VARIATIONAL DERIVATION OF MEAN FIELD THEORIES WITH MIXED STATES

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ABSTRACT — A variational approach to the dynamics of many-fermion systems appropriate to physical situations requiring a description in terms of mixed states has been developed. The formalism presented here leads in a straightforward way to a mean field theory for mixed states. In this framework, the well-known Hartree-Fock and RPA results for pure states are generalized to the case of mixtures.

1 — INTRODUCTION

D. Brink has suggested in 1955 that one could build collective excitations on top of any stationary state of the nucleus, not necessarily its ground state [1].

In this vein, one may consider collective excitations, which have as "ground state" a mixture of pure states, chosen such as to make the energy of the system stationary. This conjecture has received strong support in 1981, with the experimental discovery at Berkeley of resonances in heavy ion collisions, which could be explained in terms of a dipole displacement of protons against neutrons in compound nuclei [2]. Indeed, γ-ray spectra from deexcitation of compound nuclei with excitation energies of ~ 50 MeV, have been measured and could be fitted by a bump superimposed on a statistical background. The same research group has been able to study the spectra of γ-rays associated with products of deep-inelastic reactions, concluding that the giant dipole resonance strength function is temperature dependent [3]. The experiment indicates that the collective frequency decreases

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with the increase of excitation energy, while the resonance width becomes larger.

Such studies have added a new dimension to our knowledge of nuclear structure. It is then important to know how the theoretical nuclear response function can be formulated for excited systems, and how does it compare with experimental results.

These calculations, which begun only recently, are expected to provide a guide for future observations in the field [4, 5, 6]. For example it is not excluded that other resonance multipolarities may be found in hot nuclei, although the techniques involved should be more sophisticated. In this context one may recall that the experimental discovery of the normal giant dipole mode preceded by 25 years the detection of the quadrupole resonance.

Within the range of theoretical methods available to tackle the problem of nuclear collective motion at zero excitation, the variational approaches distinguish themselves because of their wide flexibility [7]. They provide an unified frame for a lot of approximation schemes, which are established according to the intuitive view one may have of the physical situation.

In this paper we present a variational approach to collective excitations in hot nuclei, putting the emphasis on the derivation of mean-field theories appropriate to that kind of situations.

As we have already presented the method in another publication [8] — where we have also applied it to a schematic two-level model — we limit ourselves here to present in detail the calculations which lead, in the independent-particle approximation, to the self-consistent mean field picture of stationary and quasi-stationary states.

The Hartree-Fock mean-field so obtained differs from the result with pure states (Slater determinants) through the introduction of occupation numbers of the single-particle levels. We call special attention to the fact that this occupation parameters must not be prescribed by the usual assumptions of the grand canonical ensemble. We stress this point, because it is not sure that there is always complete thermalization of the nuclear systems occuring in heavy ion reactions. This is in contrast with the case of matter inside massive stars, where statistical equilibrium is reached during its late evolutive stage.

Small oscillation of the mean-field due to an external perturbation are accounted for, leading to the response function of

the excited system (Random Phase Approximation (RPA) for mixed states).

Specializing the results to mixed states corresponding to thermal equilibrium, the occupation numbers are given by the Fermi-Dirac distribution and the thermal Hartree-Fock and RPA formulae are readily obtained.

The paper is organized as follows. In section 2 we sketch the method. This is based on the density matrix formalism, which is the natural tool to deal with mixed states. In section 3 the response function for mixed states is discussed. In section 4 the features of thermal equilibrium are presented. In section 5 we introduce the notation needed within the independent particle approximation. The static Hartree-Fock theory for mixed states is derived in section 6, while the corresponding RPA is derived in section 7. The conclusions, which are formulated in section 8, contain some perspectives of further work in the field.

