm{P})^{\frac{1}{4}}\,\mathrm{W}^{(1)}(t)\,e^{i\omega_\lambda t} \tag{37}$$

This equation is easily integrated. Assuming the field $W(t)$ is switched on at time $-T$, we get for $c_\lambda(T)$,

$$c_\lambda(T) = -i\frac{\lambda}{M}\left(\frac{N}{P}\right)^{\frac{1}{4}} \int_{-T}^{+T} W^{(1)}(t)\ e^{i\omega_\lambda t}\ dt$$

$$\cong -i\frac{\lambda}{M}\left(\frac{N}{P}\right)^{\frac{1}{4}} 2\pi\, W^{(1)}(\omega_\lambda)\ , \tag{38}$$

where we denote by $f(\omega)$ the FOURIER transform of $f(t)$,

$$f(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(t)\ e^{i\omega t}\ dt \tag{39}$$

In order to interpret eq. (29) we consider now the change in the expectation value of the unperturbed hamiltonian. A simple calculation yields

$$\frac{<\Phi \mid H \mid \Phi>}{<\Phi \mid \Phi>} - E_o = \frac{1}{2}(\zeta^* \quad \zeta)\begin{pmatrix} \frac{1}{2}(N+P) & \frac{1}{2}(N-P) \\ \frac{1}{2}(N-P) & \frac{1}{2}(N+P) \end{pmatrix}\begin{pmatrix} \zeta \\ \zeta^* \end{pmatrix} \tag{40}$$

$$= \omega_o M\, c_{+1}\, c_{-1}$$
$$= \omega_o M \mid c_{+1} \mid^2 \ .$$

This result shows that the matrix element of an operator W, between the groundstate $|0)$ and the excited (dipole) state $|d)$, should be identified with

$$(d \mid W \mid 0) = \frac{1}{\sqrt{M}}\left(\frac{N}{P}\right)^{\frac{1}{4}} W^{(1)} \ . \tag{41}$$

We note, finally, that under the hypothesis of eq. (19), $W^{(1)}$ may be written

$$W^{(1)} = -i \sum_{in} <i \mid \varkappa \mid n> <n \mid W \mid i> \ . \tag{42}$$

4. *NUMERICAL EXAMPLE: THE DIPOLE STATE OF* ^{16}O. *CONCLUSIONS.*

As a numerical example we will investigate the dipole state of ^{16}O. We will represent the groundstate of this nucleus by a Slater determinant of harmonic oscillator wave functions and we will neglect the spin orbit splitting (this is permissible because ^{16}O is a closed shell nucleus in both *j-j* and *L-S* coupling schemes). The single particle wave functions may, therefore, be represented by

$$|\, i\,) = |\, t_i\,)\, |\, s_i\,)\, |\, \mu_i\,) \tag{43}$$

were $|\, t_i)$ denotes an isospin statevector, $|\, s_i)$ a spin statevector and $|\, \mu_i)$ an orbital wave function. Actually $|\, \mu_i) = |\, \mu_i', \mu_i'', \mu_i''')$ the quantum numbers μ_i', μ_i'' and μ_i''' denoting the number of oscillator quanta in the three spacial directions. We only need the following one-dimensional oscillator wave functions

$$\varphi_o(q) = \sqrt{\frac{\alpha}{\pi}}\, e^{-\frac{1}{2}\alpha q^2} \tag{44}$$

$$\varphi_1(q) = \sqrt{\frac{\alpha}{\pi}} \cdot \sqrt{2\alpha}\, q\, e^{-\frac{1}{2}\alpha q^2} \tag{45}$$

$$\varphi_2(q) = \sqrt{\frac{\alpha}{\pi}} \cdot \frac{1}{\sqrt{2}} (2\alpha q^2 - 1)\, e^{-\frac{1}{2}\alpha q^2} \tag{46}$$

We assume a δ-function 2-body interaction, which we write in standard notation,

$$v_{12} = V_o (a + b\, \vec{\sigma}_1 \cdot \vec{\sigma}_2 + c\, \vec{\tau}_1 \cdot \vec{\tau}_2 + d\, (\vec{\sigma}_1 \cdot \vec{\sigma}_2)\, (\vec{\tau}_1 \cdot \vec{\tau}_2))\, \delta(\vec{r}_1 - \vec{r}_2) \tag{47}$$

