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DERIVATION OF AN ADIABATIC TIME-DEPENDENT HARTREE-FOCK FORMALISM FROM A VARIATIONAL PRINCIPLE

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ABSTRACT

A derivation of the adiabatic time dependent Hartree-Fock formalism is given, which is based on a variational principle analogous to Hamilton's principle in classical mechanics. The method leads to a Hamiltonian for collective motion which separates into a potential and a kinetic energy and gives mass and potential parameters in terms of the nucleon-nucleon interaction. The adiabatic approximation assumes slow motion but not small amplitudes and can therefore describe anharmonic effects. The RPA is a limiting case where both amplitudes and velocities are small. The variational approach provides a consistent way of extracting coordinates and momenta from the density matrix and of obtaining equations of motion when particular trial forms for this density matrix are chosen. One such choice leads to Thouless-Valatin formula. An other choice leads to irrotational hydrodynamics.

1 - Introduction

If one assumes that the wave function of a many-body system is a Slater determinant varying with time, its self-consistent motion is given by the time-dependent Hartree-Fock (TDHF) formalism which was first formulated by Dirac[1] in 1930. In recent years TDHF has often been used to derive the random phase approximation (RPA). This approximation, which has many applications in nuclear physics, describes small vibrations about a static Hartree-Fock solution. Many collective motions however do not have small amplitudes and most low energy spectra are not harmonic. We have in mind for instance the dynamics of soft nuclei, of fission and of fusion. These processes are characterized by the fact that their collective velocity is slow compared to some single-particle velocity. In these cases the adiabatic time-dependent Hartree-Fock (ATDHF) approximation, which does not require small amplitudes, is valid. In this paper we will closely follow the spirit and notations of refs[2-3] where ATDHF was derived and studied.

There have already been several applications of the ATDHF approximation to nuclear physics problems. Thouless and Valatin[4] showed the existence of rotating solutions of the TDHF equations and used the adiabatic approximation to derive a formula for the moment of inertia of a slowly rotating nucleus. The adiabaticity is also at the root of the cranking formula[5]. However inconsistencies in this formula have often been discussed[6-7], and indeed the ATDHF formalism gives corrections to the cranking formula. The works of Baranger and Kumar[7], Belyaev[8] and Villars[9] are closely related to the present formulation. In their investigation of soft nuclei Baranger and Kumar used a separable quadrupole force, neglecting the exchange matrix elements. The present work originated in an attempt to generalize their formalism to an arbitrary interaction. In fact no assumption about the interaction was made in Belyaev's work in which the pairing

correlations were also included by using the Hartree-Bogolyubov formalism. Many of the ideas underlying the present work were already contained in Belyaev's paper which does not seem to have received enough attention. There is also a close connection with Villars' work although we will not attempt a detailed comparison between his work and ours. The recent investigations of nuclear hydrodynamics by Bertsch[10] and Wong et al.[11] are related to ATDHF. Other recent works concerned with ATDHF can be found in refs.[12,13]. The main feature of the present paper is the derivation of the ATDHF equations from a variational procedure analogous to Hamilton's principle in classical mechanics.

One of the aims of the ATDHF formalism is to provide a microscopic foundation for successful phenomenological models and at the same time to derive directly from the two-body force the potential an inertial parameters occuring in these models[14]. In the ATDHF theory an adiabatic expansion is made which allows the collective energy to be separated into potential and kinetic parts. In ref[3] equations of motion were derived by carrying this adiabatic expansion in the time-even and time-odd parts of the TDHF equation. The coherence of the formalism was established by verifying that these equations of motion could be written in a Lagrangian form. In the present paper we proceed in a somewhat different way by deriving the adiabatic Lagrangian and the corresponding Hamilton equations directly from a variational principle[15]. We believe that this procedure clarifies and simplifies the derivation of the entire formalism. The connection between ATDHF and classical mechanics, which has been discussed in ref[3], is established here through the Hamiltonian formalism. The Hamilton equations obtained here have a different form from the equations of motion of ref[3] and are shown to be equivalent. Moreover the form of the adiabatic Lagrangian which we obtain makes it clear that the matrix elements of ρ_o and χ, which are the operators entering the fundamental transformation (2-13), correspond respectively to classical coordinates and momenta.

In their most general form the equations of motion would be very difficult to solve. Particular kinds of collective motion can be studied by introducing trial forms for the operators ρ_o and χ . In this case the variational approach has the added advantage of leading unambiguously to a collective Hamiltonian. We consider two examples of restrictions on ρ_o and χ . In the first ρ_o is assumed to be a function of a single real variable and χ is unrestricted. In the second χ is assumed to be local in coordinate space and ρ_o is unrestricted. In the second case one obtains hydrodynamical equations similar to those of ref[10].

The present paper is self-contained except for a proof of the existence and the uniqueness of the decomposition (2-13). This proof can be found in ref[3] together with more detailed discussions of the physical content of the theory.

2 - The time-dependent Hartree-Fock [illegible]

Consider the [illegible]

$$I = \int_{t_1}^{t_2} \mathcal{L} \, dt \qquad [illegible]$$

with $\mathcal{L} = (\Psi(t), (i \frac{\partial}{\partial t} - H) \Psi(t))$.

In this equation and throughout the paper we [illegible]. For an arbitrary variation [illegible] of $\Psi(t)$ between t_1 and t_2 [illegible] the fixed end point conditions [illegible], the stationarity condition [illegible] leads to the time-dependent Schrödinger equation,

$$i \frac{\partial \Psi}{\partial t} = H \Psi . \qquad [illegible]$$

If $\Psi(t)$ is restricted to be a single Slater determinant then the variational principle [illegible] leads to the time-dependent Hartree-Fock (TDHF) equation[1,2] .

To the Slater determinant $\Psi(t)$ there corresponds a time-dependent density matrix $\rho(t)$ such that

$$\rho = \rho^{+} , \qquad \rho = \rho^2 , \qquad \mathrm{Tr}\,\rho = n , \qquad (2-4)$$

n being the number of particles of the system (in this paper we shall only consider cases for which n is even). The properties (2-4) express the well-known fact that ρ is a projector which can be written as

$$\rho(t) = \sum_{M=1}^{n} | \psi_M(t) > < \psi_M(t) | , \qquad (2-5)$$

where $\psi_M(t)$ are single-particle wave functions and the index M refers to the occupied states.

In terms of the density matrix ρ, the TDHF equation reads

$$i \dot{\rho} = [W, \rho] , \qquad (2-6)$$

where W is the Hartree-Fock Hamiltonian. Its matrix elements are given in an arbitrary single-particle basis $|\alpha\rangle$ by

$$\langle\alpha|W|\gamma\rangle = \langle\alpha|T|\gamma\rangle + \sum_{\beta\delta} \langle\alpha\beta|\tilde{V}|\gamma\delta\rangle \langle\delta|\rho|\beta\rangle . \qquad (2\text{-}7a)$$

In eq. (2-7a) the operator T is the kinetic energy and $\langle\alpha\beta|\tilde{V}|\gamma\delta\rangle$ is an antisymmetrized matrix element of the interaction V (for reasons of simplicity we will assume that H includes only two-body forces). The expectation of H for the Slater determinant $\Psi(t)$ is given by the expression

$$E=\langle\Psi|H|\Psi\rangle=\sum_{\alpha\gamma}\langle\alpha|T|\gamma\rangle\langle\gamma|\rho|\alpha\rangle + \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\gamma|\rho|\alpha\rangle\langle\alpha\beta|\tilde{V}|\gamma\delta\rangle\langle\delta|\rho|\beta\rangle . \qquad (2\text{-}8a)$$

In a more symbolic notation we will write

$$W = T + \mathrm{Tr}\,\tilde{V}\rho, \qquad (2\text{-}7b)$$

$$E = \mathrm{Tr}\,T\rho + \frac{1}{2}\mathrm{Tr}\,\mathrm{Tr}\,\rho\tilde{V}\rho . \qquad (2\text{-}8b)$$

for eqs. (2-7a) and (2-8a) respectively.

