THEORY OF LARGE AMPLITUDE COLLECTIVE VIBRATIONS: CLASSICAL ANALOG OF THE CONCEPT OF COLLECTIVE PATH.

J. da Providência and J.N. Urbano
Departamento de Física
Universidade de Coimbra
P 3000 Coimbra, Portugal

1. Introduction

Marumori's and Villars theories of large amplitude collective oscilations[1,2] are here examined within the framework of time dependent Hartree-Fock (TDHF) theory. It is not our purpose to provide new results. We believe, however, it is useful to translate to a language as simple and familiar as possible, the concepts involved in those theories. In particular, the invariance principle postulated by Marumori is here explained in elementary terms. In section 2, TDHF theory is briefly reviewed and applied to the description of large amplitude collective oscillations.
In section 3, an interpretation of the equations for the "collective path" and of the concept of collective variables is developed on the basis of Hamilton equations of Classical Mechanics.

2. TDHF Theory of large amplitude collective motion

Time-dependent Hartree-Fock equations, which govern the time evolution of Slater determinants $|\Phi(t)\rangle$, may be derived from the action principle

$$\delta \int_{t_1}^{t_2} L \, dt = 0 \qquad (2.1)$$

with

$$L = i\langle\Phi|\dot{\Phi}\rangle - \langle\Phi|H|\Phi\rangle, \qquad (2.2)$$

where H is the hamiltonian.
These equations are summarized by the variational equation

$$i(\langle\Phi|\delta S|\dot{\Phi}\rangle + \langle\dot{\Phi}|\delta S|\Phi\rangle) = \langle\Phi|[\delta S, H]|\Phi\rangle, \qquad (2.3)$$

δS being an arbitrary one body operator.

If $|\Phi(t)\rangle$ is a TDHF state, solution of eq. (2.3) and we require that also the Slater determinant

$$|\Psi(t)\rangle = \exp\ (iS(t))\,|\Phi(t)\rangle$$

is a TDHF state, S(t) being an infinitesimal hermitian one body operator, the linear equation for the time evolution of S(t), which arises from such a requiremente, is written, in variational form,

$$i\langle\Phi|[\delta S,\dot{S}]|\Phi\rangle = \langle\Phi|[\delta S,[H,S]\,]|\Phi\rangle, \tag{2.4}$$

where δS is again an arbitrary one body operator. Although this equation is formally analogous to the RPA equations, there is an important difference. Indeed, since $|\Phi(t)\rangle$ is a function of time, the equation satisfied by $S(t)$ is a linear differential equation with time dependent coefficients.

We observe in passing that it is possible to rewrite eq. (2.3) in a more familiar form if we introduce an hermitian one-body operator $K(t)$ such that

$$|\Phi(t+\delta t)\rangle = \exp\,(-i\delta t K(t))\,|\Phi(t)\rangle. \tag{2.5}$$

We have, therefore,

$$\partial_t|\Phi(t)\rangle = -iK(t)\,|\Phi(t)\rangle\ . \tag{2.6}$$

We obtain, finally

$$\langle\Phi(t)|[\delta S,[K(t) - H]\,]|\Phi(t)\rangle = 0\ . \tag{2.7}$$

We discuss now large amplitude collective motion. We denote by Σ a set of normalized Slater determinants such that their time evolution as TDHF states takes place inside Σ. If $|\Phi(0)\rangle$ belongs to Σ then $|\Phi(t)\rangle$ remains in Σ for all times t. We assume, for simplicity, that the elements of the invariant set Σ are labeled by two real parameters α,β.

The time evolution of the parameters α,β is determined by the following effective Lagrangean

$$\mathcal{L}(\alpha,\beta,\dot{\alpha},\dot{\beta}) = i[\langle\Phi(\alpha,\beta)|\partial_\alpha\Phi(\alpha,\beta)\rangle\,\dot{\alpha}$$

$$+ \langle\Phi(\alpha,\beta)|\partial_\beta\Phi(\alpha,\beta)\rangle\dot{\beta}] - \langle\Phi(\alpha,\beta)|H|\Phi(\alpha,\beta)\rangle\ . \tag{2.8}$$

The parametrization α,β of Σ is chosen such that

$$i\langle\Phi(\alpha,\beta)|\partial_\alpha\Phi(\alpha,\beta)\rangle = 0, \tag{2.9}$$

$$i\langle\Phi(\alpha,\beta)|\partial_\beta\Phi(\alpha,\beta)\rangle = \alpha. \tag{2.10}$$

This choice is permissible according to Darboux theorem, and implies the following relation

$$i[\langle\partial_\alpha\Phi|\partial_\beta\Phi\rangle - \langle\partial_\beta\Phi|\partial_\alpha\Phi\rangle] = 1. \tag{2.11}$$

