

## MEAN-FIELD THEORIES WITH MIXED STATES AND ASSOCIATED BOSON EXPANSIONS

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**Abstract:** A variational derivation of the Liouville-von Neumann equation of quantum-statistical mechanics is presented, in order to formulate mean-field approximations appropriate to mixed states. The Hartree-Fock and the RPA at finite temperatures are particular cases of the general formalism. A thermal boson expansion is defined, which allows us to describe anharmonic motion around a thermal excited state. In a numerical application on the basis of the Lipkin model, temperature-dependent phase transitions are observed.

### 1. Introduction

Studies of the decay of the compound nuclei formed in heavy-ion reactions have added a new dimension to the field of nuclear structure. The temperature of the compound nucleus at a given excitation energy rises from zero at the yrast state to a few MeV at angular momentum zero.

Recently the decay of high-excited states above the yrast line, like the giant dipole resonance, has been observed<sup>1,2</sup>). These measurements were carried out making use of sum-spectrometer multiplicity techniques, thus allowing to determine the average angular momentum of the system and from this knowledge the temperature of the nucleus. One can then study experimentally the nuclear structure at finite values of both the angular momentum and temperature, and the corresponding theoretical analysis of giant resonances above thermal excited states is now the object of intensive research<sup>3-7</sup>).

On the other hand, the observation of deep-inelastic reactions has been an important source of information on the behaviour of nuclei under strong external fields. In these reactions the two interacting ions emerge after the collision with approximately the same charge and mass, but having lost a large fraction of the energy and angular momentum of relative motion they had in the entrance channel [cf. e.g. ref. <sup>8</sup>) and references therein].

Different mechanisms play a role in these reactions, like the transfer of particles and the excitation of giant resonances [cf. ref. <sup>9</sup>) and references therein]. Because these vibrations have a damping width the energy and angular momentum absorbed through them into the nuclei lead to a finite temperature and to rigid rotation. This

is also the case for a large number of the events where uncorrelated particles are exchanged between the systems.

Because the nuclear response is relevant for studying the reaction process, it is important to know how it changes with temperature and angular momentum<sup>7)</sup>.

In the present paper we present a new variational derivation of static and dynamical mean field theories appropriate to general mixed states. Our approach may be useful to achieve a detailed description of compound-nuclear decay and of deep-inelastic reactions. Small oscillations of the mean field due to external perturbations are accounted for, leading to the response function of the excited system. This response may be described by means of a sum rule. Particularizing the results to Fermi-Dirac distributions the standard static Hartree-Fock and random-phase approximations at finite temperatures<sup>10)</sup> are readily obtained. We show further how to define a thermal boson expansion, which is in principle able to provide corrections to the mean-field approximation.

In sect. 2 we present the general formalism which is based on density matrix techniques. The significance of thermal equilibrium is briefly discussed. In sect. 3 the response function for mixed states is presented and the energy-weighted sum rule appropriate to mixed states is derived. In sect. 5 we introduce a thermal boson expansion, which may be used to treat anharmonicities in the collective spectrum of excited systems.

The formalism is applied in sect. 6 to the Lipkin model. The conclusions are collected in sect. 7.

## 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:

$$\text{Tr } D = 1. \quad (2.1)$$

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

$$[H, D_0] = 0. \quad (2.2)$$

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

$$D = UD_0U^+ = e^{-iF}D_0e^{iF}, \quad (2.3)$$

where  $F$  is an arbitrary hermitean operator. The stationarity condition for the energy, which is necessary to assure minimal energy,

$$\delta \text{Tr } (DH) = \delta \text{Tr } (e^{-iF}D_0e^{iF}H) = 0, \quad (2.4)$$

leads to

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

Since this equation must hold for all variations  $\delta F$  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

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

which is equivalent to

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

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 by writing the time-dependent density matrix in terms of the stationary density matrix which satisfies eq. (2.2):