The static H F equation

$$[W,\rho] = 0, \qquad (2\text{-}9)$$

obviously corresponds to a particular solution of eq. (2-6).

It is easily shown from eq. (2-6) that if $\rho^2 = \rho$ at t = 0, this remains true at all times. It is also easy to see from eqs. (2-6) and (2-8) that the energy E is constant in time. Indeed from the relation

$$\delta E = \mathrm{Tr}\,W\,\delta\rho , \qquad (2\text{-}10)$$

one has

$$\frac{dE}{dt} = \mathrm{Tr}\,W\frac{d\rho}{dt} , \qquad (2\text{-}11)$$

and, using eq. (2-6)

$$\frac{dE}{dt} = -i\,\mathrm{Tr}\,W[W,\rho] = 0. \qquad (2\text{-}12)$$

If the determinant $\Psi(t)$ is given at t = 0,

the first order eq. (2-6) determines the trajectory followed by the system in the non-linear space of determinants. This situation is reminiscent of classical mechanics. In this case the trajectory in phase space is determined by Hamilton's equations once the initial coordinates and momenta are given. In eq. (2-6) however we have only one set of variables, i.e. the matrix elements of ρ, instead of the usual sets of coordinates and momenta. The analogy with classical mechanics suggests extracting from $\rho(t)$ a part which corresponds to a set of classical coordinates and a part which corresponds to their momenta.

We can find a transformation which makes this extraction possible by using the fact that the density operator is non-invariant under time reversal. Moreover this transformation can be chosen in such a way that our coordinates still correspond to a determinant. For this purpose the decomposition

$$\rho(t) = U^{+}(t)\rho_{o}(t)U(t) \ , \tag{2-13a}$$

was introduced in refs[2-3] where

$$U(t) = e^{-i\chi(t)} \ . \tag{2-13b}$$

In eqs. (2-13) the single-particle operators $\rho_{o}(t)$ and $\chi(t)$ are both hermitian and even under time-reversal. More precisely ρ_{o} and χ are assumed to satisfy the conditions

$$\rho_{o} = \rho_{o}^{+} = K\,\rho_{o}\,K^{+} \ , \tag{2-14a}$$

$$\chi = \chi^{+} = K\,\chi\,K^{+} \ , \tag{2-14b}$$

where K is the usual antiunitary quantal time-reversal operator $K=-i\sigma_{y}K_{o}$ [17].

Equations (2-13) and conditions (2-14) do not determine $\rho_{o}(t)$ and $\chi(t)$ in a unique way ; we will come back to this point at the end of sect. 5.

It is clear from eqs. (2-13) and conditions (2- 4) that ρ_{o} is also a projector. Therefore the wave function corresponding to ρ_{o} is a time-even Slater determinant $\Psi_{o}(t)$

which is related to $\Psi(t)$ by

$$\Psi(t) = e^{i\chi(t)} \Psi_o(t) \ . \qquad (2\text{-}15)$$

The density ρ_o can be written as

$$\rho_o(t) = \sum_{M=1}^{N} |\varphi_M(t)\rangle\langle\varphi_M(t)| \ , \qquad (2\text{-}16)$$

where the set of the single-particle wave functions φ_M is left invariant by the time-reversal operator K. In terms of the single-particle wave functions eq. (2-13a) reads

$$\varphi_M(\underset{\sim}{x},t) = U(t)\varphi_M(\underset{\sim}{x},t) \ . \qquad (2\text{-}17)$$

With this notation the first term of $\mathcal{L}$ (see eq. (2-2)) can be written under the form

$$\begin{aligned}(\Psi|\frac{\partial}{\partial t}|\Psi) &= \sum_M \langle\varphi_M|\frac{\partial}{\partial t}|\varphi_M\rangle = \sum_M \langle\varphi_M, U\frac{\partial}{\partial t} U^+|\varphi_M\rangle \\ &= \sum_M \langle\varphi_M|\dot{U}U^+|\varphi_M\rangle + \sum_M \langle\varphi_M|\frac{\partial}{\partial t}|\varphi_M\rangle \ .\end{aligned} \qquad (2\text{-}18)$$

The last term of eq. (2-18) vanishes because of the time-reversal property of the set φ_M. Inserting a closure relation in the remaining term we have

$$(\Psi|\frac{\partial}{\partial t}|\Psi) = \sum \mathrm{Tr}\ \dot{U}^+|\varphi_M\rangle\langle\varphi_M|U = \mathrm{Tr}\ \dot{U}^+\rho_o\ U \ , \qquad (2\text{-}19)$$

and finally obtain

$$i(\Psi|\frac{\partial}{\partial t}|\Psi) = i\ \mathrm{Tr}\ \dot{e}^{iX}\ \rho_o\ e^{-iX} \ . \qquad (2\text{-}20)$$

3 - The adiabatic approximation

Although it would be of great interest, we are not looking in this paper for an exact solution of eq. (2-6), but for a microscopic description of certain types of collective motion. We would like, through this description, to establish

a connection with successful phenomenological models, and in particular with the Copenhagen collective model[14]. We would then have microscopic expressions for various inertial parameters entering into these models. As in the Copenhagen hamiltonian we want our collective energy to separate into potential and kinetic parts, the potential part depending only on some "coordinates" and the kinetic part being quadratic in the corresponding velocities (or conjugate momenta) with coefficients depending only on the coordinates. There is no a priori reason why the expression (2-8) should be of this form unless it is simplified by some approximation taking into account the specific character of the collective motion we intend to describe. Most instances of collective motion are slow compared to single-particle motion and it is natural to introduce the adiabatic approximation. This we do by assuming that in the decomposition (2-13) the dimensionless operator χ is small so that $U(t)$ can be expanded as a rapidly converging power series in χ.

Indeed for an even nucleus in the static situation of eq. (2-9) the nuclear density would be completely time-even. This cannot be the case for the matrix ρ, solution of eq. (2-6). However, if the motion is adiabatic, the time-odd part of ρ should be small.

Let us begin then by expanding eq. (2-13) up to second order in χ :

$$\rho(t) = \rho_0(t) + \rho_1(t) + \rho_2(t) + \ldots \qquad (3-1)$$

with

$$\rho_1(t) = i[\chi, \rho_0] \ , \qquad (3-2)$$

$$\rho_2(t) = -\frac{1}{2}[\chi[\chi, \rho_0]] \ . \qquad (3-3)$$

To this order, $\rho_1(t)$ is the time-odd part of $\rho(t)$.