Then we have

$$\mathcal{L} = \alpha\dot{\beta} - \mathcal{H}(\alpha,\beta), \tag{2.12}$$

$$\dot{\alpha} = -\frac{\partial\mathcal{H}}{\partial\beta}\ ,\ \dot{\beta} = \frac{\partial\mathcal{H}}{\partial\alpha} \tag{2.13}$$

with

$$\mathcal{H}(\alpha,\beta) = \langle\Phi(\alpha,\beta)|H|\Phi(\alpha,\beta)\rangle\ . \tag{2.14}$$

Since we have

$$\partial_t|\Phi(\alpha,\beta)> = |\partial_\alpha\Phi(\alpha,\beta)>\dot{\alpha} + |\partial_\beta\Phi(\alpha,\beta)>\dot{\beta}$$

$$= - |\partial_\alpha\Phi(\alpha, \beta)>\partial_\beta\mathcal{H} + |\partial_\beta\Phi(\alpha,\beta)>\partial_\alpha\mathcal{H} , \qquad (2.15)$$

the condition that $|\Phi(\alpha,\beta)>$ is a TDHF state becomes

$$-(<\Phi(\alpha,\beta)|\delta S|\partial_\alpha\Phi(\alpha,\beta)> + <\partial_\alpha\Phi(\alpha,\beta)|\delta S|\Phi(\alpha,\beta)>)\partial_\beta\mathcal{H}$$

$$+ (<\Phi(\alpha,\beta)|\delta S|\partial_\beta\Phi(\alpha,\beta)> + <\partial_\beta\Phi(\alpha,\beta)|\delta S|\Phi(\alpha,\beta)>)\partial_\alpha\mathcal{H}$$

$$+ i<\Phi(\alpha,\beta)|[\delta S,H]|\Phi(\alpha,\beta)> = 0 . \qquad (2.16)$$

This is equivalent to the equation which has been proposed by Marumori[1)] for the collective path, and reduces to a simpler form if we introduce hermitian one body operators $A(\alpha,\beta)$, $B(\alpha,\beta)$, such that

$$|\Phi(\alpha+\delta\alpha,\beta)> = \exp(-i\delta\alpha B(\alpha,\beta))|\Phi(\alpha,\beta)>, \qquad (2.17)$$

$$|\Phi(\alpha,\beta + \delta\beta) > = \exp(i\delta\beta A(\alpha,\beta))|\Phi(\alpha,\beta)> . \qquad (2.18)$$

We have, therefore

$$\partial_\alpha|\Phi(\alpha,\beta)> = -iB(\alpha,\beta)|\Phi(\alpha,\beta)> , \qquad (2.19)$$

$$\partial_\beta|\Phi(\alpha,\beta)> = iA(\alpha,\beta)|\Phi(\alpha,\beta)> , \qquad (2.20)$$

so that eq. (2.16) reduces to

$$<\Phi(\alpha,\beta)|[\delta S, (B\partial_\beta\mathcal{H} + A\partial_\alpha\mathcal{H} - H)]|\Phi(\alpha,\beta)> = 0 . \qquad (2.21)$$

This is another version of the equation of the path. With the help of the operators A,B, eq. (2.11) may also be given a more meaningful form,

$$- i<\Phi|[B,A]|\Phi> = 1 . \qquad (2.22)$$

3. Classical analog of the concept of collective degrees of freedom

Let us consider the classical Hamiltonian

$$H = \frac{1}{2}\sum_{i,j=1}^{n} p_i (M^{-1})_{ij}\, p_j + V(q_1,\ldots,q_n), \qquad (3.1)$$

where the matrix M_{ij} may be some function of the coordinates $q_1,\ldots,q_n$. We denote by Σ a surface such that if $(p_1(0),\ldots,p_n(0), q_1(0),\ldots,q_n(0))$ belongs to Σ, then $(p_1(t),\ldots,p_n(t), q_1(t),\ldots,q_n(t))$ will remain on Σ for all times t. Here, the functions $p_i(t)$, $q_i(t)$, $i = 1,\ldots,n$, describe a possible motion of the system under investigation, i.e, they are a solution of Hamilton equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}\,,\quad \dot{q}_i = \frac{\partial H}{\partial p_i}\,. \tag{3.2}$$

There are many such surfaces, but it may happen that only a few of them are physically interesting. Let the equations of the surface be

$$p_i = f_i(\alpha,\beta)\,,\quad q_i = g_i(\alpha,\beta)\,,\quad i = 1,\ldots,n. \tag{3.3}$$

