A NOTE ON THERMAL BOSONS

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Abstract: We call attention to an alternative way of formulating the thermal boson expansion presented in a previous article. The new formulation involves a parametrization of a mean field density matrix by classical canonical variables. The thermal mean-field energy of the Lipkin model is evaluated as well as the excitation energy associated with the thermal bosons, correcting an error in the previous article. An approximation to the free energy of the model is presented, including the contribution of the thermal bosons.

1. Introduction

There has been recently some interest in describing nuclear collective excitations at finite temperature. Various extensions of standard zero temperature formalisms have been proposed in order to deal with mixed states.

We have proposed in ref. ¹⁾ a variational approach to the quantal statistical many-body problem. This has the advantage of being the generalization of the well-known variational formulation of the time-dependent Schroedinger equation for cold systems, which has been considered as a conceptual basis for the mean field approximation. Therefore it was straightforward to derive within our approach mean-field results at finite temperature: thermal time-dependent Hartree-Fock, thermal static Hartree-Fock and thermal RPA. They arise naturally by taking adequate ansätze for the trial density matrix.

Boson expansions are known to be useful tools to formulate the harmonic approximation (embodying quantal features) to oscillations around mean-field solutions and to go beyond that approximation ²⁾. We have proposed in ref. ¹⁾ a simple extension to generalize the boson concept and the method of boson expansions to a hot system.

Boson expansions at $T = 0$ consist essentially in establishing a mapping between fermion operators (it may be applied to spin systems as well) and boson operators in a given Fock space. The Belyaev-Zelevinsky mapping is defined by the following prescription:

(i) The commutation algebra fulfilled by the operators should be the same in both spaces, i.e. if

$$[A, B] = C \quad (1a)$$

then

$$[(A)_B, (B)_B] = (C)_B \quad (1b)$$

where the subscript B refers to the boson image;

(ii) expectation values of observables are the same in both spaces

$$\langle 0|A|0\rangle = \langle 0|(A)_B|0\rangle, \quad (2)$$

where $|0\rangle$ refers to the independent-particle approximation (Hartree-Fock) to the ground state and $|0\rangle$ is the boson vacuum.

For a situation described by a mixed state, only (ii) should be modified. Instead of an expectation value in the Hartree-Fock state, a statistical average over an adequate density matrix (the independent-particle density matrix) is used

$$\text{Tr}(D_0 A) = \langle 0|(A)_B|0\rangle. \quad (3)$$

Eqs. (1) and (3) define unambiguously a thermal boson expansion.

Note that in eq. (3) the boson vacuum is associated with a density matrix describing a mean field at finite temperature. There is therefore a redefinition of the boson vacuum for each temperature.

It is known that the variational formulation of mean field results may be cast in the form of classical equations of motion³⁾. The independent-particle density matrices D are parametrized by a set of complex numbers α , which should be chosen in such a way that α and α^* are canonically conjugate to each other, and variation is performed with respect to these quantities.

Alternatively, the thermal boson expansion proposed in ref.¹⁾ may be formulated in terms of the following ingredients: (i) fermion states described by the mean field density matrices $D(\alpha)$; (ii) coherent states $|\alpha\rangle$ belonging to the boson Fock space constructed with the aid of appropriate boson operators $a_i, a_i^\dagger$ (we have $a_i|\alpha\rangle = \alpha_i|\alpha\rangle$). A mapping is established:

- between mean field states $D(\alpha)$ and coherent states $|\alpha\rangle$.
- between fermion operators A and their boson images $(A)_B$ in such a way that the relation

$$\text{Tr}(D(\alpha)A) = \langle \alpha|(A)_B|\alpha\rangle \quad (4)$$

is satisfied for arbitrary α .

It follows that the thermal boson expansion proposed in ref.¹⁾ is obtained by replacing Poisson brackets $\{\alpha_i, \alpha_j\}$, and $\{\alpha_i, \alpha_j^*\}$, respectively, by commutators $[a_i, a_j]$ and $[a_i, a_j^\dagger]$. That expansion is therefore nothing else than the natural quantization scheme of the classical dynamical system described by the mean field equations. We hope that the quantized hamiltonian embodying the main quantal correlations provides a useful model of the quantal dynamics of the hot system and describes well such properties as the strength distribution of collective states built on a hot reference state.

We obtain classical equations of motion in the case of the Lipkin model at finite temperature and show how the quantization of the classical hamiltonian leads to the thermal boson expansion. Since ref. ¹⁾ contains an error in the application of the method to the Lipkin model, our approach has been subject to some criticism (see refs. ^{2,4)}). In the present work we correct the error and try to clarify the meaning and purpose of our method of thermal bosons.