In order to derive the adiabatic Lagrangian we now expand eq. (2-2) to the same order in χ .

For the first term (2-20) we obtain

$$i\,\mathrm{Tr}\ [illegible] \ldots +\ldots)\rho_o(1-i\chi-\frac{\chi^2}{2}+\ldots)$$

$$= [illegible] -\frac{1}{2}\ \mathrm{Tr}\ \rho_o[\dot\chi,\chi] +\ldots \quad (3-4)$$

The second term of eq. (3-4) vanishes. Indeed if the operators A and B are hermitian and if A is time-even and B time-odd one always has

$$\mathrm{Tr}\ AB = 0 . \quad (3-5)$$

Since the operators ρ_o and $i[\dot\chi,\chi]$ fulfil these conditions, we are left with

$$i(\Psi|\frac{\partial}{\partial t}|\Psi) = -\mathrm{Tr}\ \rho_o\dot\chi = \mathrm{Tr}\ \dot\rho_o\chi - \frac{d}{dt}\mathrm{Tr}\ \rho_o\chi . \quad (3-6)$$

In deriving eq. (3-6) we have neglected terms of the type $\dot\chi\rho_o\chi^2$ i.e. we have assumed that $\dot\chi$ is small, at least to the same extent as χ .

Carrying the expansion in χ to the second term (2-8) of $\mathcal{L}$, we obtain in terms of the operators ρ_o, ρ_1 and ρ_2

$$E_a = \mathrm{Tr}\ T\rho_o + \frac{1}{2}\mathrm{Tr}\mathrm{Tr}\rho_o\tilde V\rho_o + \mathrm{Tr}T\rho_2 + \frac{1}{2}\mathrm{Tr}\mathrm{Tr}\rho_1\tilde V\rho_1 + \mathrm{Tr}\mathrm{Tr}\rho_o\tilde V\rho_2 . \quad (3-7)$$

All the first order terms have disappeared because of their time-reversal properties (see eq. (3-5)).

We can divide the adiabatic energy E_a into two terms

$$E_a = \mathcal{K} + \mathcal{V} , \quad (3-8)$$

where $$\mathcal{V} = \mathrm{Tr}\ T\rho_o + \frac{1}{2}\ \mathrm{Tr}\ \mathrm{Tr}\ \rho_o\ \tilde V\ \rho_o , \quad (3-9)$$

$$\mathcal{K} = \mathrm{Tr}\ T\rho_2 + \mathrm{Tr}\mathrm{Tr}\rho_o\tilde V\rho_2 + \frac{1}{2}\mathrm{Tr}\mathrm{Tr}\rho_1\tilde V\rho_1 = \mathrm{Tr}W_o\rho_2 + \frac{1}{2}\mathrm{Tr}W_1\rho_1 , \quad (3-10)$$

with $W_o = T + \mathrm{Tr}\ \tilde V\ \rho_o$, (3-11a) $\qquad W_1 = \mathrm{Tr}\ \tilde V\ \rho_1$. (3-11b)

The term $\mathcal{V}$ is independent of χ . One sees

moreover that eq. (3-9) is the expression of the Hartree-Fock energy for the density ρ_o. Hence

$$\mathcal{V}(\rho_o) = (\Psi_o|H|\Psi_o) \quad , \tag{3-12}$$

where Ψ_o is the Slater determinant corresponding to the density ρ_o. The important point is that the second term $\mathcal{K}(\rho_o,\chi)$ is now quadratic in χ.

We have thus obtained for the adiabatic Lagrangian the expression

$$\mathcal{L}_a = -\mathrm{Tr}\rho_o\dot{\chi} - E_a(\rho_o,\chi) = \mathrm{Tr}\chi\dot{\rho}_o - \mathcal{V}(\rho_o) - \mathcal{K}(\rho_o,\chi) - \frac{d}{dt}\mathrm{Tr}\rho_o\chi \quad , \tag{3-13}$$

which, except for the total derivative, is similar to the expression

$$L = \sum_i p_i\dot{q}_i - H(q_i,p_i) = \sum_i p_i\dot{q}_i - V(q) - T(p,q) \tag{3-14}$$

of a Lagrangian in classical mechanics, V and T being respectively the potential and kinetic energies.

From the analogy between eqs. (3-13) and (3-14) we can immediately draw several important consequences. It first suggests that matrix elements of the operators ρ_o and χ correspond respectively to classical coordinates and to their conjugate momenta. The energy $\mathcal{V}(\rho_o)$ appears as a potential energy and $\mathcal{K}(\rho_o,\chi)$, which is quadratic in the momentum χ, as the associated kinetic energy.

Independent variations of the action integral A

$$A = \int_{t_1}^{t_2} L \; dt \quad , \tag{3-15}$$

with respect to q_i and p_i lead to Hamilton's equations. Consequently we will obtain the "adiabatic Hamilton equations" by performing separate variations of ρ_o and χ in the

corresponding action integral

$$I_a = \int_{t_1}^{t_2} \mathcal{L}_a \, dt \quad . \tag{3-16}$$

As is well known the variation of the action $\bar{I}_a$

$$\bar{I}_a = \int_{t_1}^{t_2} \bar{\mathcal{L}}_a \, dt = \int_{t_1}^{t_2} (\mathrm{Tr}\chi\dot{\rho}_o - E_a(\rho_o,\chi))dt \quad , \tag{3-17}$$

with fixed end points for ρ_o leads to the same Hamilton equations as the variation of I_a with fixed end points for χ. Our coordinates being ρ_o we prefer to use the Lagrangian $\bar{\mathcal{L}}_a$ which corresponds more closely to the classical Lagrangian (3-14). Another important consequence of the analogy between (3-13) and (3-14) is that

$$\mathcal{H}(\rho_o,\chi) = \frac{1}{2}\,\mathrm{Tr}\,\chi\dot{\rho}_o \quad . \tag{3-18}$$

This can be verified simply by making the scale variation $\rho_o = \alpha\rho_o$ in eq. (3-17) where α is a small real number. Since $\mathcal{H}(\rho_o,\chi)$ is homogeneous and quadratic in χ

$$\delta\mathcal{H} = 2\alpha\mathcal{H} \, . \tag{3-19}$$

Hence $\delta\bar{\mathcal{L}}_a = \mathrm{Tr}\,(\delta\chi\dot{\rho}_o) - \delta\mathcal{H} = \alpha(\mathrm{Tr}\chi\dot{\rho}_o - 2\mathcal{H})$, (3-20)

and $\delta\bar{I}_a = 0$ gives eq. (3-18).

At the beginning of this section we introduced the adiabatic approximation as an expansion in powers of χ. Since we have shown that χ plays the role of a momentum such an expansion now appears to be completely appropriate for the description of adiabatic motion.