The parameters α,β may, under some circumstances, be regarded as collective variables or generator coordinates.
It is well known that Hamilton equations are derived from an action principle related to the following Lagrangean

$$L = \sum_{i=1}^{n} p_i\,\dot{q}_i - H. \tag{3.4}$$

An effective Lagrangean $\mathcal{L}$, describing the evolution in time of the parameter α,β is obtained when we combine equations (3.3) and (3.4),

$$\mathcal{L} = \Big(\sum_{i=1}^{n} f_i\,\frac{\partial g_i}{\partial\alpha}\Big)\,\dot{\alpha} + \Big(\sum_{i=1}^{n} f_i\,\frac{\partial g_i}{\partial\beta}\Big)\,\dot{\beta} - \mathcal{H}(\alpha,\beta) \tag{3.5}$$

where $\mathcal{H}(\alpha,\beta)$ is given by

$$\mathcal{H}(\alpha,\beta) = \frac{1}{2}\sum_{i,j} f_i(\alpha,\beta)\,(M^{-1})_{ij}\,f_j(\alpha,\beta) + V(g_1(\alpha,\beta),\ldots,g_n(\alpha,\beta)). \tag{3.6}$$

Also in M_{ij} the replacement $q_i = g_i\ (\alpha,\beta)$ is assumed. According to Darboux theorem, the parametrization α,β of the surface Σ may be chosen in such a way that

$$\sum_{i=1}^{n} f_i\,\frac{\partial g_i}{\partial\alpha} = 0 \tag{3.7}$$

$$\sum_{i=1}^{n} f_i\,\frac{\partial g_i}{\partial\beta} = \alpha. \tag{3.8}$$

If this choice is made, the effective Lagrangean becomes

$$\mathcal{L} = \alpha\,\dot{\beta} - \mathcal{H}(\alpha,\beta) \tag{3.9}$$

so that α is the effective momentum, β is the effective coordinate and $\mathcal{H}(\alpha,\beta)$ is the effective Hamiltonian corresponding to the particular collective motion under consideration. The time evolution of the parameters α,β is described by Hamilton equations

$$\dot{\alpha} = -\frac{\partial\mathcal{H}}{\partial\beta}\,,\quad \dot{\beta} = \frac{\partial\mathcal{H}}{\partial\alpha}\,. \tag{3.10}$$

These equations are of interest even if the surface Σ is not exactly, but only approximately, invariant. From eqs. (3.7) and (3.8) the following normalization condition (analogous to eqs. (2.11) or (2.22)) is obtained

$$\sum_{i=1}^{n} \left(\frac{\partial f_i}{\partial\alpha} \frac{\partial g_i}{\partial\beta} - \frac{\partial f_i}{\partial\beta} \frac{\partial g_i}{\partial\alpha}\right) = 1 \ . \tag{3.11}$$

We present now the classical equivalent to Marumori's equations of the collective path.

Imposing that the exact equations of motion are satisfied by the parametrization α,β, we find

$$\begin{aligned} \frac{\partial f_i}{\partial\alpha}\dot{\alpha} + \frac{\partial f_i}{\partial\beta}\dot{\beta} &= -\left(\frac{\partial H}{\partial q_i}\right)_{(f,g)} , \\ \frac{\partial g_i}{\partial\alpha}\dot{\alpha} + \frac{\partial g_i}{\partial\beta}\dot{\beta} &= \left(\frac{\partial H}{\partial p_i}\right)_{(f,g)} , \end{aligned} \tag{3.12}$$

where $i = 1,\ldots, n$, and the subscript (f,g) means that the replacement $p_i = f_i$ and $q_i = g_i$ has been made. A convenient set of equations for the surface Σ is now obtained if we take into account eqs. (3.10)

$$\begin{aligned} \left(\frac{\partial f_i}{\partial\alpha} \frac{\partial g_i}{\partial\beta} - \frac{\partial f_i}{\partial\beta} \frac{\partial g_i}{\partial\alpha}\right) \frac{\partial \mathcal{H}}{\partial\alpha} &= \frac{\partial H}{\partial q_i} \frac{\partial g_i}{\partial\alpha} + \frac{\partial H}{\partial p_i} \frac{\partial f_i}{\partial\alpha} , \\ \left(\frac{\partial f_i}{\partial\alpha} \frac{\partial g_i}{\partial\beta} - \frac{\partial f_i}{\partial\beta} \frac{\partial g_i}{\partial\alpha}\right) \frac{\partial \mathcal{H}}{\partial\beta} &= \frac{\partial H}{\partial q_i} \frac{\partial g_i}{\partial\beta} + \frac{\partial H}{\partial q_i} \frac{\partial g_i}{\partial\beta} . \end{aligned} \tag{3.13}$$

Analogous sets of equations have been given in ref. 3). These equations for an invariant surface Σ are equivalent to Marumori's equations of the path. This may be seen as follows. Introduce generators

$$A = A\ (p_1,\ldots,p_n,q_1,\ldots,q_n),\ B = B\ (p_1,\ldots,p_n,q_1,\ldots,q_n)$$

such that

$$\frac{\partial h}{\partial\alpha} = \{B,h\},\ \frac{\partial h}{\partial\beta} = -\ \{A,h\},$$

where $h = h\ (p_1,\ldots,\ p_2,\ q_1,\ldots,\ q_n)$.

