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Resonant states in the thermo field dynamics

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Abstract

The formalism of the thermo field dynamics (TFD) is extended in order to accommodate resonant states belonging to the spectrum of a single-particle Hamiltonian. It is shown that the rules of the TFD can be applied to a fermionic basis where resonant states are described as complex eigenvalues. The consequences for the definition of TFD thermodynamical observables, due to the inclusion of resonant states, are studied. © 1998 Elsevier Science B.V.

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1. Introduction

The theoretical treatment of thermal excitations in quantum many-body systems has been the subject of various studies in different fields of physics [1]. Among the theories used to treat thermal excitations, the thermo field dynamics (TFD) developed by Umezawa and co-workers has received attention in a number of publications [2]. A comparison between the TFD and other theories based on the use of contours in the time–temperature plane can be found in Ref. [3].

The advantage of the use of TFD, in dealing with quantum systems at finite temperature, has been presented in Ref. [4], where the gauge structure of the theory was discussed in detail. Several other aspects of the TFD can be found in Refs. [2,17] and references therein.

The experimental study of nuclear properties at finite temperature has produced new interest in TFD and it has already been shown that the theory exhibits some advantages

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as compared, for example, with Matsubara's techniques or with other complex- or real-time formalisms [5]. One particular problem associated with the treatment of nuclei at finite temperature is the inclusion of the continuum [6]. Recently, we have investigated the suitability of a representation of resonant states [7] which is based on the theory of ultradistributions and on Dirac's formulation of quantum mechanics. The formulation of quantum mechanics in the rigged Hilbert space (RHS) has been presented, among others, by Bohm [14]. In Ref. [14] it is shown that idealized resonances can be described in the RHS representation by generalized eigenvectors of a self-adjoint Hamiltonian with complex eigenvalues. These states are included in the Hamiltonian eigenvalue density as Breit–Wigner energy distributions around the real value of their energies. The spreading of these distributions around the centroids is given by the imaginary part of the energies. In Ref. [7] we show that this representation of resonances is indeed valid and that it is consistent with Dirac's formulation. In the present work we shall adopt the same definition of a resonance and assume that the spectrum of the Hamiltonian includes complex eigenvalues. Since we are dealing with a Fock representation this condition (complex eigenvalues) suffices for the identification of resonances, since generalized spectral functions can be constructed without explicit reference to wave functions [6–8,13,14].

In the present paper we are mostly concerned with the question about the inclusion of resonant states [8] in the framework of the TFD, with reference to the calculation of nuclear partition functions and Green functions at finite temperatures. These elements, and the need of a rigorous procedure to describe the effects due to the continuum at finite temperature, are frequently found in articles specifically devoted to nuclear structure studies [9,10].

In Section 2 we shall discuss the meaning of thermal Bogoliubov transformations in the presence of resonant states and extend the rules of the TFD to include resonant states. The TFD invariance of a Hamiltonian with complex eigenstates will be shown in Section 3. The TFD representation in Fock space, the occupation numbers and the partition functions will be given in Section 4. Conclusions are drawn in Section 5.

2. On the TFD with complex eigenvalues

We shall start our presentation of the subject with the definition of the TFD Hamiltonian $\hat{H}$, associated with a physical system described by a Hamiltonian H and its TFD dual $\tilde{H}$. For the sake of completeness we shall briefly review the main steps of the TFD procedure as they have been formulated by Umezawa and coworkers [1,17]. Details can be found in Refs. [12,15]. The main features of TFD are the following [3–5].

(i) TFD physical and dual spaces are related in such a manner that one has always to calculate vacuum expectation values instead of the usual statistical averages.

(ii) Fermion degrees of freedom are expressed in terms of thermal quasi-particles. The normal ordering of these operators is defined with respect to the TFD vacuum given by the G-transformation. The thermal quasi-particles are constructed by acting thermal

Bogoliubov transformations on the original and dual fermion degrees of freedom. Finally, the meaning of the various operations which are used in TFD calculations, such as the TFD tilde-transformation which relates dual and physical degrees of freedom, can be found in Ref. [1]. In the following we shall assume that the density of eigenvalues of the starting Hamiltonian represents both bound states, which correspond to real eigenvalues, and resonant states, which are represented by complex eigenvalues. This situation is found, for instance, in the single-particle solutions of the central nuclear potential which includes centrifugal and Coulomb terms in addition to the bulk and spin–orbit contributions. The superposition of these terms generates a central potential of finite deep and finite range with a dense distribution of eigenvalues around the surface. It has been shown that bound states and a few isolated resonances, with complex energies, can be used to define a basis [8]. It has also been shown that the corresponding Hamiltonian distribution of eigenvalues can be represented by a delta function on discrete states (i.e. states with zero imaginary part of the energy) and a Breit–Wigner distribution for the few narrow resonances near the real axis [6–10]. The energies of these non-overlapping resonances are complex and their imaginary parts are much smaller than the real parts. In the above-mentioned works they have been introduced in configuration space and they were adopted as a representation of the continuum. The full implication of this assumption can be found in Berggren's works [8,13]. It is the aim of the present work to include these states in a Fock's representation and use it to calculate TDF vacuum expectation values. Therefore, by assuming that the Hamiltonian density includes both discrete states and resonances, we can write, for a single-particle (free) Hamiltonian, the expression

$$\hat{H} = H - \tilde{H} = \sum_{n=1} (E_n a_n^+ a_n - E_n^* \tilde{a}_n^+ \tilde{a}_n), \tag{1}$$

where E_n is the eigenvalue associated with the linear momentum $p_n = k_n - i\eta_n$, with $\eta_n \geqslant 0$. The quantity η_n entering in this definition of p_n is related to the imaginary part of the energy, $E(p_n) = \epsilon_n - i\gamma_n/2$, and its value is given by the solution of the central potential eigenvalue problem. Therefore, η_n does not represent the imaginary shift of the energy variable appearing in the spectral density distribution [16]. Rather, it is a physical parameter associated with the single-particle scape-width [6].