2 — GENERAL FORMALISM

Let H denote the hamiltonian of a general N particle system. According to the principles of quantum mechanics, an arbitrary mixed state of the system is described by a density matrix D whose trace is unity

$$\mathrm{Tr}\ D = 1 . \tag{2.1}$$

The density matrix D_0 describing a stationary mixed state satisfies the condition

$$[\,H\,,\,D_0\,] = 0 . \tag{2.2}$$

This condition may be formulated variationally. For this purpose we consider the set of all density matrices having a fixed spectrum of eigenvalues given a priori. If D_0 belongs to that set, so does the matrix

$$D = U\,D_0\,U^+ = e^{-iF}\,D_0\,e^{iF}, \tag{2.3}$$

where F is an arbitrary hermitean operator. The stationarity

condition for the energy, which is necessary to assure minimum energy,

$$\delta \, \text{Tr} \, (DH) = \delta \, \text{Tr} \, (e^{-iF} \, D_0 \, e^{iF} \, H) = 0 \qquad (2.4)$$

leads to

$$\text{Tr} \, ([D_0, \delta F] \, H) = \text{Tr} \, ([H, D_0] \, \delta F) = 0 \qquad (2.5)$$

Since this equation must hold for all variations δF one obtains finally eq. (2.2).

We will discuss now the time evolution of D. According to the rules of quantum-dynamics the operator D should satisfy the Liouville-von Neumann equation

$$\dot{D} = i \, [D, H] \qquad (2.6)$$

which is equivalent to

$$D(t) = e^{-iHt} \, D(0) \, e^{iHt} . \qquad (2.7)$$

We see that the eigenvalue spectrum of D remains unchanged with the time. Our aim is to obtain a variational formulation of (2.6) which could be used as a source of reliable approximation schemes to the exact dynamical equation. We begin with writing the time-dependent density matrix in terms of the stationary density matrix which satisfies eq. (2.2):

$$D(t) = U(t) \, D_0 \, U^+(t) , \qquad (2.8)$$

where $U(t)$ is a variational unitary operator (the unitarity of U assures the time-invariance of the eigenvalue spectrum of D).

Let us consider the action integral

$$I = \int_{t_1}^{t_2} L \, dt , \qquad (2.9)$$

where the lagrangian is given by

$$L = i \, \text{Tr} \, (U \, D_0 \, \dot{U}^{+}) + \text{Tr} \, (U \, D_0 \, U^{+} H) \, . \tag{2.10}$$

The least action principle $\delta I = 0$ with L given by (2.10) does lead to the correct equation of motion (2.6) as we shall prove in the following.

We denote now by δF an infinitesimal hermitean time-dependent operator which satisfies

$$U + \delta U = U \, e^{-i \, \delta F} \, . \tag{2.11}$$

We have therefore

$$\delta U = -i \, U \, \delta F \, , \tag{2.12}$$

$$U^{+} \, \delta U = - \, \delta U^{+} \, U = - i \, \delta F \, . \tag{2.13}$$

The following boundary condition may be imposed on δF:

$$\text{Tr} \, [\, D_0 \, \delta F \, (\, t_1 \,) \,] = \text{Tr} \, [\, D_0 \, \delta F \, (\, t_2 \,) \,] = 0 \, . \tag{2.14}$$

The variation of the action integral may be written

$$\delta I = \int_{t_1}^{t_2} dt \, [\, i \, \text{Tr} \, (\, \delta U \, D_0 \, \dot{U}^{+} + U D_0 \, \delta \dot{U}^{+}) +$$

$$+ \, \text{Tr} \, (\, \delta U \, D_0 \, U^{+} H + U D_0 \, \delta U^{+} H) \,] = i \, \text{Tr} \, (\, D_0 \, \delta U^{+} U) \Big|_{t_1}^{t_2} +$$

$$+ \int_{t_1}^{t_2} dt \, \text{Tr} \, \{ \, \delta U \, U^{+} \, [\, i \, (U D_0 \, \dot{U}^{+} + \dot{U} D_0 \, U^{+}) +$$

$$+ \, (U D_0 \, U^{+} H - H U D_0 \, U^{+}) \,] \, \}$$

$$= - \, \text{Tr} \, (\, \delta F \, D_0) \Big|_{t_1}^{t_2} + i \int_{t_1}^{t_2} dt \, \text{Tr} \, \{ \, U \, \delta F \, U^{+} \, (- i \dot{D} - [\, D \, , \, H \,]) \, \}$$

$$= \int_{t_1}^{t_2} dt \, \text{Tr} \, \{ \, U \, \delta F \, U^{+} \, (\dot{D} - i \, [\, D \, , \, H \,]) \, \} = 0 \, , \tag{2.15}$$

where use has been made of (2.13) and of the boundary condition (2.14). Since the variation δF is arbitrary for $t_1 < t < t_2$ one gains indeed the Liouville-von Neumann equation (2.6) from the action principle.