Then eqs. (3.12) may be written

$$\begin{aligned} \{B,p_i\} \frac{\partial \mathcal{H}}{\partial\beta} + \{A,p_i\} \frac{\partial \mathcal{H}}{\partial\alpha} &= \{H,p_i\} \\ \{B,q_i\} \frac{\partial \mathcal{H}}{\partial\beta} + \{A,q_i\} \frac{\partial \mathcal{H}}{\partial\alpha} &= \{H,q_i\} \ . \end{aligned} \tag{3.14}$$

These equations are clearly of the same form as eqs. (2.21).

We assume that H is invariant under time reversal. The invariant surface Σ will reflect the time reversal simmetry of the Hamiltonian, so that

$$f_i(\alpha,\beta) = - f_i(-\alpha,\beta)$$

$$g_i(\alpha,\beta) = g_i(-\alpha,\beta) \ .$$

We look now for a power series solution of eqs. (3.13) by expanding $f_i(\alpha,\beta)$ and $g_i(\alpha,\beta)$ in powers of α. Retaining only the zeroth and first order terms we arrive at equations which are equivalent to Villars [2)] equations. We write, therefore,

$$f_i(\alpha,\beta) = \alpha\, f_i^{(1)}(\beta) + \mathcal{O}(\alpha^3)$$
$$g_i(\alpha,\beta) = g_i^{(0)}(\beta) + \mathcal{O}(\alpha^2) \qquad (3.15)$$

From eq. (3.11) we find

$$\sum_{i=1}^{n} f_i^{(1)}(\beta)\, \frac{dg_i^{(0)}(\beta)}{d\beta} = 1 \ , \qquad (3.16)$$

while the Hamiltonian $\mathcal{H}(\alpha,\beta)$ becomes replaced by

$$\mathcal{H}(\alpha,\beta) = \frac{\alpha^2}{2\mathcal{M}} + \mathcal{V}(\beta) \qquad (3.17)$$

where

$$\frac{1}{2\mathcal{M}} = \sum_{i,j} f_i^{(1)}(\beta)\, f_j^{(1)}(\beta)\, (M^{-1})_{ij} \ , \qquad (3.18)$$

$$\mathcal{V}(\beta) = V\,(g_1^{(0)}(\beta),\ldots,g_n^{(0)}(\beta)) . \qquad (3.19)$$

In this approximation, eqs. (3.13) are replaced by

$$\frac{dg_i^{(0)}}{d\beta}\,\frac{1}{\mathcal{M}} = \sum_j (M^{-1})_{ij}\, f_j^{(1)}$$

$$f_i^{(1)} \frac{\partial \mathcal{V}}{\partial \beta} = \frac{\partial V}{\partial q_i} .$$

One easily verifies that these equations are analogous to Villars equations for the collective path[2,3).]

We end this section with a reference to the stability of a particular solution $p_i(t)$, $q_i(t)$, $i = 1,\ldots,n$, of eqs. (2.2). Let $\delta p_i(t)$, $\delta q_i(t)$ be infinitesimal quantities such that also $p_i(t) + \delta p_i(t)$, $q_i(t) + \delta q_i(t)$, is a solution of eqs. (3.2). It follows that $\delta p_i(t)$, $\delta q_i(t)$ satisfy the following equations

$$\delta\dot{p}_i = - \sum_j \frac{\partial^2 H}{\partial q_i \partial p_j}\, \delta p_j - \sum_j \frac{\partial^2 H}{\partial q_i \partial q_j}\, \delta q_j$$

$$\dot{\delta q_i} = \sum_j \frac{\partial^2 H}{\partial p_i \partial p_j} \delta p_j + \sum_j \frac{\partial^2 H}{\partial q_i q_j} \delta q_j .$$

The trajectory $p_i(t)$, $q_i(t)$ is stable if all possible quantities $\delta p_i(t)$, $\delta q_i(t)$ remain infinitesimal for all times.

It seems natural to require that the collective path is a surface Σ which not only is invariant bot also stable.

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References

1) T. Marumori et. al., Prog. Theor. Phys. 64 (1980) 1294

2) F. Villars, Nucl. Phys. A 285 (1977) 269

3) L.P. Brito and C.A. de Sousa, J. Phys. A 14 (1981) 2239