MEAN FIELD THEORIES WITH MIXED STATES

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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 theory at finite temperatures is a particular case of the general formalism. A thermal boson expansion is defined, which allows to derive the RPA and 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.

The decay of high excited states above the yrast line has been observed [1,2] in recent studies of the compound nuclei formed in heavy ion reactions. These states have been interpreted on the basis of mean field theories as collective oscillations of mixed states. A renewed interest [3-7] in the quantum mechanics of mixed states has originated from the new dimension which such studies have added to the field of nuclear structure.

On the present talk a variational derivation of static and dynamic mean field theories appropriate to mixed states [8] is presented.

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,

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

In order to introduce the important notion of equilibrium for mixed states we consider the statistical matrix D_U unitarily similar to D,

$$D_U = U\, D\, U^+, \tag{2}$$

where U is an arbitrary unitary matrix, (we remark, in passing, that transformations generated by unitary matrices do not change the entropy, i.e. they are adiabatic in the thermodynamic sense). The density matrix $D_o = D_{U_o}$ describes an equilibrium state if and only if

$$E_o = \mathrm{Tr}\, (D_o\, H) \leq \mathrm{Tr}\, (D_U\, H) \tag{3}$$

for all unitary operators U. From this property it follows that

$$[\, H,\, D_o\,] = 0. \tag{4}$$

Indeed, let $D_U = e^{iF}\, D_o\, e^{-iF}$, where F is an infinitesimal hermitian operator such that $U = e^{iF}$. The expansion

$$\mathrm{Tr}\, (e^{iF} D_o\, e^{-iF} H) = E_o + \mathrm{Tr}\, ([F, D_o]\, H) + \ldots \geq E_o$$

leads to

$$\mathrm{Tr}\, ([\, F,\, D_o\,]\, H) = \mathrm{tr}\, (F\, [\, D_o, H\,]\,) = 0.$$

Since F is arbitrary, eq. (4) follows trivially.

We will discuss now the time evolution of D. According to quantum mechanics, the operator D satisfies the Liouville-von-Neumann equation

$$\dot{D} = i\, [\, D,\, H\,]. \tag{5}$$

Our aim is to obtain a variational formulation of eq. (5) which can be used as a source of reliable approximation schemes to the exact dinamical equation. We begin with writing the time-dependent density matrix in terms of the stationary density matrix D_o which satisfies eq. (4):

$$D\, (t) = U\, (t)\, D_o\, U^+\, (t),$$

where U (t) is a variational unitary operator.

Let us consider the action integral

$$I = \int_{t_1}^{t_2} L\, dt$$

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where the lagrangian L is given by

$$L = i\, Tr\, (U\, D_o\, \dot{U}^+) + Tr\, (U\, D_o\, U^+ H). \qquad (6)$$

The variation of the action integral induced by arbitrary variations of the unitary operator U at intermediate instants of time ($t_1 < t < t_2$) may be written

$$\delta I = i \int_{t_1}^{t_2} dt\, Tr\, \{\delta U U^+ (\dot{D} - i [D, H])\}.$$

Since the skew-hermitian time-dependent operator $\delta U U^+$ is arbitrary, the action principle $\delta I = 0$ is equivalent to the Liouville-von-Neumann equation.

We are now in a position to discuss the linear response function for mixed states.

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

$$D\,(t) = e^{-iF\,(t)}\, D_o\, e^{iF\,(t)} \qquad (7)$$

where F (t) is a hermitian infinitesimal operator. Since F is infinitesimal, the lagrangian (6) may be replaced by its leading order terms. The following quadratic lagrangian is obtained (the linear terms give no contribution)

$$L^{(2)} = \frac{i}{2}\, tr\, (D_o\, [F, \dot{F}])$$

$$- \frac{1}{2}\, Tr\, (D_o\, [F, [H, F]]) \qquad (8)$$

From the action condition

$$\delta \int_{t_1}^{t_2} L^{(2)}\, dt = 0 \qquad (9)$$

we obtain the equation

$$i\, tr (D_o [\delta F, \dot{F}]) - tr\, (D_o [\delta F, [H,F]]) = 0, \qquad (10)$$

or, since δF is arbitrary,

$$[\dot{F}, D_o] = - i\, [H\, [F, D_o]]. \qquad (11)$$

Here, the Jacobi identity for double commutators has been used together with the short term equilibrium condition (4).