4 - Variation of the adiabatic action $\bar{I}_a$

We now proceed to calculate the variation of the adiabatic action $\bar{I}_a$ with respect to ρ_o and χ. In making this variation one has to bear in mind the restrictions

(2-14) on ρ_o and χ and also the condition $\rho_o^2 = \rho_o$. This last constraint implies that $\delta\rho_o$ has only particle-hole matrix elements with respect to the projector ρ_o since the relation

$$\rho_o \delta\rho_o \rho_o = \sigma_o \delta\rho_o \rho_o = 0 \ , \qquad (\sigma_o = 1 - \rho_o) \tag{4-1}$$

follows from

$$\delta\rho_o = \rho_o \delta\rho_o + \delta\rho_o \rho_o \ . \tag{4-2}$$

By expanding eq. (2-10) up to second order we obtain the variation of the collective energy E_a

$$\delta E_a = \mathrm{Tr}\ (W_o \delta\rho_o + W_2 \delta\rho_o + W_1 \delta\rho_1 + W_c \delta\rho_2) \ . \tag{4-3}$$

In eq. (4-3) W_o, W_1, W_2 are the zero, first and second-order parts of the Hartree-Fock hamiltonian W ; also W_o, W_2 , $\delta\rho_o$, $\delta\rho_2$ are time-even while W_1 and $\delta\rho_1$ are time-odd. These time reversal properties are a consequence of restrictions (2-14) on ρ_o and χ . The first order terms $\mathrm{Tr}W_1\delta\rho_o$ and $\mathrm{Tr}W_o\delta\rho_1$ have disappeared from eq. (4-3) because of eq. (3-5).

We will denote by δ^I and δ^{II} the variations at constant ρ_o and χ respectively that is :

$$\begin{aligned} &\delta^I \rho_o = 0 \qquad \text{hence} \quad \delta\rho_o = \delta^{II}\rho_o \ , \\ &\delta^{II}\chi = 0 \qquad \text{hence} \quad \delta\chi = \delta^I\chi \ , \end{aligned} \tag{4-4}$$

and the total variation of the adiabatic Lagrangian $\overline{\mathcal{L}}_a$ is

$$\delta\overline{\mathcal{L}}_a = \delta^I\overline{\mathcal{L}}_a + \delta^{II}\overline{\mathcal{L}}_a = \mathrm{Tr}\left(\frac{\partial\overline{\mathcal{L}}_a}{\partial\rho_o}\,\delta\rho_o + \frac{\partial\overline{\mathcal{L}}_a}{\partial\chi}\,\delta\chi\right), \tag{4-5}$$

where eq. (4-5) defines the operators $\dfrac{\partial\overline{\mathcal{L}}_a}{\partial\rho_o}$ and $\dfrac{\partial\overline{\mathcal{L}}_a}{\partial\chi}$.

I) We first vary χ keeping ρ_o constant. We have

$$\delta^I\rho_o = 0 \ , \tag{4-6a}$$

$$\delta^I\rho_1 = i[\delta\chi, \rho_o], \tag{4-6b}$$

$$\begin{aligned} \delta^I\rho_2 &= -\tfrac{1}{2}[\delta\chi,[\chi,\rho_o]] - \tfrac{1}{2}[\chi,[\delta\chi,\rho_o]] \\ &= i[\delta\chi,\rho_1] + \tfrac{1}{2}\rho_o \ldots \rho_o \end{aligned} \tag{4-6c}$$

... the Jacobi identity has been used in eq. (4-6c).

We now vary E_a with respect to χ. Using ... we obtain

$$\delta_{\chi} \ldots = \ldots + \tfrac{1}{2}\,\mathrm{Tr}\,W_0[\rho_0,[\chi,\delta\chi]] + \mathrm{Tr}W_1[\chi,[\chi,\delta\chi]] + \tfrac{1}{2}\,\mathrm{Tr}W_0[\rho_0,[\chi,\delta\chi]]$$

$$= -i\,\mathrm{Tr}\{[W_1,\rho_0] + [W_0,\chi] + \tfrac{i}{2}[[W_0,\rho_0],\chi]\}\delta\chi \quad , \tag{4-7}$$

where we have used the property $\mathrm{Tr}[A,B]C = \mathrm{Tr}\,A[B,C]$. (4,8)
It only remains to vary the kinetic term of $\mathcal{L}_a$, which gives

$$\delta^{I}(\mathrm{Tr}\dot{\rho}_0\chi) = \mathrm{Tr}\,\dot{\chi}\delta\rho_0 \quad . \tag{4-9}$$

We have therefore

$$\delta\mathcal{L}_a = \mathrm{Tr}\{\dot{\rho}_0\chi + i[W_1,\rho_0] + i[W_0,\chi] - \tfrac{1}{2}[[W_0,\rho_0],\chi]\}\delta\chi \quad . \tag{4-10}$$

(II) Let us now vary ρ_0 keeping χ constant. We have

$$\delta^{II}\ldots = i[\chi,\ldots]\ldots \quad , \tag{4-11a}$$

$$\delta^{II}W_1 = -\tfrac{1}{2}[\chi,[\chi,\delta\rho_0]] \quad . \tag{4-11b}$$

Using eqs. (4-3) and (4-11) we obtain for the energy E_a

$$\delta^{II}E_a = \mathrm{Tr}\frac{\delta E_a}{\delta\rho_0}\delta\rho_0 = \mathrm{Tr}W_0\delta\rho_0 - \tfrac{1}{2}\mathrm{Tr}W_0[\chi,[\chi,\delta\rho_0]] + i\mathrm{Tr}W_1[\chi,\delta\rho_0] + \mathrm{Tr}W_2\delta\rho_0$$

$$= \mathrm{Tr}\{W_0 + W_2 + i[W_1,\chi] - \tfrac{1}{2}[[W_0,\chi],\chi]\}\delta\rho_0 \quad , \tag{4-12}$$

and for the kinetic energy term

$$\delta^{II}(\mathrm{Tr}\dot{\rho}_0\chi) = -\mathrm{Tr}\,\dot{\chi}\delta\rho_0 + \frac{d}{dt}\,\mathrm{Tr}(\chi\delta\rho_0) \quad . \tag{4-13}$$

We have therefore

$$\delta^{II}\mathscr{L}_a = \frac{d}{dt}\,\mathrm{Tr}(\chi\,\delta\rho_o) + \mathrm{Tr}(-\dot{\chi} - W_o - W_2 - i[W_1,\chi] + \tfrac{1}{2}[[W_o,\chi],\chi])\,\delta\rho_o \quad (4\text{-}14)$$

Using eqs. (4-10) and (4-14) the total variation of the adiabatic action $\bar{I}_a$ finally reads

$$\begin{aligned}\delta\bar{I}_a = \delta^{I}\bar{I}_a + \delta^{II}\bar{I}_a &= 0 = \int_{t_1}^{t_2}\mathscr{L}_a\,dt \\ &= \mathrm{Tr}(\chi\,\delta\rho_o)\Big]_{t_1}^{t_2} + \int_{t_1}^{t_2}\mathrm{Tr}\{(\dot{\rho}_o + i[W_1,\rho_o] - i[W_o,\chi] \\ &\quad - \tfrac{1}{2}[[W_o,\rho_o],\chi])\,\delta\chi \\ &\quad + (-\dot{\chi} - W_o - W_2 - i[W_1,\chi] + \tfrac{1}{2}[[W_o,\chi],\chi])\,\delta\rho_o\}dt \quad . \qquad (4\text{-}15)\end{aligned}$$

The first term vanishes because of the fixed end-point conditions and eq. (4-15) can be rewritten as

$$\delta\bar{I}_a = \int_{t_1}^{t_2}\mathrm{Tr}\{(\dot{\rho}_o - \frac{\partial E_a}{\partial\chi})\,\delta\chi - (\dot{\chi} + \frac{\partial E_a}{\partial\rho_o})\,\delta\rho_o\}\;dt = 0 \quad . \qquad (4\text{-}16)$$