3 – THE LINEAR RESPONSE FUNCTION FOR MIXED STATES

If a quantal system stays in a stationary state described by the time-independent density matrix D_0 and at some later occasion is slightly perturbed, the density matrix of the perturbed system may be written

$$D(t) = e^{-iF(t)} D_0 \, e^{iF(t)} \tag{3.1}$$

where $F(t)$ is a hermitean infinitesimal operator. Since F is infinitesimal the lagrangian (2.10) may be replaced by its leading order terms. The following quadratic lagrangian is obtained (the linear terms give no contribution):

$$L^{(2)} = (-i/2) \, \text{Tr} \, (D_0 \, [F, \dot{F}]) + 1/2 \, \text{Tr} \, (D_0 \, [F, [H, F]]). \tag{3.2}$$

The principle of least action will then lead to linear equations of motion which are the small amplitude limit of the Liouville-von Neumann equation. From the variation

$$\delta \int L^{(2)} \, dt = 0 \tag{3.3}$$

we obtain

$$i \, \text{Tr} \, (D_0 \, [\delta F, \dot{F}]) - \text{Tr} \, (D_0 \, [\delta F, [H, F]]) = 0, \tag{3.4}$$

so that

$$i \, \text{Tr} \, \{ \delta F \, ([\dot{F}, D_0] + i \, [[H, F], D_0]) \} = 0, \tag{3.5}$$

or, since δF is arbitrary,

$$[\dot{F}, D_0] = -i \, [H, [F, D_0]] \tag{3.6}$$

Here the Jacobi identity for double commutators has been used together with the equilibrium condition (2.2).

We consider now the eigenmode solutions of (3.6). We insert the appropriate ansatz

$$F_r(t) = e^{-i\omega_r t} \Theta_r^+ + e^{i\omega_r t} \Theta_r \qquad (3.7)$$

and obtain

$$\omega_r [\Theta_r^+, D_0] = [H, [\Theta_r^+, D_0]]$$

$$-\omega_r [\Theta_r, D_0] = [H, [\Theta_r, D_0]] \qquad (3.8)$$

where we can consider $\omega_r > 0$. The following normalization condition for the operators Θ_r and Θ_s^+ may be imposed:

$$\mathrm{Tr}\,(D_0 [\Theta_r, \Theta_s^+]) = \delta_{rs}$$

$$\mathrm{Tr}\,(D_0 [\Theta_r, \Theta_s]) = \mathrm{Tr}\,(D_0 [\Theta_r^+, \Theta_s^+]) = 0. \qquad (3.9)$$

The general solution of eq. (3.6) can be written as

$$F(t) = \sum_r (f_r\, e^{-i\omega_r t}\, \Theta_r^+ + f_r^*\, e^{i\omega_r t}\, \Theta_r). \qquad (3.10)$$

The normalization (3.9) leads to the following expression for the mixed state transition amplitudes

$$f_r = \mathrm{Tr}\,(D_0 [\Theta_r, F(0)])$$

$$f_r^* = \mathrm{Tr}\,(D_0 [F(0), \Theta_r^+]) . \qquad (3.11)$$

The energy-weighted sum-rule for these transition amplitudes may now be derived. Indeed from eq. (3.4) with F instead of δF we conclude that

$$i\,\mathrm{Tr}\,(D_0 [F, \dot{F}]) = \mathrm{Tr}\,(D_0 [F, [H\ F]]) \qquad (3.12)$$

It may be easily checked that $i \, \mathrm{Tr} \, (D_0 \, [\, F , \dot{F} \,]) = 2 \sum_r \omega_r \, | \, f_r \, |^2$. Therefore

$$\sum_r \omega_r \, | \, f_r \, |^2 = 1/2 \ \mathrm{Tr} \ (\, D_0 \, [\, F , \, [\, H , \, F \,] \,] \,) \ . \qquad (3.13)$$

We emphasize that this sum-rule is exact and not restricted to the RPA, in which $\log D_0$ and F are one-body operators.

Since the operators H and D_0 commute they may be simultaneously diagonalized. Denoting by $\{ \, | \, m > \, \}$ a set of common eigenvalues

$$H \, | \, m > \, = E_m \, | \, m >$$

$$D_0 \, | \, m > \, = P_m \, | \, m > \qquad (3.14)$$

the solutions of the equations of motion (3.8) are given by

$$\omega_r = E_m - E_n$$

$$\Theta_r^+ = (\, P_n - P_m)^{-1/2} \, | \, m > < n \, | \qquad (3.15)$$

with $E_m > E_n$ and $P_n > P_m$. The index r labels the pair $(\, m, n \,)$.