We consider now the eigenmode solution of (11). We insert the appropriate ansatz

$$F_r (t) = e^{-iw_r t}\, O_r^+ + e^{iw_r t}\, O_r \qquad (12)$$

and obtain

$$w_r\, [O_r^+, D_o] = [H, [O_r^+, D_o]] \qquad (13)$$

$$- w_r\, [O_r, D_o] = [H, [O_r, D_o]].$$

We may require, without loss of generality, that $w_r \neq 0$. The following normalization condition for the operators O_r may then be imposed

$$Tr\, (D_o\, [O_r, O_r^+]) = \delta_{rs}, \qquad (14)$$

$$Tr\, (D_o\, [O_r, O_s]) = Tr\, (D_o\, [O_r^+, O_s^+]) = 0. \qquad (15)$$

The general solution of eq. (11) may be written as

$$F\,(t) = \sum_r (f_r\, e^{-iw_r t}\, O_r^+ + f_r^*\, e^{iw_r t}\, O_r) \qquad (16)$$

where,

$$f_r = tr\, (D_o\, [O_r\, , F(0)]). \qquad (17)$$

The energy-weighted sum rule for these transition amplitudes may now be derived. Indeed, from eq. (10) with δF replaced by F we conclude that

$$i\, tr\, (D_o\, [F, \dot{F}]) = tr\, (D_o\, [F, [H,F]]). \qquad (18)$$

It may easily be checked that

$$i\, tr\, (D_o\, [F, \dot{F}]) = 2 \sum_r w_r\, |f_r|^2. \qquad (19)$$

Therefore

$$\sum_r w_r\, |f_r|^2 = \frac{1}{2}\, tr\, (D_o\, [F, [H,F]]). \qquad (20)$$

We emphasize that this sum rule is exact and not restricted to the RPA in which log D_o and F are one body operators.

Indeed, the RPA describes small amplitude oscillations around the Hartree-Fock ground state. Now, the Hartree-Fock approximation for mixed states is obtained when the variational space in (3) only includes independent - particle density matrices. Therefore, in order to arrive at the RPA, log D_o should be a one body hermitian operator which may be written in the form

$$\log D_o = \log K + \sum_i \log \left(\frac{n_i}{1 - n_i}\right) a_i^+\, a_i, \qquad (21)$$

where K is a normalization factor, n_i is the occupation number of level i, and a_i, a_i^+ are fermion operators.

If the hamiltonian is given by

$$H = \sum_{ij} t_{ij} a_i^+ a_j + \frac{1}{2} \sum_{ijke} v_{ij,ke} a_i^+ a_j^+ a_e a_k \quad (22)$$

it is easy to arrive, in the framework of the independent particle approximation, at the following Hartree-Fock equations

$$t_{ij} + \sum_k n_k v^A_{ik,jk} = \varepsilon_i \delta_{ij} \quad (23)$$

where

$$v^A_{ij,ke} = v_{ij,ke} - v_{ij,ek} . \quad (24)$$

These equations are obtained if we require that

$$E_o = tr\ (D_o H) < tr\ (e^{iS} D_o e^{-iS}) \quad (25)$$

for all hermitian one body operators S.

We will now derive the RPA for mixed states by the method of boson expansions. This implies replacing the equilibrium density matrix in the independent particle approximation, D_o, by a boson vacuum state vector $|0)$ and substituting operators on the Hilbert space of fermion state vectors by boson images with the same commutation properties. More specificaly, if i,j are such that $n_i \neq n_j$ we introduce the boson operators A_{ij} with the following properties

$$A_{ij} = A^+_{ji} , \quad (26)$$

$$| A_{ij}, A_{k\ell} | = \delta_{i\ell} \delta_{jk} (n_i - n_j), \quad (27)$$

$$A_{ij}|0) = 0 \text{ if } n_i > n_j . \quad (28)$$

Having in mind that

$$Tr\ (D_o[a_i^+ a_j, a_k^+ a_e]) = \delta_{ie} \delta_{jk}(n_i - n_j) \quad (29)$$

we obtain the following expansion for $n_i \neq n_j$

$$(a_i^+ a_j)_B = (a_i^+ a_j)^{(1)}_B + (a_i^+ a_j)^{(2)}_B + \ldots \quad (30)$$

where

$$(a_i^+ a_j)^{(1)}_B = A_{ij} \quad (31)$$

$$(a_i^+ a_j)^{(2)}_B = - \frac{1}{3} \sum_k A_{ik} A_{kj} \left(\frac{1}{n_i - n_k} + \frac{1}{n_j - n_k}\right) + + \frac{1}{3} \delta_{ij} \sum_k \frac{2\ \Theta(n_i - n_k)}{n_i - n_k} \quad (32)$$

whith $\Theta(x) = 1$ if $x > 0$, $\Theta(x) = 0$ if $x < 0$.