Since $\delta\chi$ and $\delta\rho_o$ are independent variations, we must have separately

$$\mathrm{Tr}(\dot{\rho}_o - \frac{\partial E_a}{\partial\chi})\,\delta\chi = \mathrm{Tr}(\dot{\rho}_o + i[W_o,\rho_1] + i[W_1,\rho_o] - \tfrac{1}{2}[[W_o,\rho_o],\chi])\,\delta\chi = 0 \quad , \qquad (4\text{-}17a)$$

$$\mathrm{Tr}(\dot{\chi} + \frac{\partial E_a}{\partial\rho_o})\,\delta\rho_o = \mathrm{Tr}(\dot{\chi} + W_o + W_2 + i[W_1,\chi] - \tfrac{1}{2}[[W_o,\chi],\chi])\,\delta\rho_o = 0 \,. \qquad (4\text{-}17b)$$

5 - The adiabatic Hamilton equations in the general case

5.1) Derivation of the Hamilton equations

In the most general case, that is when no constraints other than conditions (2-14) and $\rho_o = \rho_o^2$ are imposed on ρ_o and χ, eqs. (4-17) have to be satisfied for all hermitian and time-even variations of the operators ρ_o and χ. However because of eq. (4-1), the condition (4-17b) can be satisfied if, and only if, the particle-hole matrix elements of the

operator multiplying $\delta\rho_o$ vanish. Therefore the extremum condition (4-17) lead to the equations :

$$\dot{\rho}_o - \frac{\partial E_1}{\partial \rho_o} = \dot{\rho}_o + i[W_o, \rho_o] - \frac{1}{2}[[W_o, \rho_o], \chi] = 0 \,, \qquad (5\text{-}1a)$$

$$\dot{\rho}_o - \frac{\partial E_1}{\partial \rho_o} = \dot{\rho}_o + i[W_o, \rho_o] - \frac{1}{2}[[W_o, \rho_o], \chi]) \rho_o = 0 \,, \qquad (5\text{-}1b)$$

where eq. (5-1b) holds only between hole-particle and (by hermitian conjugation) particle-hole matrix elements.

From eq. (3-2), ρ_1 is of the same order as χ (and from eq. (3-3) χ is of order χ^2). The last three terms of eq. (5-1a) are then at least of first order. We assume that there is no accidental cancellation in these terms and that their sum is of first order. Therefore, if eq. (5-1) is to be satisfied, $\dot{\rho}_o$ should be of the same order as $\Delta\chi$, where Δ is some frequency characteristic of the single particle motion determined by the operator W_o.

Let us now turn our attention to eq. (5-1b). Its last three terms are clearly at least of order two. As for the first term, we have already assumed in sect.3 that $\dot{\chi}$ is at least of the same order as $\Delta\chi$. All the terms in eq. (5-1b) are therefore obviously at least of first order in χ except $\dot{\rho}_o W_o \rho_o$. This shows that if the motion is adiabatic, the particle-hole matrix elements of W_o should be small, at least of first order in χ. It is also equivalent to saying that the commutator $[W_o, \rho_o]$ is at least of first order.

This is reasonable because in the static case the Hartree-Fock equation is

$$[W_o, \rho_o] = 0 \,. \qquad (5\text{-}2)$$

In the adiabatic case this condition cannot be fulfilled exactly but the commutator $[W_o(t), \rho_o(t)]$ is small : the system is almost in equilibrium at all times.

The smallness of $[W_o, \rho_o]$ has two other

important consequences. The first is that the last term of the first order eq. (5-1a) can be neglected since it is at least of second order. The second consequence is that in the remaining equation

$$i\dot{\rho}_o = [W_o,\rho_1] + [W_1,\rho_o] \quad , \tag{5-3}$$

only the particle-hole and hole-particle matrix elements are meaningful. This is obvious for the term $[W_1,\rho_o]$. For $\dot{\rho}_o$ it results from the relation

$$\dot{\rho}_o = \rho_o\dot{\sigma}_o + \dot{\rho}_o\sigma_o \quad , \tag{5-4}$$

which is obtained by differentiating the condition $\rho_o^2 = \rho_o$ with respect to the time. Finally the Jacobi identity

$$[W_o,\rho_1] = i[W_o,[\chi,\rho_o]] = i[[W_o,\chi],\rho_o] + i[\chi,[W_o,\rho_o]] \tag{5-5}$$

and eqs. (5-8) and (5-9) show that the particle-particle and hole-hole matrix elements of $[W_o,\rho_1]$ are at least second order and hence should be neglected.

The Hamilton equations (5-1) resulting from the extremum condition $\delta\bar{I}_a = 0$ can therefore be rewritten

$$\dot{\rho}_o\dot{\rho}_o\sigma_o = \rho_o \frac{\partial E_a}{\partial \chi}\sigma_o \quad , \tag{5-6A}$$

$$\rho_o\dot{\chi}\sigma_o = -\rho_o \frac{\partial E_a}{\partial \rho_o}\sigma_o \quad , \tag{5-6B}$$

where $$\rho_o \frac{\partial E_a}{\partial \chi}\sigma_o = -i[\rho_o W_o\rho_o+\sigma_o W_o\sigma_o,\rho_1]-i[W_1,\rho_o] \quad , \tag{5-7a}$$

$$\rho_o \frac{\partial E_a}{\partial \rho_o}\sigma_o = \rho_o(W_o+W_2+i[W_1,\chi]-\tfrac{1}{2}[[W_o,\chi]\chi))\sigma_o \, . \tag{5-7b}$$

Notice that, when the auxiliary conditions (5-16) are chosen, the last term of eq. (5-7b) can be neglected. Indeed it is easily shown, again using the smallness of $\rho_o W_o \sigma_o$, that this last term is at least third order.

By taking the hermitian conjugates of eqs. (5-6) we obtain the corresponding equations for the particle-hole matrix elements.

5.2) A different form for the second Hamilton equation

In ref.[3] equations of motion have been obtained in a somewhat different way by carrying out directly the expansion (3-1) in the time-odd and time-even parts of eq. (2-1). The first order equation was the same as (5-6A). To show the equivalence of the other equation we write eq. (5-6B) in a different form.