4 – THERMAL EQUILIBRIUM

The stationarity condition (2.2) should not be confused with the condition for statistical equilibrium.

It is well-known that thermal equilibrium occurs when the entropy

$$S = - \mathrm{Tr} \ (D \, \log D) \qquad (4.1)$$

is maximal for a given value of the energy $E = \mathrm{Tr} \, (DH)$. In order to determine the states of thermal equilibrium the function

$$W = \beta \ \mathrm{Tr} \ (DH) + \mathrm{Tr} \ (D \, \log D) \qquad (4.2)$$

should, therefore, be minimized with respect to variations of D satisfying the normalization condition (2.1). The parameter β is a Lagrange multiplier which fixes the energy and should be interpreted as the inverse of the temperature. The function W is proportional to the well-known Helmholtz function.

The minimization of (4.2) may be viewed as consisting of two steps:

i) Minimization with respect to D for a fixed eigenvalue spectrum. This stage is identical to the time-independent variational procedure formulated in section 2 because the entropy is not affected by canonical transformations. We determine, within the class of all density matrices with a given spectrum, the density matrix D_0 which minimizes the energy and commutes with the hamiltonian H, so that it may be simultaneously diagonalized with H (see eqs. (3.14)). In this first stage we obtain the eigenvectors $|m>$ of H and D_0 and the corresponding eigenenergies E_m.

ii) Minimization with respect to the eigenvalues of D, the set of eigenvectors being kept fixed. We determine the eigenvalues P_m of D_0 which are suitable to describe thermal equilibrium. The function (4.2) may be written

$$W = \beta \sum_m P_m E_m + \sum_m P_m \log P_m \qquad (4.3)$$

and the normalization condition (2.1) reads as

$$\sum_m P_m = 1 \qquad (4.4)$$

Minimization of W with respect to the eigenvalue spectrum P_m is now easily performed leading to

$$P_m = Z^{-1} e^{-\beta E_m} \quad , \quad Z = \sum_m e^{-\beta E_m} \qquad (4.5)$$

Finally we arrive at the following inequality

$$-\log \left(\sum_m e^{-\beta E_m} \right) < \beta \, \text{Tr} \, (DH) + \text{Tr} \, (D \log D)$$

which is precisely the well known Peierls variational principle for the free energy.

We observe that the equilibrium condition (2.2) is a necessary but not sufficient condition for statistical equilibrium. That condition may be interpreted as indicating short-term equilibrium around which the system may oscillate due to a small external perturbation. On the other hand thermal equilibrium should be understood as long-term equilibrium. The composition of the mixed state is in this case specified by (4.5).

5 — INDEPENDENT PARTICLE APPROXIMATION FOR MIXED STATES : NOTATION

In the independent particle approximation we assume that the density-matrix has the following form

$$D = C \, e^{K} ; \qquad (5.1)$$

here K is a one-body hermitean operator and C is a normalization constant.

As this approximation is most conveniently discussed for a variable number of particles in the formalism of second quantization we represent the hamiltonian as

$$H = T + V$$

$$T = \sum_{\mu\nu} t_{\mu\nu} \, a_{\mu}^{+} \, a_{\nu} \qquad (5.2)$$

$$V = 1/2 \sum_{\mu\nu\rho\sigma} v_{\mu\nu\rho\sigma} \, a_{\mu}^{+} \, a_{\nu}^{+} \, a_{\sigma} \, a_{\rho}$$

where a_i^{+}, a_j are respectively creation and annihilation fermion operators corresponding to an orthonormal set of single particle states.

If the number of particles is kept fixed we can write

$$T = \sum_{i=1}^{N} t_i \tag{5.3}$$

$$V = 1/2 \sum_{i \neq j=1}^{N} v_{ij}$$

where the operators t_i and v_{ij} act respectively on functions of the coordinates of the particle i and of the particles i and j. The symbols t and v denote therefore, respectively, the restriction of T and V to one-body and two-body Hilbert spaces.