We emphasize that the method of thermal bosons has appeared as a simple extension of the boson theory for zero temperature and does not have such a firm foundation on the principles of statistical mechanics as the works based on "thermofield dynamics" ⁴⁻⁶⁾. However, since the invoked variational principle leads in the most general case to the Liouville-von Neumann equation, the possibility exists to improve towards the exact quantal statistical results any approximations made in practical problems.

The variational approach is presented in sect. 2 leading to the boson expansion through a requantization process. In sect. 3, this procedure is applied to the Lipkin model. A brief discussion of the results, together with a comparison with other works, is presented in sect. 4.

2. Variational approach

The basic idea of ref. ¹⁾ is centered on the derivation of the mean field solutions for mixed states (time-dependent Hartree-Fock at finite temperature) from the lagrangian

$$L = i \operatorname{Tr} (D_0 U \dot{U}^\dagger) - \operatorname{Tr} (D_0 U H U^\dagger), \quad (5)$$

where H is the hamiltonian of the system, D_0 is a density matrix (such that $\operatorname{Tr} D_0 = 1$ and the eigenvalues of D_0 are non-negative) and U is a time-dependent unitary matrix. The mean field approximation in this context means that D_0 and U are restricted to the form

$$D_0 = \exp(A) / \operatorname{Tr}(\exp A), \quad U = \exp(iS), \quad (6)$$

where A and S are hermitian one-body operators. The most general U of the specified form may be parametrized by a set of complex quantities $\alpha_1, \dots, \alpha_n$. We write $U = U(\alpha, \alpha^*)$ to indicate that U is an analytical function of $2n$ variables (α_k^* is the complex conjugate of α_k), so that both derivatives $\partial U / \partial \alpha_k$ and $\partial U / \partial \alpha_k^*$ are well defined operators. Without any loss of generality, the parameters $\alpha_1, \dots, \alpha_n$ may be chosen such that

$$\operatorname{Tr} (D_0 U \delta U^\dagger) = \frac{1}{2} \sum_k (\alpha_k \delta \alpha_k^* - \alpha_k^* \delta \alpha_k). \quad (7)$$

The parameters α_k, α_k^* may therefore be viewed as canonical variables. It is convenient to introduce the function

$$\mathcal{H}(\alpha, \alpha^*) = \operatorname{Tr} (D_0 U(\alpha, \alpha^*) H U^\dagger(\alpha, \alpha^*)). \quad (8)$$

Then, the time evolution of the variables $\alpha_1, \dots, \alpha_n$ is determined by the action principle, which leads to Hamilton's equations

$$i\dot{\alpha}_k^* = \frac{\partial \mathcal{H}}{\partial \alpha_k}, \quad -i\dot{\alpha}_k = \frac{\partial \mathcal{H}}{\partial \alpha_k^*}. \quad (9)$$

The boson image of H (denoted by H_B) is obtained by replacing the classical variables α_k, α_k^* by boson operators $a_k, a_k^\dagger$ ordered in such a way that

$$\langle \alpha | H_B | \alpha \rangle = \mathcal{H}(\alpha, \alpha^*), \quad (10)$$

where $|\alpha\rangle$ is a boson coherent state defined by

$$a_k |\alpha\rangle = \alpha_k |\alpha\rangle. \quad (11)$$

One has $H_B =: \mathcal{H}(a_k, a_k^\dagger) :$, where $: :$ denotes normal order. The boson images of any other operator may be obtained in the same way.

Care should be taken to ensure that α_k corresponds to a destruction operator and α_k^* to a creation operator. This distinction arises naturally in practice. For instance, if we denote by $c_i^\dagger, c_i$ fermion operators related to the single-particle state i and by n_i the corresponding occupation number such that $\text{Tr}(D_0 c_i^\dagger c_j) = n_i \delta_{ij}$, it follows from the commutation relation

$$\text{Tr}(D_0 [c_i^\dagger c_j, c_k^\dagger c_l]) = (n_i - n_j) \delta_{il} \delta_{jk} \quad (12)$$

that $c_i^\dagger c_j$ should be associated with a boson destruction operator A_{ij} if $n_i > n_j$. On the other hand, $c_i^\dagger c_j$ is related to a boson creation operator $A_{ji}^\dagger$ if $n_j > n_i$.