We have already used the property that the condition

$$\rho_0 G \rho_0 = 0 \quad , \tag{5-8}$$

where G is hermitian, is equivalent to

$$[\rho_0, G] = 0 \quad . \tag{5-9}$$

We can then write eq. (5-6B) as

$$[\dot{\chi}, \rho_0] + [W_0 + W_2, \rho_0] + i[[W_1, \chi], \rho_0] - \tfrac{1}{2}[[[W_0, \chi], \chi], \rho_0] = 0 \quad . \tag{5-10}$$

After some manipulations involving Jacobi identities, we obtain for the different terms of eq. (5-10) :

$$[\dot{\chi}, \rho_0] = -i\dot{\rho}_1 + [\dot{\rho}_0, \chi] \quad , \tag{5-11}$$

$$[[W_1, \chi], \rho_0] = [[W_1, \rho_0], \chi] - i[W_1, \rho_1] \quad , \tag{5-12}$$

$$-\tfrac{1}{2}[[[W_0, \chi], \chi], \rho_0] = [W_0, \rho_2] + i[[W_0, \rho_1], \chi] - \tfrac{1}{2}[[[W_0, \rho_0], \chi], \chi] \quad . \tag{5-13}$$

Finally eq. (5-10) can be written as

$$-i\dot{\rho}_1 + [W_0, \rho_0] + [W_2, \rho_0] + [W_1, \rho_1] + [W_0, \rho_2]$$

$$+[\dot{\rho}_0 + i[W_1, \rho_0] + i[W_0, \rho_1] - \tfrac{1}{2}[[W_0, \rho_0], \chi]), \chi] = 0 \quad . \tag{5-14}$$

If eq. (5-7a) is satisfied then eq. (5-14) reduces to

$$i\dot{\rho}_1 = [W_0, \rho_0] + [W_2, \rho_0] + [W_1, \rho_1] + [W_0, \rho_2] \quad , \tag{5-15}$$

which is precisely the second equation of motion of ref.[3].

5.3) Some comments on the equations of motion

[illegible] the validity of the adiabatic approximation is the smallness of the dimensionless operator χ. Indeed through eq. (5-3) it ensures the smallness of $\dot{\rho}_0$ and of the collective velocities. Because $\dot{\rho}_0$ involves products of amplitudes by frequencies there are two interesting limiting cases which are both compatible with adiabatic motion.

In the first case the amplitudes of the motion are small but the frequencies can be comparable with single-particle frequencies. The operator $\dot{\chi}$ (or equivalently $\dot{\rho}_1$), which is of order χ times a collective frequency, is in this case of first order. In eq. (5-7b) the terms

$$\rho_0 (W_2 + i[W_1,\chi_1] - \frac{1}{2}[[W_0,\chi_1],\chi_1])\rho_0$$

are of second order in χ and can be neglected. The remaining term $\rho_0 W_0 \rho_0$ (or equivalently the commutator $[W_0,\rho_0]$ in eq. (5-15)) must be of first order. In this limit eqs. (5-6) reduce to R.P.A.

In the second case the amplitudes of the motion are large but [illegible] frequencies are small compared with characteristic single particle frequencies. Then $\dot{\chi}$ (and $\dot{\rho}_1$) is of second order because both χ and the collective frequencies are small. All terms on the right hand side of eq. (5-7b) (or (5-15)), including $\rho_0 W_0 \rho_0$ (or $[W_0\rho_0]$), must then be small of second order and all must be retained when solving the equations. These two limiting cases are studied in more detail in ref.[3].

Clearly the equations (5-6A) and (5-6B) do not determine all the matrix elements of χ. Both have only particle-hole matrix elements. The number of independent equations in each set is equal to the number of independent matrix elements of $\dot{\rho}_0$, which is less than the total number of matrix elements of χ (see eq. (5-4)). Hence the matrix elements

of χ need to be restricted by some auxiliary conditions. One natural way of doing this is to impose on χ the supplementary conditions

$$\rho_o \chi \rho_o = \bar{\rho}_o \chi \bar{\rho}_o = 0 \quad , \tag{5-16}$$

which mean that, as in the case of $\dot{\rho}_o$, the particle-particle and hole-hole matrix elements of χ are zero.

The arbitrariness for χ which we have just mentionned is related to the non-uniqueness of the decomposition (2.13). In fact the supplementary conditions (5-16) make this decomposition unique as shown in ref.[3]. The conditions (5-16) are compatible with the equations of motion (5-6). Differentiating $\rho_o \chi \rho_o$ with respect to time gives

$$\frac{d}{dt}(\rho_o \chi \rho_o) = \rho_o \dot{\chi} \rho_o + \dot{\rho}_o \chi \rho_o + \rho_o \chi \dot{\rho}_o \quad . \tag{5-17}$$

Since the equations (5-6) do not provide any information on the first term of the right hand side of eq. (5-17), the left hand side is not restricted by the equations of motion and conditions (5-16) can be imposed at all times.

Once the conditions (5-16), or perhaps some other ones, are imposed, eqs. (5-6) determine the adiabatic path $\rho_o(t)$ and the momentum $\chi(t)$ when the initial conditions are fixed.

6 - Restricted choices of ρ_o and χ

The equations obtained in the preceding section are very general and difficult to solve numerically with unrestricted ρ_o and χ. If additional constraints are imposed on ρ_o and χ equations of motion are still obtained from the variational principle $\delta I_a = 0$ and are just the eqs. (4-17) where the constraints on ρ_o and χ imply supplementary restrictions on $\delta\rho_o$ and $\delta\chi$.

6.1) Density depending on a single parameter

A particularly interesting case is to pick a trial family of time-even Slater determinants $\rho_o(q_1 \ldots q_n)$ depending on n real collective parameters q_α and to leave χ unrestricted (except for the supplementary conditions (5-16)). In this case eq. (4-17a) still leads to eqs. (5-6A) and (5-7a), or equivalently to eq. (5-3). On the other hand the restricted choice of ρ_o implies that $\delta\rho_o$ in eq. (4-17b) must have the form

$$\delta\rho_o = \sum_\alpha \frac{\partial\rho_o}{\partial q_\alpha} \delta q_\alpha \quad . \tag{6-1}$$

The variational eqs. (4-17) lead therefore to the following set of equations :

$$\frac{\partial\rho_o}{\partial q} \dot{q} - \frac{\partial E_a}{\partial \chi} = 0 \quad , \tag{6-2a}$$

$$\mathrm{Tr} \left\{ (\dot{\chi} + \frac{\partial E_a}{\partial \rho_o}) \frac{\partial \rho_o}{\partial q_\alpha} \right\} = 0 \quad . \tag{6-2b}$$

We look at eqs. (6-2) in more detail and discuss their consequences. For simplicity the discussion is restricted to the case where $\rho_o(q)$ depends on just one real parameter q. The eqs. (6-2a) determine χ in terms of q and $\dot{q}$. Indeed the equivalent eqs. (5-3) can be written in the form

$$[W_1, \rho_o] + [W_o, \rho_1] = i \frac{\partial\rho_o}{\partial q} \dot{q} \quad . \tag{6-3}$$

This is a set of linear equations for the matrix elements of ρ_1, and χ is uniquely determined when ρ_1 is known provided the supplementary conditions (5-16) are imposed. Hence inverting eq. (6-3) gives

$$\chi = k(q)\, \dot{q} \quad , \tag{6-4}$$

where $k(q)$ is a matrix depending only on q and which satisfies the same supplementary conditions (5-16) as χ .

One of the main aims of this paper is to obtain a collective hamiltonian for the nucleus. To do this it is necessary to introduce canonical variables. We have assumed that q is the collective coordinate and it is necessary to find its conjugate momentum. From eq. (3-18) the term $\mathcal{K}(\rho_o, \chi)$ of E_a is seen to be

$$\mathcal{K} = \frac{1}{2} \mathrm{Tr}\chi \dot{\rho}_o = \frac{1}{2} \dot{q} \mathrm{Tr}\chi \frac{\partial \rho_o}{\partial q} \quad , \tag{6-5}$$

which suggests that q and

$$p = \mathrm{Tr}\chi \frac{\partial \rho_o}{\partial q} \quad , \tag{6-6}$$

are conjugate variables. We will now verify this by deducing Hamilton equations from eqs. (6-2).