On the other hand, if $n_i = n_j$,

$$(a_i^+ a_j)_B = (a_i^+ a_j)^{(0)} + (a_i^+ a_j)^{(2)}_B + \ldots, \quad (33)$$

where

$$(a_i^+ a_j)^{(0)}_B = n_i \delta_{ij} \quad (34)$$

$$(a_i^+ a_j)^{(2)}_B = \sum_k \frac{A_{ik}A_{kj}}{n_k - n_i} - \delta_{ij} \sum_k \frac{\Theta(n_i - n_k)}{n_k - n_i} . \quad (35)$$

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

$$Tr\ (D_o H) = E_o \quad (36)$$

$$Tr\ (D_o [H, a_i^+ a_j]) = 0 \quad (37)$$

$$Tr\ (D_o[[H, a_i^+ a_j], a_k^+ a_\ell]) = = (\varepsilon_j - \varepsilon_i) (n_i - n_j) \delta_{jk} \delta_{i\ell} + v^A_{ik,j\ell}(n_k - n_\ell) (n_i - n_j). \quad (38)$$

We require, therefore,

$$(0| H_B | 0) = E_o \quad (39)$$

$$(0| [H_B, A_{ij}] |0) = 0 \quad (40)$$

$$(0| [[H_B, A_{ij}], A_{k\ell}] |0) = (\varepsilon_j - \varepsilon_i)(n_i - n_j)\delta_{jk}\delta_{i\ell} + v^A_{ik,j\ell}(n_k - n_\ell) (n_i - n_j), \quad (41)$$

and find

$$H_B = E_o + \Delta + \frac{1}{2} \sum_{ij} \frac{\varepsilon_j - \varepsilon_i}{n_j - n_i} A_{ij} A_{ji} + + \frac{1}{2} \sum_{ijk\ell} v^A_{ik,j\ell} A_{ij} A_{k\ell} + \ldots \quad (42)$$

where

$$\Delta = - \frac{1}{2} \sum_{ij} [\varepsilon_j - \varepsilon_i + v^A_{ij,ji} (n_j - n_i)] \Theta(n_i - n_j) . \quad (43)$$

The diagonalization of H_B is straightforward and leads to the well known RPA equations for mixed states

$$\begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix} \begin{bmatrix} X_r \\ Y_r \end{bmatrix} = \omega_r \begin{bmatrix} X_r \\ Y_r \end{bmatrix} \quad (44)$$

Here, the matrices A and B have the following elements

$$A_{k\ell,ij} = (\varepsilon_k - \varepsilon_\ell)\, \delta_{\ell j}\, \delta_{ik} + v^A_{ki,\ell j}\, (n_i - n_j), \quad (45)$$

where i,j,k,ℓ are such that $n_\ell > n_k$, $n_i > n_j$, and

$$B_{k\ell,ij} = v^A_{ki,\ell j} \quad (46)$$

where i,j,k,ℓ are such that $n_\ell > n_k$, $n_j > n_i$. It may be shown that the stability condition (25) insures that the eigenvalues w_r are real.

As an example of the ideas involved in this approach we are going to consider the schematic two-level model which is due to Lipkin et al (10).

The hamiltonian of the Lipkin model reads as

$$H = J_z + \frac{V}{2}\, (J_+^2 + J_-^2) \quad (47)$$

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

$$[J_-, J_+] = -2 J_z, \quad [J_z, J_+] = J_+. \quad (48)$$

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

$$D = C\, e^{\alpha J_z}, \quad (49)$$

where C and α 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 (49) does not describe an exactly stationary state because $|H, D| = 0$. Such a state is described by $D_o = U^+ D\, U$, with $U U^+ = U^+ U = 1$, provided we choose U in order to have Tr $(D_o H)$ as a minimum of the energy.