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

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

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

where the lagrangian is given by

$$L = i \text{Tr} (UD_0 \dot{U}^+) + \text{Tr} (UD_0 U^+ H). \quad (2.10)$$

We denote now by  $\delta F$  an infinitesimal hermitean time-dependent operator satisfying

$$U + \delta U = U e^{-i\delta F}. \quad (2.11)$$

We have therefore

$$\delta U = -iU\delta F, \quad (2.12)$$

$$U^+ \delta U = -\delta U^+ U = -i\delta F. \quad (2.13)$$

We show that the density matrix (2.8) satisfies the Liouville-von Neumann equation (2.6), if (and only if)  $\delta I$  does not depend on  $\delta F(t)$ , for  $t_1 < t < t_2$ . More precisely, the following statement is valid: If (and only if) we have up to order  $(\delta F)^2$

$$\delta I + \text{Tr} [\delta F(t_2) D_0] - \text{Tr} [\delta F(t_1) D_0] = 0 \quad (2.14)$$

for arbitrary values of  $\delta F$ ,  $t_1 \leq t \leq t_2$ , then  $D = UD_0 U^+$  obeys the correct equation of motion (2.6). The proof reads as follows: The variation of the action integral

may be written

$$\begin{aligned}
 \delta I &= \int_{t_1}^{t_2} dt [i \text{Tr} (\delta U D_0 \dot{U}^+ + U D_0 \delta \dot{U}^+) + \text{Tr} (\delta U D_0 U^+ H + U D_0 \delta U^+ H)] \\
 &= i [\text{Tr} (D_0 \delta U^+ U)]_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \text{Tr} \{ \delta U U^+ [i (U D_0 \dot{U}^+ + \dot{U} D_0 U^+) \\
 &\quad + (U D_0 U^+ H - H U D_0 U^+)] \} \\
 &= - [\text{Tr} (\delta F D_0)]_{t_1}^{t_2} + i \int_{t_1}^{t_2} dt \text{Tr} \{ U \delta F U^+ (-i \dot{D} - [D, H]) \} \\
 &= -\text{Tr} [\delta F(t_2) D_0] + \text{Tr} [\delta F(t_1) D_0] + \int_{t_1}^{t_2} dt \text{Tr} \{ U \delta F U^+ (\dot{D} - i [D, H]) \},
 \end{aligned}
 \tag{2.15}$$

where use has been made of (2.13). Since the variation  $\delta F$  is arbitrary, for  $t_1 \leq t \leq t_2$ , the action principle (2.14) is equivalent to the Liouville-von Neumann equation.

The quantities  $\text{Tr} [\delta F(t_2) D_0]$  and  $\text{Tr} [\delta F(t_1) D_0]$  do not play a physically relevant role and therefore we may, without loss of generality, impose that

$$\text{Tr} [\delta F(t_2) D_0] - \text{Tr} [\delta F(t_1) D_0] = 0.
 \tag{2.16}$$

Then the action principle (2.14) reduces to the simplest form

$$\delta I = 0.
 \tag{2.17}$$

The following comment about the meaning of the eq. (2.2) is in order. This so-called stationarity condition should not be confused with the condition for statistical equilibrium, which is more restrictive. Indeed it is well known that thermal equilibrium occurs when the energy  $E = \text{Tr} (DH)$  is minimal for a fixed value of the entropy  $S = -\text{Tr} (D \log D)$ . In order to determine the states of thermal equilibrium, the function  $W = E - \beta S$ , with  $\beta$  a Lagrange multiplier, must therefore be minimized with respect to variations of  $D$  satisfying the normalization condition (2.1). The composition of the mixed state is then unambiguously prescribed.

The condition (2.2), which is required to minimize the energy, may be interpreted as indicating short-term equilibrium. On the other hand, thermal equilibrium should be understood as long-term equilibrium. In both cases the system may oscillate around the equilibrium due to some small external perturbation.

### 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):

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

The condition of least action (2.17) will then lead to linear equations of motion which are the small-amplitude limit of the Liouville-von Neumann equation. From the variation

$$\delta \int_{t_1}^{t_2} L^{(2)} dt = 0 \quad (3.3)$$

we obtain

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

so that

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

or, since  $\delta F$  is arbitrary,

$$[\dot{F}, D_0] = -i[H, [F, D_0]] . \quad (3.6)$$

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

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

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

and obtain

$$\begin{aligned} \omega_r [\Theta_r^+, D_0] &= [H, [\Theta_r^+, D_0]] , \\ -\omega_r [\Theta_r, D_0] &= [H, [\Theta_r, D_0]] , \end{aligned} \quad (3.8)$$

where we can consider  $\omega_r > 0$ . The following normalization condition for the operators  $\Theta_r$  and  $\Theta_s$  may be imposed:

$$\begin{aligned} \operatorname{Tr} (D_0[\Theta_r, \Theta_s^+]) &= \delta_{rs} , \\ \operatorname{Tr} (D_0[\Theta_r, \Theta_s]) &= \operatorname{Tr} (D_0[\Theta_r^+, \Theta_s^+]) = 0 . \end{aligned} \quad (3.9)$$