The expectation values of T and V in the mixed state described by an independent-particle density matrix D may be written

$$< T > = \text{Tr} \ (DT) = \sum_{\mu\nu} \rho_{\mu\nu} \ t_{\nu\mu} = \text{tr} \ (\rho t) \tag{5.4}$$

$$< V > = \text{Tr} \ (DV) = 1/2 \sum_{\mu\nu\rho\sigma} \rho_{\mu\nu} \ \rho_{\rho o} v_{\nu\sigma, \ \mu\rho}^{A} = 1/2 \ \text{tr}_1 \ \text{tr}_2 \ (\rho_1 \ \rho_2 \ v_{12}^{A})$$

where $\rho_{\mu\nu}$ are the elements of the one-body density matrix

$$\rho_{\mu\nu} = < \mu | \rho | \nu > = \text{Tr} \ (D \ a_{\nu}^{+} \ a_{\mu}) \tag{5.5}$$

and v^A is the antisymmetrized interaction defined through

$$v_{\mu\nu, \ \rho\sigma}^{A} = v_{\mu\nu, \ \rho\sigma} - v_{\mu\nu, \ \sigma\rho} \tag{5.6}$$

We should call attention to the distinction between "Tr" and "tr". "Tr" denotes trace in the Hilbert space of state vectors corresponding to an arbitrary number of particles (which is the direct sum of Hilbert spaces of state vectors corresponding to definite numbers of particles). On the other hand "tr" means trace in the Hilbert space of single-particle state vectors.

The relationship between D and ρ indicated by (5.5) can be made more explicit. If k is the restriction of K to the one-body Hilbert space then

$$\rho = e^{k} / (1 + e^{k})$$

(5.7)

The average number of particles, which must be kept fixed in all the calculations, is

$$N = \text{Tr} \left(D \sum_{\mu} a_{\mu}^{+} a_{\mu} \right) = \text{tr } \rho$$

(5.8)

6 — HARTREE-FOCK APPROXIMATION FOR MIXED STATES

The Hartree-Fock approximation for mixed states requires that the variational space in (2.4) only includes independent-particle density matrices. Therefore $\log D_0$ should be a one-body hermitian operator while F is an arbitrary hermitian one-body operator.

The variational equation (2.5) with δF a one-body operator determines the independent-particle density matrix D_0 which commutes as nearly as possible with H. Let us start with

$$\text{Tr} \left(D_0 \, [H, F] \right) = 0$$

(6.1)

which can be obtained from (2.5) using the cyclic property of the trace and replacing δF by F. For fixed N the hamiltonian is given by (5.3) and we have

$$F = \sum_{i=1}^{N} f_{i}$$

(6.2)

Then elementary algebraic manipulations lead to

$$[H, F] = \sum_{i=1}^{N} [t_{i}, f_{i}] + 1/2 \sum_{i \neq j=1}^{N} [v_{ij}, f_{i} + f_{j}]$$

(6.3)

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so that

$$\text{Tr} (D_0 [H, F]) = \text{tr}_1 (\rho_{0,1} [t_1, f_1]) +$$

$$+ 1/2 \; \text{tr}_1 \; \text{tr}_2 (\rho_{0,1} \; \rho_{0,2} [\overset{A}{v_{12}}, f_1 + f_2]) = 0 \tag{6.4}$$

where ρ_0 is related to D_0 as in (5.5). From (6.4) we obtain further

$$\text{Tr} (D_0 [H, F] = \text{tr}_1 (f_1 [\rho_{0,1}, h_1]) = 0 \tag{6.5}$$

where

$$h_1 = t_1 + \text{tr}_2 (\overset{A}{v_{12}} \rho_{0,2}) \tag{6.6}$$

Since f_1 is arbitrary (6.5) implies finally

$$[h, \rho_0] = 0 \tag{6.7}$$

These are the Hartree-Fock equations for mixed states. Let us consider now a representation in which h and ρ_0 are simultaneously diagonal:

$$h |\mu> = \varepsilon_\mu |\mu>$$

$$\rho_0 |\mu> = n_\mu |\mu> \tag{6.8}$$

Then the Hartree-Fock equations may be written in the matricial form

$$t_{\mu\nu} + \underset{k}{\Sigma} \; n_k \; \overset{A}{v_{\mu k, \nu k}} = \varepsilon_\mu \; \delta_{\mu\nu} \tag{6.9}$$