3. The Lipkin model revisited

The Lipkin model has been invented to imitate the many-nucleon system and to investigate different many-body techniques. The hamiltonian of this model may be written as

$$H = T_z + V(T_+^2 + T_-^2), \quad (13)$$

where T_z, T_+ and T_- are quasi-spin operators. These are constructed as pairs of fermionic operators

$$\begin{aligned} T_+ &= \sum_{n=1}^N c_{n,+1}^\dagger c_{n,-1}, \\ T_- &= \sum_{n=1}^N c_{n,-1}^\dagger c_{n,+1}, \\ T_z &= \frac{1}{2} \sum_{n=1}^N (c_{n,+1}^\dagger c_{n,+1} - c_{n,-1}^\dagger c_{n,-1}). \end{aligned} \quad (14)$$

The fermions occupy two sets of N degenerate levels labeled by -1 and $+1$. The operators $c_{n,i}^\dagger$, $c_{n,i}$ fulfill therefore the anticommutation relations

$$\begin{aligned}\{c_{n,i}, c_{n',i'}^\dagger\} &= \delta_{nn'}\delta_{ii'}, \\ \{c_{n,i}, c_{n',i'}\} &= 0.\end{aligned}\quad (15)$$

A possible one-body density matrix is given by

$$D_0 = \exp(-\beta T_z) / \text{Tr}(\exp(-\beta T_z)), \quad (16)$$

with β a real parameter, measuring the occupation probability. An unitary transformation defined by an operator U may be necessary in order to obtain a lower mean field energy but, for the sake of simplicity, let us consider now a phase which is well described by the density matrix D_0 . The commutation relation

$$\text{Tr}(D_0[T_+, T_-]) = 2 \text{Tr}(D_0 T_z) < 0 \quad (17)$$

implies that T_+ is related to a creation operator, while T_- is related to a destruction operator (assuming $\beta > 0$).

Any parametrization of the time-dependent density matrix, built up on D_0 ,

$$D(\alpha) = U^\dagger(\alpha, \alpha^*) D_0 U(\alpha, \alpha^*), \quad (18)$$

with U a unitary operator parametrized by the complex variable α , leads to the following classical equations of motion:

$$i\dot{\alpha}^* = \partial \mathcal{H} / \partial \alpha, \quad -i\dot{\alpha} = \partial \mathcal{H} / \partial \alpha^*, \quad (19)$$

with $\mathcal{H} = \text{Tr}(D_0 U(\alpha, \alpha^*) H U^\dagger(\alpha, \alpha^*))$, providing condition (7) is imposed.

Now, the prescription

$$\text{Tr}(D_0 U(\alpha, \alpha^*) T_{(+,-,z)} U^\dagger(\alpha, \alpha^*)) = \langle \alpha | (T_{(+,-,z)})_{\text{B}} | \alpha \rangle, \quad (20)$$

in agreement with eq. (4), leads to a boson representation of the operators T_+ , T_- , T_z . An example of such a boson representation is given by the operators $(T_+)_{\text{B}}$, $(T_-)_{\text{B}}$, $(T_z)_{\text{B}}$ obtained in ref. ¹⁾

$$\begin{aligned}(T_+)_{\text{B}} &= (NP)^{1/2} a^\dagger (1 - a^\dagger a / NP)^{1/2}, \\ (T_-)_{\text{B}} &= (NP)^{1/2} (1 - a^\dagger a / NP)^{1/2} a, \\ (T_z)_{\text{B}} &= -\frac{1}{2} NP + a^\dagger a,\end{aligned}\quad (21)$$

where $P = P_- - P_+$ is the difference between the occupation probabilities of the two levels of the Lipkin model. The parameter P is clearly related to β by

$$P = \text{th } \frac{1}{2}\beta. \quad (22)$$

We observe that eqs. (21) are a generalization, to a finite temperature, of the well-known Holstein-Primakoff boson representation.

The fact that the eigenvalues of $(T_z)_B$ need not be integers or half integers seems to be in conflict with the fact that the commutation relations of the boson representation $(T_+)_z, (T_-)_B, (T_z)_B$ reproduce precisely the commutation relations of the quasi-spin operators T_+, T_-, T_z . This means that the boson representations are mathematically ill-defined. In practice, this problem does not arise since a truncation is always made in the boson expansion.