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

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

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

$$\begin{aligned} f_r &= \operatorname{Tr} (D_0[\Theta_r, F(0)]) , \\ f_r^* &= \operatorname{Tr} (D_0[F(0), \Theta_r^+]) . \end{aligned} \quad (3.11)$$

The energy-weighted sum rule for these transition amplitudes may now be derived.

Indeed from eq. (3.4) with  $F$  instead of  $\delta F$  we conclude that

$$i \operatorname{Tr} (D_0[F, \dot{F}]) = \operatorname{Tr} (D_0[F, [H, F]]) . \quad (3.12)$$

It may easily be checked that

$$i \operatorname{Tr} (D_0[F, \dot{F}]) = 2 \sum_r \omega_r |f_r|^2 . \quad (3.13)$$

Therefore

$$\sum_r \omega_r |f_r|^2 = \frac{1}{2} \operatorname{Tr} (D_0[F, [H, F]]) . \quad (3.14)$$

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  $\{|m\rangle\}$  a set of common eigenvalues

$$\begin{aligned} H|m\rangle &= E_m|m\rangle , \\ D_0|m\rangle &= P_m|m\rangle , \end{aligned} \quad (3.15)$$

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

$$\begin{aligned} \omega_r &= E_m - E_n , \\ \Theta_r^+ &= \frac{|m\rangle\langle n|}{\sqrt{P_n - P_m}} , \end{aligned} \quad (3.16)$$

with  $E_m > E_n$  and  $P_n > P_m$ .

#### 4. Hartree-Fock and random-phase 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 hermitean operator while  $F$  is an arbitrary hermitean one-body operator.

In the framework of this approximation it is easy to arrive at the following Hartree-Fock equations:

$$t_{ij} + \sum_k n_k v_{ik,jk}^A = \varepsilon_i \delta_{ij} , \quad (4.1)$$

where  $t$  is the single-particle kinetic energy and  $v^A$  the antisymmetrized interaction. The occupation numbers differ from the case of pure states (Slater determinants), which is characterized by  $n_k = 0, 1$ . For statistical equilibrium these numbers are given by the Fermi-Dirac distribution, but in general they may be given by some other prescription, if situations of non-thermal equilibrium are under consideration.

If we assume that  $\log D_0$  and  $F$  are one-body operators in the lagrangian (3.2), it is possible to derive the following RPA equations from the variational principle:

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_r \\ Y_r \end{pmatrix} = \omega_r \begin{pmatrix} X_r \\ Y_r \end{pmatrix}, \quad (4.2)$$

$$\begin{aligned} A_{kl,ij} &= (\varepsilon_k - \varepsilon_l) \delta_{ij} \delta_{kl} + v_{kl,ij}^{\wedge} (n_i - n_j), & n_l > n_k, n_i > n_j, \\ B_{kl,ij} &= v_{kl,ij}^{\wedge} (n_i - n_j), & n_l > n_k, n_j > n_i, \end{aligned} \quad (4.3)$$

where the  $\omega_r$  denote collective frequencies of the excited system.

It can also be seen that the RPA preserves the energy-weighted sum rule [cf. refs. <sup>6,7,11</sup>].

### 5. Boson expansions for mixed states

The method of boson expansions for mixed states involves the replacement of the density matrix for independent-particles  $D_0$  by a boson vacuum-state vector  $|0\rangle$ . Operators acting in the Hilbert space of fermion state vectors are replaced by boson images having the same commutation properties.