The occupation numbers n_ν are easily determined in the case of statistical equilibrium through the minimization of the function

$$W' = \beta E - S - \beta\mu \; N \tag{6.10}$$

The last term appears because a constraint in the mean number of particles must be included when using a formalism with a

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variable number of particles. The function (6.10) is clearly proportional to the grand canonical potential. Following the arguments given at section 4 and using (5.1) and (5.7) it is straightforward to arrive at

$$n_\nu = [\, 1 + e^{\beta\,(\,\varepsilon_\nu^{\,-}\,\mu\,)}\,]^{-1} \tag{6.11}$$

which is just the Fermi-Dirac distribution function. Our general mixed-state formalism provides a rigorous justification to the introduction of Fermi-Dirac occupation numbers in the Hartree-Fock equations (6.9), which are then called thermal Hartree-Fock equations. We emphasize however that the occupation numbers which appear in (6.9) may be given by some other prescription when situations of non-thermal equilibrium are under consideration. The occupation numbers $n_\nu = 1$, $\nu \leqslant N$ and $n_\nu = 0$, $\nu > N$, correspond to the $T = 0$ situation.

7 – RANDOM PHASE APPROXIMATION FOR MIXED STATES

Let us consider again the lagrangian (3.2), but we are now going to assume that both $\log D_0$ and F are one-body operators.

For a fixed number of particles we have the following values for the commutators involved in $L^{(2)}$:

$$[\,F,\,\dot{F}\,] \;=\; \sum_{i=1}^{N}\,[\,f_i,\,\dot{f}_i\,] \tag{7.1}$$

$$[\,F,\,[\,H,\,F\,]\,] = \sum_{i=1}^{N}\,[\,f_i,\,[\,t_i,\,f_i\,]\,] + \\ + \,1/2 \sum_{i\neq j=1}^{N}\,[\,f_i + f_j,\,[\,\overset{A}{v_{ij}},\,f_i + f_j\,]\,] \tag{7.2}$$

so that

$$L^{(2)} = (-i/2) \, tr_1 \, (\rho_{0,1} \, [\, f_1 \, , \, \dot{f}_1 \,]) + 1/2 \, tr_1 \, (\rho_{0,1} \, [\, f_1 \, , \, [\, t_1 \, , \, f_1 \,]])$$

$$(7.3)$$

$$+ 1/4 \, tr_1 \, tr_2 \, (\rho_{0,1} \, \rho_{0,2} \, [\, f_1 + f_2 \, , \, [\, \overset{A}{v}_{12} \, , \, f_1 + f_2 \,]])$$

The condition of least action leads now to

$$i \, tr_1 \, (\rho_{0,1} \, [\, \delta f_1 \, , \, f_1 \,]) - tr_1 \, (\rho_{0,1} \, [\, \delta f_1 \, , \, [\, t_1 \, , \, f_1 \,]])$$

$$(7.4)$$

$$- tr_1 \, tr_2 \, (\rho_{0,1} \, \rho_{0,2} \, [\, \delta f_1 \, , \, [\, \overset{A}{v}_{12} \, , \, f_1 + f_2 \,]]) = 0$$

After some straightforward algebraic manipulations we obtain

$$i \, [\, \dot{f}_1 \, , \, \rho_{0,1} \,] - [\, [\, h \, , \, f_1 \,] \, , \, \rho_{0,1} \,] - [\, tr_2 \, (\rho_{0,2} \, [\, \overset{A}{v}_{12} \, , \, f_2 \,]) \, , \, \rho_{0,1} \,] = 0$$

$$(7.5)$$

Finally in the representation in which ρ_0 and h are both diagonal

$$i \, \dot{f}_{\mu\nu} \, (n_\nu - n_\mu) - (\varepsilon_\mu - \varepsilon_\nu) \, f_{\mu\nu} \, (n_\nu - n_\mu) - \underset{\rho\sigma}{\Sigma} \, (n_\rho - n_\sigma)$$

$$(7.6)$$

$$(n_\nu - n_\mu) \, \overset{A}{v}_{\mu\rho, \, \nu\sigma} \, f_{\sigma\rho} = 0$$