Let us examine the boson representation of the energy of the system. Since, for a non-vanishing temperature, the boson image of the product does not necessarily agree with the product of the boson images, one should be careful, not just inserting in H the boson expansion (21). We have to expand the hamiltonian H itself. The first term of the expansion is clearly the thermal Hartree-Fock energy (mean-free energy). This value is achieved with the aid of an unitary transformation of the density matrix (or equivalently the hamiltonian H)

$$U(\theta) = \exp(i\theta T_y). \quad (23)$$

The thermal Hartree-Fock energy $E_0 = \langle 0|H_B|0 \rangle$ is the minimum of the function

$$E(\theta) = \text{Tr}(D_0 U(\theta) H U^\dagger(\theta)). \quad (24)$$

In order to evaluate correctly the traces, we note that we may construct a convenient invariant subspace of H in the following way. Denoting the vacuum by $|0\rangle$ ($c_{n,\gamma}|0\rangle = 0$), let us consider the subspace spanned by the kets

$$|\gamma_1, \dots, \gamma_N\rangle = c_{1,\gamma_1}^\dagger c_{2,\gamma_2}^\dagger \dots c_{N,\gamma_N}^\dagger |0\rangle; \quad \gamma_i = \pm 1. \quad (25)$$

We define

$$X = \left\{ \sum_{\gamma_1, \dots, \gamma_N} \mathcal{C}_{\gamma_1, \dots, \gamma_N} |\gamma_1, \dots, \gamma_N\rangle \right\}. \quad (26)$$

Clearly, if a vector $|x\rangle \in X$, then we also have $H|x\rangle \in X$. Although the total Hilbert space of the N -particle system is spanned by the kets

$$|n_1 \gamma_1, \dots, n_N \gamma_N\rangle = c_{n_1, \gamma_1}^\dagger \dots c_{n_N, \gamma_N}^\dagger |0\rangle \quad (27)$$

it is enough, for calculating the traces, to consider the above-defined invariant subspace. The trace of any operator is taken to be

$$\text{Tr}(A) = \sum_{i=1}^N \langle i|A|i \rangle, \quad (28)$$

where the set $\{|i\rangle\}$ is some basis of X ($i \in \{1, \dots, 2^N\}$). We obtain

$$\begin{aligned} \text{Tr}(\exp(\beta T_z)) &= \sum_{\gamma_1, \dots, \gamma_N} \langle \gamma_1 \dots \gamma_N | \exp(\beta T_z) | \gamma_1 \dots \gamma_N \rangle \\ &= (2 \cosh \tfrac{1}{2} \beta)^N. \end{aligned} \quad (29)$$

Therefore (see eq. (16))

$$\text{Tr} (D_0 T_z) = \frac{1}{2} N \text{th} \frac{1}{2} \beta = \frac{1}{2} NP. \quad (30)$$

On the other hand,

$$\text{Tr} (D_0 T_+) = \text{Tr} (D_0 T_-) = 0 \quad (31)$$

and

$$\text{Tr} (D_0 (T_+ T_- + T_- T_+)) = NP. \quad (32)$$

The energy (24) is finally given by

$$E(\theta) = -\frac{1}{2} NP \cos \theta + \frac{1}{4} VN(N-1)P^2 \sin^2 \theta. \quad (33)$$

This expression agrees with eq. (6.2) of ref. ⁴⁾ (or eq. (24.77) of ref. ²⁾). Minimizing with respect to θ , we conclude that there are two possible phases: a normal phase with $\cos \theta_0 = 1$ if $-1 \leq \chi(P) = VP(1-N) \leq 1$ and an abnormal phase with $\cos \theta_0 = -1/\chi(P)$ if $|\chi(P)| > 1$. When the system for $P=1$ is at the abnormal phase, there is a phase transition for decreasing P .

There is an error in ref. ¹⁾ in connection with the computation of the traces (31) and (32). This however does not invalidate the conceptual foundation of the method.

We could as well have calculated the traces using the space spanned by the kets (27), instead of the subspace X . The result for the energy would be the same, as it may be easily verified.

In the sequel, we write $U_0 = U(\theta_0)$. We observe that there are no linear terms in the boson expansion, due to equations like $\text{Tr} (U_0^\dagger D_0 U_0 [H, T_+]) = 0$, which express the stationarity condition for the energy $E(\theta)$. The quadratic term may be calculated from the trace of the double commutators

$$\begin{aligned} \text{Tr} (U_0^\dagger D_0 U_0 [[H, T_+], T_-]) &= (0 | [[(H)_B, (T_+)_B], (T_-)_B] | 0) \\ &= NP(\cos \theta_0 + \frac{3}{2} \chi(P) \sin^2 \theta_0), \end{aligned} \quad (34)$$

$$\begin{aligned} \text{Tr} (U_0^\dagger D_0 U_0 [[H, T_+], T_+]) &= (0 | [[(H)_B, (T_+)_B], (T_+)_B] | 0) \\ &= NP\chi(P)(1 - \frac{1}{2} \sin^2 \theta_0). \end{aligned} \quad (35)$$