The boson image of the fermion pair  $a_i^+ a_j$  is a complicated operator. However, in leading order the image of  $a_i^+ a_j$  is some boson operator

$$a_i^+ a_j = A_{ij} + O(A^2), \quad (5.1)$$

such that

$$A_{ij} = A_{ji}^+. \quad (5.2)$$

The commutation relation for the boson operators are such as to preserve the relation

$$\text{Tr} (D_0 [a_i^+ a_j, a_k^+ a_l]) = \delta_{jk} \delta_{il} (n_i - n_j). \quad (5.3)$$

Therefore,

$$[A_{ji}^+, A_{kl}] = \delta_{jk} \delta_{il} (n_i - n_j). \quad (5.4)$$

the boson operators are not normalized to unity and therefore they do not describe normalized states. We also require

$$A_{ij}|0\rangle = 0, \quad (5.5)$$

if  $n_i > n_j$  (if  $n_i = n_j$ , the object  $A_{ij}$  does not exist).

The boson image of  $H$ , denoted by  $H_B$ , is constructed so as to preserve the following relations:

$$\begin{aligned} \text{Tr} (D_0 H) &= E_0, \\ \text{Tr} (D_0 [H, a_i^+ a_j]) &= 0, \\ \text{Tr} (D_0 [[H, a_i^+ a_j], a_k^+ a_l]) &= (\varepsilon_j - \varepsilon_i) (n_i - n_j) \delta_{jk} \delta_{il} + v_{ik,jl}^{\wedge} (n_k - n_l) (n_i - n_j). \end{aligned} \quad (5.6)$$

We find

$$H_B = E_0 + \Delta + \frac{1}{2} \sum_{i \neq j} \frac{\epsilon_j - \epsilon_i}{n_j - n_i} A_{ij} A_{ji} + \frac{1}{2} \sum_{ijkl} v_{ik,jl}^{\Lambda} A_{ij} A_{kl} + \dots, \quad (5.7)$$

where

$$\Delta = -\frac{1}{2} \sum_{\substack{ij \\ \epsilon_i > \epsilon_j}} [\epsilon_j - \epsilon_i + v_{ij,ji}^{\Lambda} (n_j - n_i)] \quad (5.8)$$

is a quantity which assures that the vacuum expectation value of  $H_B$  is the Hartree-Fock energy  $E_0$ . Diagonalization of  $H_B$  is in principle straightforward. The eigenenergies of (5.7) agree with the RPA frequencies given by (4.2).

It should, however, be emphasized that the correlation energy so obtained is not reliable because the convergence of the boson expansion is very poor when the bosons describe both collective and single-particle degrees of freedom.

A boson expansion dealing only with collective bosons, images of appropriate linear combinations of fermion pair operators, may also be formulated along the lines of the derivation which has been presented. Equations of the RPA type, but restricted to the collective degrees of freedom, are then obtained and an improved convergence of the boson expansion is achieved. The cost for the better convergence is the artificial freezing of the single-particle excitations.

In this spirit we can consider terms of the boson expansion which go beyond the RPA and which should be useful to describe anharmonicities.

A boson expansion around a state corresponding to statistical equilibrium may be called a thermal boson expansion.

### 6. Thermal Hartree-Fock, RPA and boson expansion in the Lipkin model

As an example of the ideas involved in sects. 2 to 5 we are going to consider the schematic two-level model due to Lipkin *et al.*<sup>12)</sup>

The hamiltonian of the Lipkin model reads as

$$H = J_z + \frac{1}{2} V (J_+^2 + J_-^2), \quad (6.1)$$

where  $J_z, J_{\pm}$  are the SU(2) generators

$$[J_-, J_+] = -2J_z, \quad [J_z, J_{\pm}] = J_{\pm}. \quad (6.2)$$

The density matrix in the independent-particle approximation can be written as an exponential of a one-body operator

$$D = C e^{\alpha J_z}, \quad (6.3)$$

where  $C$  and  $\alpha$  are chosen such that the occupation number of the upper level is  $P_+$  and the occupation number of the lower level is  $P_- = 1 - P_+$ .



The density matrix (6.3) does not describe an exactly stationary state because  $[H, D] \neq 0$ . Such a state is described by  $D_0 = U^+ D U$ , with  $U U^+ = U^+ U = 1$ , provided we choose  $U$  in order to have  $\text{Tr}(D_0 H)$  as a minimum of the energy.