Taking p and q as independent variables, we can write from the definition (4-5) of $\frac{\partial}{\partial \chi}$ and $\frac{\partial}{\partial \rho_o}$

$$\frac{\partial E_a}{\partial p} = \mathrm{Tr} \frac{\partial E_a}{\partial \chi} \frac{\partial \chi}{\partial p} + \mathrm{Tr} \frac{\partial E_a}{\partial \rho_o} \frac{\partial \rho_o}{\partial p} \quad . \tag{6-7}$$

Since ρ_o is only a function of q, the second term of expression (6-7) is zero. Multiplying eq. (6-2a) by $\partial\chi/\partial p$ and taking the trace, we get :

$$\frac{\partial E_a}{\partial p} = \dot{q} \mathrm{Tr} \frac{\partial \rho_o}{\partial q} \frac{\partial \chi}{\partial p} \quad , \tag{6-8}$$

and using

$$\frac{\partial p}{\partial p} = 1 = \mathrm{Tr} \frac{\partial \chi}{\partial p} \frac{\partial \rho_o}{\partial q} \quad , \tag{6-9}$$

we obtain the first Hamilton equation :

$$\dot{q} = \frac{\partial E_a}{\partial p} \quad . \tag{6-10}$$

We now calculate $\dot{p}$ by differentiating eq. (6-6)

$$\dot{p} = \mathrm{Tr}\ \dot{\chi}\ \frac{\partial \rho_o}{\partial q} + \dot{q}\ \mathrm{Tr}\ \chi\ \frac{\partial^2 \rho_o}{\partial q^2} \quad . \tag{6-11}$$

Using eq. (6-2b), the first term on the right hand side of eq. (6-11) is

$$\mathrm{Tr}\ \dot{\chi}\ \frac{\partial \rho_o}{\partial q} = -\ \mathrm{Tr}\ \frac{\partial E_a}{\partial \rho_o}\ \frac{\partial \rho_o}{\partial q} \quad . \tag{6-12}$$

To write the second term in a different form, we remember that p and q are independent variables :

$$\frac{\partial p}{\partial q} = 0 = \mathrm{Tr}\ \frac{\partial \chi}{\partial q}\ \frac{\partial \rho_o}{\partial q} + \mathrm{Tr}\ \chi\ \frac{\partial^2 \rho_o}{\partial q^2} \quad . \tag{6-13}$$

Using (6-13) and (6-2a), we get

$$\dot{q}\ \mathrm{Tr}\ \chi\ \frac{\partial^2 \rho_o}{\partial q^2} = -\ \dot{q}\ \mathrm{Tr}\ \frac{\partial \chi}{\partial q}\ \frac{\partial \rho_o}{\partial q} = -\ \mathrm{Tr}\ \frac{\partial E_a}{\partial \chi}\ \frac{\partial \chi}{\partial q} \quad , \tag{6-14}$$

and eqs. (6-11), (6-12) and (6-14) lead to the second Hamilton equation :

$$\dot{p} = -\ \frac{\partial E_a}{\partial q} \quad . \tag{6-15}$$

It remains only to write to adiabatic energy E_a explicitly in terms of p and q. The potential part $\mathcal{V}$ depends on ρ_o which depends only on q. Hence $\mathcal{V}(q)$ is a function of q :

$$\mathcal{V}(q) = \langle \Psi_o(q) | H | \Psi_o(q) \rangle \tag{6-16}$$

where $\Psi_o(q)$ is a Slater determinant corresponding to $\rho_o(q)$. From eqs. (6-4) and (6-6) we have

$$p = \dot{q} \; \mathrm{Tr}\; k(q) \frac{\partial \rho_o}{\partial q} \quad . \tag{6-17}$$

The kinetic energy part (6-5) can then be written

$$\mathcal{H} = \frac{1}{2} \frac{p^2}{\mathrm{Tr}\; k(q) \frac{\partial \rho_o}{\partial q}} \quad . \tag{6-18}$$

Hence

$$E_a = \frac{p^2}{2m(q)} + \mathcal{V}(q) \quad , \tag{6-19}$$

where

$$m(q) = \mathrm{Tr}\; k(q) \frac{\partial \rho_o}{\partial q} \quad . \tag{6-20}$$

Expression (6-19) is exactly of the form of a classical Hamiltonian with mass parameter given by eq. (6-20). The reduced Lagrangian can therefore be written as

$$\bar{\mathcal{L}}_a = p\dot{q} - \mathcal{V}(q) - \frac{p^2}{2m(q)} \quad , \tag{6-21}$$

and the Hamilton's equations have the explicit form

$$\dot{q} = \frac{p}{m(q)} \quad , \tag{6-22a}$$

$$\dot{p} = -\frac{\partial V}{\partial q} - \frac{1}{2} \frac{\partial}{\partial q} \frac{1}{m(q)} p^2 \quad . \tag{6-22b}$$

For a given trial density $\rho_o(q)$, eqs. (6-22) determine the time dependence of q and hence of ρ_o and χ.

An alternative expression for the mass m(q) can be found by expanding the total energy (2-8) to second order in χ in the form

$$E = \langle \Psi_o(q) | e^{-i\chi} H \, e^{i\chi} | \Psi_o(q) \rangle$$
$$= \mathcal{V}(q) + \frac{1}{2} \langle \Psi_o(q) | [\chi, [H, \chi]] | \Psi_o(q) \rangle \quad . \tag{6-23}$$

Comparing with eqs. (3-8) and (6-4)

$$\mathcal{K} = \frac{1}{2} \langle \Psi_o(q) | [\chi, [H, \chi]] | \Psi_o(q) \rangle \quad , \tag{6-24}$$

and

$$m(q) = \langle \Psi_o(q) | [k(q), [H, k(q)]] | \Psi_o(q) \rangle \quad . \tag{6-25}$$

We consider as an exemple the case of adiabatic rotation of a deformed nucleus about the y axis. In this case the coordinate q is the angle of rotation θ and we take

$$\rho_o(0) = e^{-i\theta J_y} \rho_{HF} e^{i\theta J_y} \quad , \tag{6-26}$$

where ρ_{HF} is the static deformed Hartree-Fock density. Then

$$\dot{\rho}_o = - i \dot{\theta} [J_y, \rho_o] \quad , \tag{6-27}$$

and eq. (6-3) becomes

$$[W_o, \rho_1] + [W_1, \rho_o] = \dot{\theta} [J_y, \rho_o] \quad , \tag{6-28}$$

which is eq. (11-c) of Thouless and Valatin[4] . Thence eq. (6-28) gives the Thouless-Valatin moment of inertia $\mathcal{J}$. From the rotational invariance of the Hamiltonian, the potential energy and the moment of inertia are both independent of θ and the Hamilton's eqs.(6-22) lead to

$$\dot{\theta} = \frac{P}{\mathcal{J}} \qquad \text{(6-29a)} \quad \text{and} \quad \ddot{\theta} = 0 \quad , \tag{6-29b}$$

as expected. Thus the present formalism is equivalent to the Thouless-Valatin theory for the special case of rotation (and translation).

In the general case we have not given any prescription for choosing the family of Slater determinants $\rho_o(q)$.