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

$$U = e^{i\Theta}\, J_y\ . \quad (50)$$

The quantity to be minimized with respect to Θ is then

$$E = \mathrm{Tr}\,(D\, H) = \mathrm{Tr}\,(D_o\, U\, H\, U^+) =$$

$$= -\frac{1}{2} N\, P \cos\Theta + \sin^2\Theta\, \frac{VN}{4}\, (NP^2 - \frac{1+P^2}{2}) \quad (51)$$

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 corresponds to T = 0; P = 0 corresponds to $T = \infty$, for the extremal values).

The parameter which determines the ground-state phase transition is

$$\chi\,(P) = V\, \left| \frac{1}{2}\, (P + \frac{1}{P}) - NP \right|.$$

The solution of the minimization problem is

$$\Theta = 0, \ |\chi\,(P)| \leq 1,$$

$$\cos\Theta = -\chi^{-1}\,(P) \quad |\chi\,(P)| > 1.$$

The ground-state energy can then be calculated

$$E_o = -\frac{1}{2}\, NP, \ |\chi\,(P)| \leq 1$$

$$E_o = -\frac{NP}{4}\, \{ \frac{1}{|\chi(P)|} + |\chi\,(P)| \}, \ |\chi\,(P)| > 1.$$

We observe temperature-dependent seconde--order phase transitions. With $|\chi(P)| > 1$ the abnormal phase, wich 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.

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

$$\omega = \{ 1 - \chi^2\,(P) \}^{1/2} \text{ if } |\chi\,(P)| \leq 1$$

$$\omega = \{ 2\, (\chi^2(P) - 1) \}^{1/2} \text{ if } |\chi\,(P)| > 1.$$

We may implement in the model the method of thermal 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 (48) order by order. This prescription is complemented by the requirements

$$(0\, |(J_z)_B|\, 0) = \mathrm{Tr}\,(D_o J_z), \quad (0\, |(J_\pm)_B|0) = \mathrm{Tr}\,(D_o J_\pm),$$

where $|\,0)$ is the boson vacuum. In this way the conditions expressed in (27) and (29) 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,

$$(0\, |(J_z)_B|0) = -\frac{NP}{2}, \ (0\, |\, (J_\pm)_B\, |\, 0) = 0.$$

It is staightforward to verify that the commutation relations and these requirements are satisfied by the following boson expansions

$$(J_+)_B = (NP)^{1/2} (A^+ - \frac{1}{2NP} A^+A^+A + \ldots) =$$

$$= (NP)^{1/2} A^+ (1 - \frac{A^+A}{NP})^{1/2}$$

$$(J_-)_B = (J_+)_B^+ = (NP)^{1/2} (1 - \frac{A^+A}{NP})^{1/2} A,$$

$$(J_z)_B = A^+A - \frac{NP}{2} .$$

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 (47) we obtain an 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 corresponding results for $T = 0$.

From the numerical[8] results the following main conclusions can be drawn:

1. The Hartree-Fock energy increases with the temperature. It must be corrected by the inclusion of the correlation energy $(\omega - A) / 2$, 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.

2. The thermal RPA frequency vanishes at transition points, as expected. 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 frequencie with the temperature has also been obtained by Vautherin and Vinh-Mau[5] in the Brown-Bolsterli model, using Green's functions methods.

For high temperature (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.

Appendix

Experience teaches us that boson expansions converge better for appropriate linear combinations of particle-hole operators,

$$T_\alpha = \sum_{ij} t_{ij}^{(\alpha)} a_i^+ a_j,$$

$$T_A = \sum_{ij} t_{ij}^{(A)} a_i^+ a_j .$$

The meaning of the two types of labels, greek and latin, will become clear from the sequel. We assume that these operators form a Lie algebra and have the following properties

$$T_\alpha = T^+_{\bar\alpha} , \; T_A = T^+_{\bar A}$$

$$Tr\,(D_o [T_\alpha , T_\beta]) = \eta_\alpha \delta_{\alpha \bar\beta} , \; \eta_\alpha = - \eta_{\bar\alpha} ,$$

$$Tr\,(D_o [T_\alpha, T_A]) = 0,$$

$$Tr\,(D_o [T_A , T_B]) = 0,$$

were $\bar\alpha = -\alpha$, $\bar A = -A$. Equivalent relations hold for the operators $a_i^+ a_j$ if we make the following correspondence.

$$T_\alpha \to a_i^+ a_j \;\; (n_i \neq n_j)$$

$$T_A \to a_i^+ a_j \;\; (n_i = n_j)$$