Let us take  $U$  to be the hermitean one-body operator

$$U = e^{i\theta J}. \quad (6.4)$$

The quantity to be minimized with respect to  $\theta$  is then

$$\begin{aligned} E &= \text{Tr}(DH) = \text{Tr}(D_0 U H U^+) \\ &= -\frac{1}{2} N P \cos \theta + \sin^2 \theta \frac{1}{4} V N (N P^2 - \frac{1}{2}(1 + P^2)), \end{aligned} \quad (6.5)$$

with  $P$  the difference between the occupation probabilities of the two levels  $P = P_- - P_+$ . Assuming thermal equilibrium, there is a well-defined relation between  $P$  and the temperature  $T$ :  $P = 1 \Rightarrow T = 0$  and  $P = 0 \Rightarrow T = \infty$  for the extremal values. The solution of the minimization problem is

$$\begin{aligned} \theta &= 0, & |P| &> |V(NP^2 - \frac{1}{2}(1 + P^2))|, \\ \cos \theta &= -\frac{P}{V(NP^2 - \frac{1}{2}(1 + P^2))}, & |P| &\leq |V(NP^2 - \frac{1}{2}(1 + P^2))|. \end{aligned} \quad (6.6)$$

The ground-state energy can then be calculated:

$$\begin{aligned} E_0 &= -\frac{1}{2} N P, & |P| &> |V(NP^2 - \frac{1}{2}(1 + P^2))|, \\ E_0 &= -\frac{1}{4} N P \left\{ \frac{1}{|V[NP - \frac{1}{2}(P + 1/P)]|} + |V[NP - \frac{1}{2}(P + 1/P)]| \right\}, \\ & & |P| &\leq |V(NP^2 - \frac{1}{2}(1 + P^2))|. \end{aligned} \quad (6.7)$$

Comparing with the  $T = 0$  result, we conclude that the effect of the temperature consists simply in the replacement of :

- (i) the number of particles  $N$  by  $NP$ ,
- (ii) the parameter characteristic of the Lipkin-model,  $\chi = V(1 - N)$ , which determines the ground-state phase transition, by

$$\chi(P) = V[\frac{1}{2}(P + 1/P) - NP]. \quad (6.8)$$

We observe therefore temperature-dependent second-order phase transitions. With  $|\chi(P)| < 1$  the normal phase is obtained, whereas with  $|\chi(P)| \geq 1$  the abnormal phase, which corresponds to a "deformed" ground state, is obtained. These phase-transitions have a thermal origin and, although analogous, differ from the ground-state phase transitions that are obtained varying the interaction strength  $V$  or the number of particles  $N$ . We can consider as order parameter  $\text{Tr}(D_0 J_x)$  because it vanishes for the symmetric situation (normal phase) and it is different from zero when the symmetry is broken.

In the model under study the  $T=0$  RPA results can be extended to finite temperatures through the temperature renormalization of the parameter  $\chi$  that has been derived. The following collective excitation energy is obtained:

$$\omega = \begin{cases} [1 - \chi^2(P)]^{1/2} & \text{if } \chi(P) \leq 1, \\ [2(\chi^2(P) - 1)]^{1/2} & \text{if } \chi(P) > 1. \end{cases} \quad (6.9)$$

We may implement in the model the method of boson expansions, which is more ambitious than the RPA.

For the present purpose this method consists in replacing the operators  $J_z, J_+$  and  $J_-$  by adequate boson operators, preserving the commutation relations (6.2) order by order. This prescription is complemented by the requirements  $\langle 0|(J_z)_B|0\rangle = \text{Tr}(D_0 J_z)$ ,  $\langle 0|(J_{\pm})_B|0\rangle = \text{Tr}(D_0 J_{\pm})$ , where  $|0\rangle$  is the boson vacuum. In this way the conditions expressed in (5.3) and (5.4) are fulfilled.

Let us assume, for simplicity, that the reference stationary state is a normal state ( $\theta=0$ ). Then, the boson expansions for  $(J_+)_B$  and  $(J_-)_B$  contain only odd powers and  $(J_z)_B$  contains only even powers of boson operators. Moreover,  $\langle 0|(J_z)_B|0\rangle = -\frac{1}{2}NP$ ,  $\langle 0|(J_{\pm})_B|0\rangle = 0$ . It is straightforward to verify that the commutation relations and these requirements are satisfied by the following boson expansions:

$$\begin{aligned} (J_+)_B &= (NP)^{1/2} \left( A^+ - \frac{1}{2NP} A^+ A^+ A + \dots \right) = (NP)^{1/2} A^+ \left( 1 - \frac{A^+ A}{NP} \right)^{1/2}, \\ (J_-)_B &= (NP)^{1/2} \left( A - \frac{1}{2NP} A^+ A A + \dots \right) = (NP)^{1/2} \left( 1 - \frac{A^+ A}{NP} \right)^{1/2} A, \\ (J_z)_B &= A^+ A - \frac{1}{2}NP. \end{aligned} \quad (6.10)$$