The parameter ξ is the distance between the centers of the wells for protons and neutrons. We describe the dipole oscilations of ^{16}O with the help of the wave function

$$\Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N/2}, \vec{r}_1', \vec{r}_2', \ldots, \vec{r}_{N/2}') =$$
$$= \Phi_o(\vec{r}_1 + \tfrac{\vec{\xi}}{2}, \vec{r}_2 + \tfrac{\vec{\xi}}{2}, \ldots, \vec{r}_{N/2} + \tfrac{\vec{\xi}}{2}, \vec{r}_1' - \tfrac{\vec{\xi}}{2}, \vec{r}_2' - \tfrac{\vec{\xi}}{2}, \ldots, \vec{r}_{N/2}' - \tfrac{\vec{\xi}}{2}),$$

where $\vec{r}$ and $\vec{r'}$ are the coordinates of protons and neutrons. The wave function Φ may also be written in the form

$$\Phi = exp\left[-i\frac{\xi}{2}\sum_{k=1}^{N}\tau_{z_k}\,p_{z_k}\right]\Phi_o\ . \tag{48}$$

Denoting now by $\mu, \nu, \lambda, \ldots$ the occupied space orbitals and by $\sigma, \rho, \ldots$ the unoccupied space orbitals, we have, with the help of eqs. (20)-(23),

$$\begin{aligned} M &= \sum_{\mu\rho}(\mu\,|\,p_z\,|\,\rho)\,(\rho\,|\,p_z\,|\,\mu) \\ &= 2\,\alpha \end{aligned} \tag{49}$$

$$\begin{aligned} N &= -\frac{V_o}{2}(a-2\,c-3\,d)\sum_{\mu\nu}(\mu\nu|\,[(p_{z_1}+p_{z_2}),[(p_{z_1}+p_{z_2}),v_{12}]]\,|\,\mu\nu) \\ &= -V_o\left(\frac{\alpha}{2\pi}\right)^{\frac{3}{2}}(a-2\,c-3\,d)\ .\ \frac{19}{2}\,\alpha \end{aligned} \tag{50}$$

$$\begin{aligned} P+N = 2\Big\{&\sum_{\mu\rho}(\mu\,|\,p_z\,|\,\rho)\Big[(\rho\,|\,\frac{\vec{p}^2}{2M}\,|\,\rho)+V_o(3\,a-3\,b-3\,c-9\,d) \\ &\sum_{\lambda}(\mu\,\lambda\,|\,\delta(\vec{r}_1-\vec{r}_2)\,|\,\rho\,\lambda) \\ &-\Big((\mu\,|\,\frac{\vec{p}^2}{2M}\,|\,\mu)+V_o(3\,a-3\,b-3\,c-9\,d) \\ &\sum_{\lambda}(\mu\,\lambda\,|\,\delta(\vec{r}_1-\vec{r}_2)\,|\,\mu\,\lambda)\Big)\Big](\rho\,|\,p_z\,|\,\mu) \\ &+V_o(-a-3\,b+5\,c+3\,d)\sum_{\mu\rho\nu\sigma}(\mu\,|\,p_z\,|\,\rho) \\ &(\rho\,\nu\,|\,\delta(\vec{r}_1-\vec{r}_2)\,|\,\mu\,\sigma)\,(\sigma\,|\,p_z\,|\,\nu)\Big\} \\ = \frac{2}{M}\alpha^2 &- V_o\left(\frac{\alpha}{2\pi}\right)^{\frac{3}{2}}(4\,a-8\,c-12\,d)\ .\ \frac{19}{8}\,\alpha\ . \end{aligned} \tag{51}$$

For the dipole operator

$$D = \frac{1}{2}\sum_i \tau_{z_i}\,z_i \tag{52}$$

we have

$$\begin{aligned} D^{(1)} &= < \partial \Phi \,/\, \partial \xi \,|\, D \,|\, \Phi >_{\zeta=0} \\ &= -i \sum_{\mu\rho} (\mu \,|\, z \,|\, \rho)\ (\rho \,|\, \dot{p}_z \,|\, \mu) \\ &= \mathrm{M}\,\alpha^{-1} \ . \end{aligned} \tag{53}$$

The size of the oscillator well and parameters of the force are given the same numerical values which had been used by BROWN, CASTILLEJO and EVANS (6)

$$\sqrt{\alpha} = 0{,}675 \ \ f^{-1} \ , \qquad a = 0{,}865 \ ,$$

$$\frac{V_o}{4\pi}\,\alpha^{\frac{3}{2}} = -8{,}5 \ Mev \ , \qquad b = 0{,}135 \ ,$$

$$c = d = 0 \ .$$

Considering also that $\mathrm{M}^{-1} = 41,\ 48\ Mev$ and using eqs. (16) and (41), we finally get

$$\omega_o = 24{,}5 \ Mev \ ,$$
$$(d \,|\, \mathrm{D} \,|\, 0) \ = \ 2\,f \ .$$

We have obtained the whole dipole strength localized in one single level because we are using a collective hamiltonian to describe the nuclear dinamics. Of course, in actual fact the dipole strength appears distributed over several levels, and if one solves the complete R. P. A. equations (7), the main features of the structure of the dipole state appear already. With the exception of this aspect our slide-rule results agree well with the results of more sophisticated calculations (consider, for instance, ref. (7)).

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