These might, for example, be obtained from a static constrained HF calculation. In general the choice of a trial density depending only on one parameter will be a severe restriction because there is no reason why a solution of eqs. (6-22) should also be a solution of the complete set (5-6). But one can still may that the choice of a Slater determinant $\rho_o(q)$ is satisfactory if eqs. (5-6B) are satisfied to a good approximation. Eqs. (5-6B) could also be useful for choosing the best constraint among several.

6.2) The case where χ is restricted to be a local operator

In the first part of this section we looked at the consequences of making a restricted choice of ρ_o and allowing χ to be determined by the equations of motion (6-2a). Another quite different possibility is to allow ρ_o to be general but to restrict χ to be local in coordinate space

$$\chi(\underset{\sim}{r},\underset{\sim}{r}') = \delta(\underset{\sim}{r}-\underset{\sim}{r}')\chi(\underset{\sim}{r}) \quad . \tag{6-30}$$

and to be independent of spin and isospin.
This restriction leads to a nuclear hydrodynamical theory similar to that of Bertsch[10]. In this case the variational eq. (4-17a) requires that the diagonal matrix elements of eq. (5-3) are zero :

$$(i\dot{\rho}_o - [W_o,\rho_1] - [W_1,\rho_o])_{\underset{\sim}{r}=\underset{\sim}{r}'} = 0 \quad . \tag{6-31}$$

For many kinds of interactions (at least for those satisfying the condition $[\chi,[\chi,V]] = 0$) eq. (6-31) reduces to the continuity equation :

$$\dot{\rho}_o(\underset{\sim}{r}) + \frac{1}{m}\,\mathrm{div}\ \underset{\sim}{j}_1(\underset{\sim}{r}) = 0 \quad , \tag{6-32}$$

where $\rho_o(\underset{\sim}{r}) = [\rho_o(\underset{\sim}{r},\underset{\sim}{r}')]_{\underset{\sim}{r}=\underset{\sim}{r}'}$; m is the nucleon mass and

$$\underset{\sim}{j}_1(\underset{\sim}{r}) = \frac{1}{2i}\,[(\underset{\sim}{\nabla}-\underset{\sim}{\nabla}')\rho_1(\underset{\sim}{r},\underset{\sim}{r}')]_{\underset{\sim}{r}=\underset{\sim}{r}'} \tag{6-33}$$

is a momentum density. When χ is local

$$\rho_1(\underset{\sim}{r},\underset{\sim}{r}') = i\langle \underset{\sim}{r}|[\chi,\rho_o]|\underset{\sim}{r}'\rangle = i[\chi(\underset{\sim}{r})-\chi(\underset{\sim}{r}')]\rho_o(\underset{\sim}{r},\underset{\sim}{r}') \qquad (6\text{-}34)$$

and

$$\underset{\sim}{j}_1(\underset{\sim}{r}) = (\underset{\sim}{\nabla}_{\underset{\sim}{r}})\rho_o(\underset{\sim}{r}) \quad . \qquad (6\text{-}35)$$

Thus the locality of χ leads to a momentum density corresponding to a hydrodynamical irrotational flow with velocity field

$$\underset{\sim}{v}(\underset{\sim}{r}) = \frac{1}{m}\underset{\sim}{\nabla}\chi \quad . \qquad (6\text{-}36)$$

The kinetic energy can be calculated from eq. (3-18)

$$\mathcal{K} = \frac{1}{2}\,\mathrm{Tr}\,(\chi\dot{\rho}_o) = \frac{1}{2}\int \chi(\underset{\sim}{r})\dot{\rho}_o(\underset{\sim}{r})d^3r \quad . \qquad (6\text{-}37)$$

Using eq. (6-32) this reduces to

$$\mathcal{K} = -\frac{1}{2m}\int \chi\,\underset{\sim}{\nabla}\cdot\underset{\sim}{j}_1\,d^3r = \frac{1}{2m}\int(\underset{\sim}{\nabla}\chi)\,\underset{\sim}{j}_1 d^3r = \frac{1}{2m}\int v^2(\underset{\sim}{r})\rho_o(\underset{\sim}{r})d^3r \quad , \qquad (6\text{-}38)$$

which is the hydrodynamical expression for the kinetic energy. The variational eq. (4-17b) leads to equations of motion for ρ_o and χ which are similar to classical hydrodynamical equations. However if χ is local, it does not seem necessary to make the adiabatic approximation in order to derive hydrodynamical-like equations. This case will therefore be discussed in more detail in a subsequent publication.

7 - Conclusion

The purpose of this paper is to give a derivation of the ATDHF formalism from a variational principle analogous to Hamilton's principle in classical mechanics and to provide a Hamiltonian for the collective motion of a nucleus with mass and potential parameters expressed in terms of the nucleon-nucleon interaction. By establishing a close connection between ATDHF and the formalism of classical mechanics, this variational approach leads to a direct way of identifying coordinates and their conjugate momenta and of writing the equations of the theory in Hamiltonian form. The variational approach is also used in section 6 to give an unambiguous way of obtaining equations of motion if trial forms are chosen for the operators Q_0 and χ.

The ATDHF formalism allows large amplitude collective motions. In the special case of rotations of a deformed nucleus it corresponds exactly to the theory of Thouless and Valatin [4]. It also leads to RPA if the amplitudes of the motion as well as the velocities are small. The Inglis cranking formula [5] for mass parameters is obtained from ATDHF by making further approximations, notably by omitting the term $[W_1, \dot{P}_0]$ in eq. (5-5). For a general force this is not self-consistent. Baranger and Kumar [7] use a separable quadrupole force λ Q.Q neglecting exchange matrix elements. In their case the term

$$W_1 = \lambda \, Q \, \mathrm{Tr} \, (\ldots)$$

is zero by eq. (3-5) and ATDHF gives back the cranking formula as found in ref. [7].

There are still a number of problems relating to ATDHF which have not been resolved by the present work. One is to understand the role and significance of the supplementary conditions (5-16) on χ. This special choice of supplementary

conditions looks somewhat arbitrary. It is consistent with the equations of motion (5-6), but we have not been able to show that different choices of supplementary conditions making the decomposition (2-13) unique lead to equivalent results for mass and potential parameters.

Another class of unresolved problems arise from the necessity of restricting the number of degrees of freedom in a practical calculation. In section 6 equations were derived corresponding to restricted trial choices of ρ_o and χ. Some criteria for deciding the adequacy of a particular trial choice were given, but in practice they seem difficult to apply. Also the way of restricting the number of degrees of freedom given in section 6 is unable to account for dissipative effects.

The theory presented in this paper produces a classical Hamiltonian for collective motion of a nucleus. This hamiltonian has to be requantized before any comparison with experiment can be made. The hamiltonian formalism is well adapted for this, but well known ambiguities remain in the order of the operators. Also the relation between the eigenstates of such a requantized collective Hamiltonian and the exact eigenstates of the original many-body system is obscure. It is possible that an improved understanding of the relations between the ATDHF and the generator coordinate method would help to answer some of these questions.

In the present paper we do not assume any special form for the two-body force. In practical applications this choice is of course crucial. A study of the ATDHF approximation with the Skyrme force can be found in ref. [12], where it was shown that the inclusion of the three-body effective interaction requires only minor modifications in the formalism.

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