The solutions for the normal modes are obtained Fourier-analysing F. The one-body approximation of (3.7) is

$$f_r \, (t) = e^{-i\omega_r t} \, \theta_r^+ + e^{i\omega_r t} \, \theta_r$$

$$(7.7)$$

which inserted in (7.6) provides the following RPA equations for mixed states

$$\omega_r \, \theta_{r, \, kl}^+ \, (n_l - n_k) - (\varepsilon_k - \varepsilon_l) \theta_{r, \, kl}^+ \, (n_l - n_k)$$

$$(7.8)$$

$$- \underset{ij}{\Sigma} \, (n_i - n_j) \, (n_l - n_k) \, \overset{A}{v}_{ki, \, lj} \, \theta_{r, \, ji}^+ = 0$$

These equations can still be written in matricial form

$$\omega_r \begin{pmatrix} X_r \\ Y_r \end{pmatrix} = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_r \\ Y_r \end{pmatrix} \tag{7.9}$$

with

$$X_{r,\,\mu\nu} = \theta^+_{r,\,\mu\nu} \,(n_\nu - n_\mu) \quad, \quad n_\nu > n_\mu$$

$$Y_{r,\,\mu\nu} = \theta^+_{r,\,\mu\nu} \,(n_\nu - n_\mu) \quad, \quad n_\mu > n_\nu$$

$$A_{\mu\nu,\,\rho\sigma} = (\varepsilon_\mu - \varepsilon_\nu)\, \delta_{\nu\sigma}\, \delta_{\mu\rho} + v^A_{\mu\rho,\,\nu\sigma} \,(n_\rho - n_\sigma) \quad, \quad n_\nu > n_\mu\,,\ n_\rho > n_\sigma$$

$$B_{\mu\nu,\,\rho\sigma} = v^A_{\mu\rho,\,\nu\sigma} \,(n_\rho - n_\sigma) \qquad\qquad\quad ,\ n_\nu > n_\mu\,,\ n_\sigma > n_\rho$$

In analogy with (3.9) the following normalization condition may be imposed:

$$\mathrm{tr}\,(\rho_0\,[\,\theta_r,\,\theta^+_s\,]) = \delta_{rs}$$

$$\tag{7.10}$$

$$\mathrm{tr}\,(\rho_0\,[\,\theta_r,\,\theta_s\,]) = \mathrm{tr}\,(\rho_0\,[\,\theta^+_r,\,\theta^+_s\,]) = 0$$

The general solution of eq. (7.6) is

$$f = \sum_r (f_r\, e^{-i\omega_r t}\, \theta^+_r + f^*_r\, e^{i\omega_r t}\, \theta_r) \tag{7.11}$$

where the mixed-state transition amplitudes are given by

$$f_r = \mathrm{tr}\,(\rho_0\,[\,\theta_r,\,f\,(0)\,])$$

$$f^*_r = \mathrm{tr}\,(\rho_0\,[\,f\,(0),\,\theta^+_r\,]) \tag{7.12}$$

We observe finally that the RPA preserves the energy-weighted sum-rule

$$\sum_r \omega_r |\,f_r\,|^2 = 1/2\ \mathrm{Tr}\,(D_0\,[\,F,\,[\,H,\,F\,]\,]) \tag{7.13}$$

where the right-hand side can be evaluated with the aid of (7.2).

If ρ_0 is the independent-particle mixed state determined by conventional equilibrium statistical mechanics then its eigenvalues n are the Fermi-Dirac occupation numbers (6.11) and eqs. (7.8) are known under the name of thermal RPA equations.

8 — CONCLUSIONS

We have developed a variational approach appropriate to physical situations requiring a description in terms of mixed states. The formalism presented leads in a straightforward way to a mean field theory for mixed states. In this framework, the well-known Hartree-Fock and RPA results for pure states are generalized to the case of mixtures.

As extensions of this work, which are presently being carried out, we would like to refer the following:

1 — The description of correlations not included in a mean-field by boson expansions adequate for mixed states. We can establish a temperature dependent Holstein-Primakoff expansion, for magnetically ordered systems, which is useful in the study of the interaction between spin waves [9].

2 — The translation of the quantal mean-field formulae into classical terms. We obtain in this way a thermal Thomas-Fermi theory, for the ground-state of a statistical system, and a fluid dynamical representation of small oscillations around it [10].

3 — The application to heavy ion collisions, such as those described in the introduction. In a realistic model, a constraint on the angular momentum must be introduced and the singe-particle states must be replaced by the single quasi-particle states of the Hartree-Fock-Bogolyubov approach.

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