These formulae are a direct generalization of the Holstein-Primakoff transformation (which is a Belyaev-Zelevinsky type of boson expansion). The only difference with respect to the  $T=0$  expansion lies on the renormalization of the number of particles. We call attention to the fact that the expansion parameter is  $1/NP$ , and, as the temperature increases, the convergence becomes poor. This convergence problem was *ab initio* expected, because the boson expansion refers to a given equilibrium state and, when departing from it, phase transitions occur.

If we insert the thermal boson expansion in the hamiltonian (6.1) we obtain a hamiltonian  $H_B$ , which, to all orders, gives results perfectly equivalent to those arising from the original  $H$ . If we make truncations, errors are of course introduced. The anharmonic terms found, which may look rather complicated, are the extension to finite temperatures of the results of ref. <sup>13</sup>).

We show in the following the numerical results obtained within the harmonic approximation. Figs. 1 to 7 were obtained for two sets of values of  $(V, N)$ , namely  $(-0.095, 20)$  and  $(-0.032, 20)$ . In the first case (strong coupling) one begins at  $T=0$  with the abnormal phase and two phase transitions occur, whereas in the second case (weak coupling) the starting point belongs to the normal phase and there is only one phase transition. The parameter  $\chi(P)$  is represented in fig. 1.

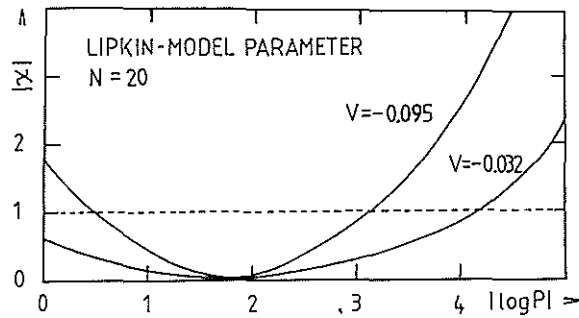


Fig. 1. The parameter of the Lipkin model (6.8), which determines the phase transitions, as a function of  $|\log P|$ , in the two cases of initial strong coupling ( $V = -0.095$ ,  $N = 20$ ) and initial weak coupling ( $V = -0.032$ ,  $N = 20$ ).

From the numerical results the following main conclusions can be drawn:

(i) The Hartree-Fock energy (figs. 2 and 3) increases with the temperature. It must be corrected by the inclusion of the correlation energy  $\frac{1}{2}(\omega - A)$ , which is temperature dependent. The RPA energy so obtained is always lower than the Hartree-Fock energy. We observe in the strong-coupling case a minimum at the second phase transition, which has a pure quantum-mechanical origin. The same phenomenon happens for the only phase transition of the weak-coupling case. However we should not take very seriously the mean-field approximation near the critical points, where large fluctuations are known to be important.

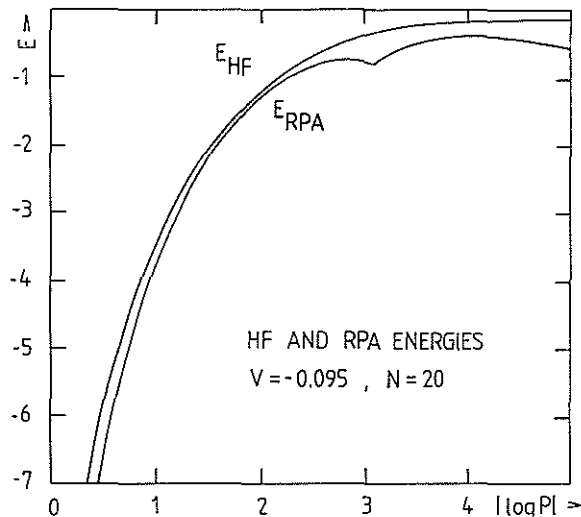


Fig. 2. The Hartree-Fock and the RPA energies as a function of  $|\log P|$  in the strong-coupling case.