It is straightforward to identify the collective frequency

$$\begin{aligned} \omega(P) &= \sqrt{1 - \chi^2(P)}, & \text{if } |\chi(P)| \leq 1, \\ \omega(P) &= \sqrt{2(\chi^2(P) - 1)}, & \text{if } |\chi(P)| > 1. \end{aligned} \quad (36)$$

Let us now make the connection between the parameter P which identifies the statistical mixture and the temperature. We consider a situation of equilibrium

described by the canonical ensemble. The free energy F of the system may be considered to consist of two parts:

(i) The free energy of the mean field

$$\begin{aligned} F_0 &= E_0 - TS_0 \\ &= -\frac{1}{2}NP + \frac{1}{4}VNP^2(N-1)\sin^2\theta_0 \\ &\quad + \frac{1}{2}Nk_B T[(1+P)\log(1+P) + (1-P)\log(1-P)]. \end{aligned} \quad (37)$$

We remark here that the mean field entropy would be a factor of two bigger, if the full Hilbert space spanned by (27) was taken instead of (26), for calculating the trace. This has consequence for the thermodynamic properties of the system and corresponds to the possible occurrence of degrees of freedom with very different relaxation times.

(ii) the free energy of the thermal bosons

$$\begin{aligned} F_2 &= E_2 - TS_2 \\ &= \omega(P)n(P) + k_B[n(P)\log n(P) - (1+n(P))\log(1+n(P))], \end{aligned} \quad (38)$$

where

$$n(P) = [\exp(\omega(P)/k_B T) - 1]^{-1} \quad (39)$$

are boson occupation numbers.

The relationship between P and the temperature T arises from the minimization of the free energy with respect to P (we remind that P was introduced to parametrize the trial density matrix and should therefore be seen as a variation parameter):

$$\frac{dF}{dP} = 0. \quad (40)$$

Admittedly, the procedure we have described has not been derived from first principles. The inclusion of the thermal bosons free energy is based on intuitive arguments but we hope that it may provide a reasonable treatment of the most relevant statistical correlations.

Let us consider the normal phase, for the sake of simplicity. We have

$$\begin{aligned} F_0 &= -\frac{1}{2}NP + \frac{1}{2}NK_B T[(1+P)\log(1+P) + (1-P)\log(1-P)], \\ F_2 &= \sqrt{1-\chi^2(P)} n(P) + k_B T[n(P)\log n(P) - (1+n(P))\log(1+n(P))]. \end{aligned} \quad (41)$$

Then eq. (40) leads to the following transcendental equation for P

$$P = \text{th} \left[\frac{1}{k_B T} \left(\frac{1}{2} - \frac{1}{NP} \frac{\chi^2(P)}{1-\chi^2(P)} \omega(P)n(P) \right) \right]. \quad (42)$$

The results presented in fig. 4 of ref.⁴⁾ correspond to considering only the mean-field free energy (37). In that case the parameter which describes the mixed

state may be identified with the temperature (compare eq. (30) with the equation which is obtained from (42) if the bosons are turned off). The inclusion of the free energy of the thermal bosons may be viewed as a way to take into account further quantal and thermal correlations. These types of corrections have been included in the treatment we have made of the Heisenberg ferromagnet (see refs. ^{8,9})).

4. Conclusions

We have in this note called attention to a possible formulation of the thermal boson expansion defined in ref. ¹), which essentially consists in using coherent states (at finite temperature) to quantize classical observables, in particular the hamiltonian.

The idea has been applied to the quasi-spins of the Lipkin model, leading to a generalization of the Holstein-Primakoff transformation, and to the boson expansion of the hamiltonian of that system.

Some authors (see e.g. refs. ^{5,6})), instead of working with density matrices in the standard form, have preferred to describe the thermal HF and RPA results using the techniques of the so-called "thermo-field dynamics". This approach seems in fact very powerful to extend the results known for pure states to the case of statistical mixtures: the mixed state is described as a pure state (Slater determinant) in an enlarged space. The cost of the method is clearly the duplication of all the degrees of freedom of the problem under study. An advantage of the formalism of thermo-field dynamics lies in its well established connection to the basic principles of quantal statistical mechanics.

The results obtained for the energy up to the harmonic order in the framework of thermo-field dynamics seem in agreement with the results of the present approach. It remains to be seen whether the two boson expansions agree when developed to higher orders. Further work is needed along this line.

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