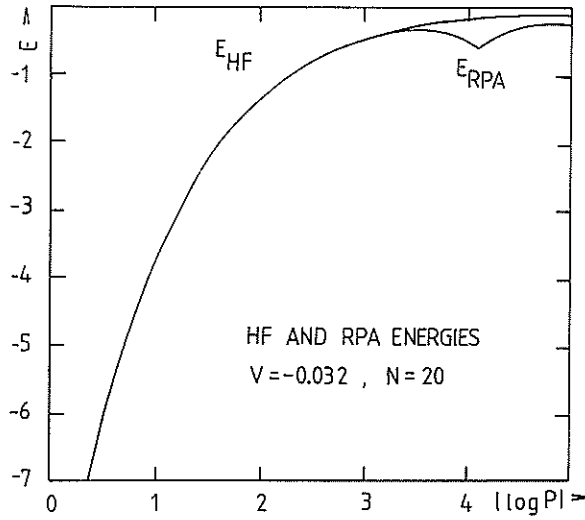


Fig. 3. The Hartree-Fock and the RPA energies as a function of  $|\log P|$  in the weak-coupling case.

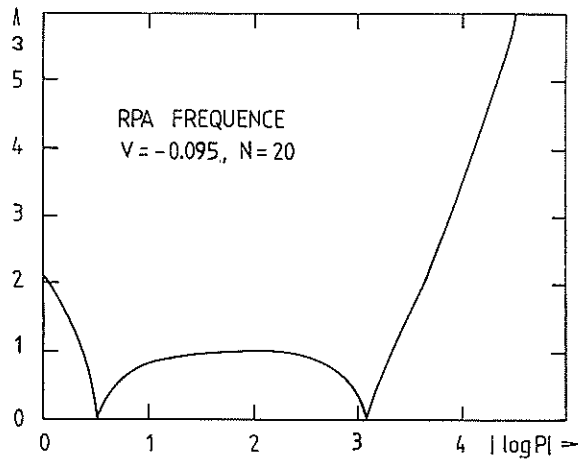


Fig. 4. The RPA frequency as a function of  $|\log P|$  in the strong-coupling case.

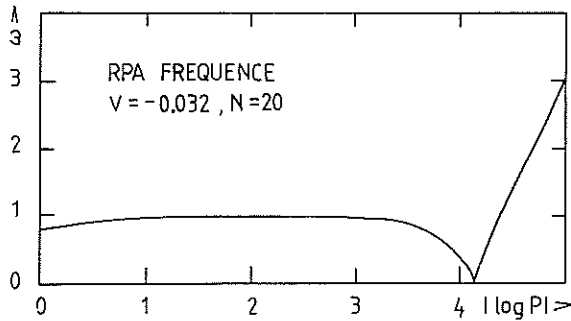


Fig. 5. The RPA frequency as a function of  $|\log P|$  in the weak-coupling case.

(ii) The thermal RPA frequency vanishes at the transition points, as expected (figs. 4 and 5). This is due to the fact that the two matrix elements of the RPA matrix are just equal at those points.

The frequency decreases in the region of low temperatures for the strong-coupling case. In the weak-coupling case, on the other hand, the frequency remains approximately constant until the vicinity of the critical point is reached, where a quick decrease occurs.

The decrease of the RPA collective frequencies with the temperature has also been obtained by Vautherin and Vinh-Mau<sup>5)</sup> in the Brown-Bolsterli model, using Green function methods. The same authors have performed more realistic calculations for  $^{40}\text{Ca}$ , using oscillator wave functions and zero-range forces<sup>6)</sup>. The isovector dipole mode was shown to decrease rather slowly in energy when increasing the temperature. For a heavier nucleus ( $^{208}\text{Pb}$ ) the data made available by Civitarese, Broglia and Dasso<sup>7)</sup>, who used an oscillator basis and separable residual forces, indicates that the isoscalar modes decrease slightly in energy, but the isovector modes have opposite behaviour. For the same nucleus, the sum-rule approach of Meyer, Quentin and Brack<sup>11)</sup>, based on a modified SkM force, both the isoscalar monopole and the isovector dipole, decrease in energy with the temperature.

For very large temperatures (i.e. after the last transition point) the thermal RPA frequency of the Lipkin model increases in the two cases considered. This fact has a clear physical meaning, namely that very hot systems are more difficult to excite collectively.

(iii) It is also interesting to examine what is the temperature dependence of the RPA and the cranking mass parameters. The mass parameter in the strong-coupling case shows a maximum at the first transition from the "deformed" to the "spherical" ground state (fig. 6), after which it decreases smoothly to zero. This fact resembles the appearance of peaks in the cranking mass parameter based on the deformed shell model (e.g. Nilsson model), which is currently used to describe the fission

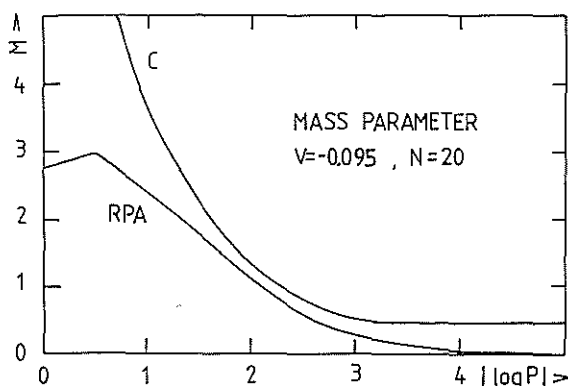


Fig. 6. The RPA and the cranking mass parameters as a function of  $|\log P|$  in the strong-coupling case.

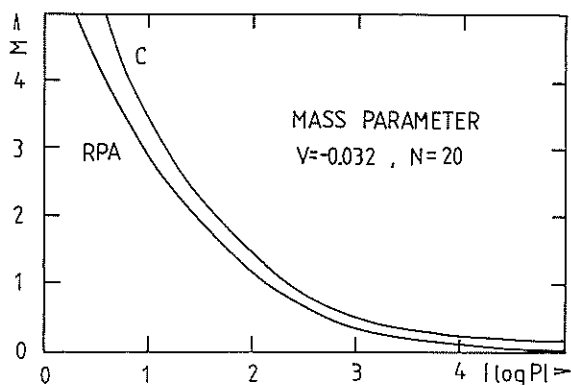


Fig. 7. The RPA and the cranking mass parameters as a function of  $|\log P|$  in the weak-coupling case.

process. In this situation the mass is proportional to the level density at the Fermi energy<sup>14</sup>). Beginning with the normal phase the mass decreases monotonously (fig. 7).

These results should be compared with the mass formula of an excited system presented by Schütte and Wilets<sup>15</sup>), who predict a decrease of the inertia with respect to the  $T=0$  value.

In the Lipkin model the cranking mass is a poor approximation to the RPA mass at  $T=0$ , as is well known<sup>16,17</sup>) (the reason lies in the fact that the correlations, which are measured by  $B$ , are in general important in the model). From the temperature-dependent treatment we may extract the conclusion that the cranking mass can become a better approximation for higher temperatures, although being always larger than the RPA mass and clearly asymptotically wrong in the strong-coupling case.

## 7. Conclusions

There have been recently some attempts to formulate variationally the Liouville-von Neumann equation<sup>18,19</sup>). In this paper we have presented a new variational derivation of the fundamental equation of quantum-statistical mechanics in order to allow for approximations to the dynamics of complicated statistical systems. We think that our treatment is not only formally very simple but also well suitable for practical calculations.

The following results were achieved:

- (i) The concept of ground state was generalized for mixed states.
- (ii) "Exact RPA equations", as the equations for the time evolution of quasi-stationary mixed states, were presented in the framework of a variational principle.
- (iii) An "exact sum rule" for mixed-state transition probabilities was derived.

(iv) A thermal boson expansion was proposed. Such an expansion is a most convenient tool to deal with dynamical correlations, which are not included in a mean-field theory.

We have emphasized that the formalism is not restricted to statistical equilibrium but can as well be applied to other situations. In particular, we can try to describe systems not very far from thermal equilibrium, for which the concepts of local temperature and entropy are useful.

The feasibility of the thermal mean-field theories and the associated boson expansions has been tested in the Lipkin model. Non-trivial temperature-dependent phase transitions were observed. The variations with the temperature of the collective excitation energy and of the collective mass have been examined in detail.

The model encourages the application to more realistic nuclear physics phenomena such as those described in the introduction. Another interesting field of application is the description of the interaction between spin waves of a ferromagnet through a thermal Holstein-Primakoff boson expansion.

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