As usual we shall denote TFD dual states by a tilde [11]. The meaning of the tilde operation has been discussed extensively by Ojima [15] and it leads to the definition of the TFD quasi-fermions as a superposition of physical and dual fields.

In order to write explicitly a TDF representation, with complex eigenvalues and at finite temperature, we shall request: (i) the invariance of $\hat{H}$ under thermal transformations [12], and (ii) real values of the expectation value of H on the TFD vacuum. These conditions can be fulfilled if and only if the following complex anticommutators are allowed in the $(a_n, \tilde{a}_n)$ basis, namely

$$\{a_n, a_m^+\} = \lambda_n \delta_{nm} \tag{2}$$

and

$$\{\tilde{a}_n, \tilde{a}_m^+\} = \lambda_n{}^* \delta_{nm}, \tag{3}$$

and the remaining anticommutators vanish.

In the present discussion of the formalism we assume that $|\lambda_n| \neq 0$. The meaning of this condition will be discussed later (see Subsection 4.2).

The algebra defined by Eqs. (2) and (3) differs from the generalized algebra used by Henning [2] and from the method of Ref. [16]. In order to draw the difference between these methods and the present one, let us mention that in Ref. [2] physical representations are constructed by the direct summation of elementary fields weighted by positive weighting functions. These elementary fields have energy and momentum not related by dispersion relations, thus they represent off-mass extensions. A similar representation, in terms of spectral functions and propagators, is used in Ref. [16]. In the present paper we shall work in a RHS [7,14] instead to define physical fields. Once the physical fields are expanded in terms of creation and annihilation operators, in both methods, the commutation relations among them require state-dependent renormalizations, which for the case of Ref. [2] are also momentum dependent (cf. Eqs. (3.28)–(3.30) of Ref. [2]). In our formalism Eqs. (2) and (3) result from conditions (i) and (ii) and they are valid at equilibrium. It should be emphasized that the commutator algebra of Eqs. (2) and (3) is not obtained by a simple rescaling, as shown at the end of Subsection 4.2).

In this representation the TFD thermal vacuum can be written as

$$|0(\beta)\rangle = \prod_{n=1} (1 + C_n a_n^+ \tilde{a}_n^+) |0\rangle,$$

$$\langle 0(\beta)| = \langle 0| \prod_{n=1} (1 + D_n \tilde{a}_n a_n). \tag{4}$$

The thermal vacuum is normalized accordingly, i.e.

$$\langle 0(\beta)|0(\beta)\rangle = 1 = \prod_{n=1} (1 + |\lambda_n|^2 D_n C_n). \tag{5}$$

The constants C_n and D_n, entering in the definition of the TFD vacuum, can be determined by transforming the single-particle operators from the TFD basis at zero temperature to a TFD basis at finite T, as is shown below.

3. Complex thermal Bogoliubov transformations

Let B and C be the matrices which define the transformation from the basis of $(a, \tilde{a})$ to the basis $(\alpha, \tilde{\alpha})$, which is the basis associated with the $\frac{1}{2}$-representation of the TFD [1,12]. As usual, $\beta = 1/T$ is the inverse temperature, in units of energy. In the following the subindex n will be omitted, for convenience. In explicit form one has, for the transformations B and C,

$$\begin{pmatrix} \alpha \\ \tilde{\alpha}^+ \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} a \\ \tilde{a}^+ \end{pmatrix} \tag{6}$$

and

$$\begin{pmatrix} \alpha^+ \\ \tilde{\alpha} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} a^+ \\ \tilde{a} \end{pmatrix} . \tag{7}$$

From the anticommutation relations (2) and (3) one obtains

$$\begin{aligned} C &= \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^* \end{pmatrix} \left(B^{-1}\right)^t \begin{pmatrix} 1/\lambda & 0 \\ 0 & 1/\lambda^* \end{pmatrix} \\ &= [\det(B)]^{-1} \begin{pmatrix} B_{22} & -(E^*/E)B_{21} \\ -(E/E^*)B_{12} & B_{11} \end{pmatrix} , \end{aligned} \tag{8}$$

with $\det(B) = B_{11}B_{22} - B_{12}B_{21}$, after transforming (1) under the conditions (i) and (ii). In (8) we have used the result $E\lambda = E^*\lambda^*$. Since we are dealing with fermions the double-tilde operation is defined by

$$\begin{aligned} &(\tilde{a})\tilde{} = -a, \qquad (\tilde{\alpha})\tilde{} = -\alpha, \\ &(\tilde{a}^+)\tilde{} = -a^+, \qquad (\tilde{\alpha}^+)\tilde{} = -\alpha^+. \end{aligned} \tag{9}$$

From these relations the elements of the matrix B fulfill the following relations:

$$\begin{aligned} &|\det(B)| = 1, \\ &\det(B) = B_{11}/B_{11}{}^* = B_{22}/B_{22}{}^* = (E^*/E)B_{21}/B_{21}{}^* = (E/E^*)B_{12}/B_{12}{}^*. \end{aligned} \tag{10}$$

Therefore,

$$\begin{aligned} &B_{22}B_{11}{}^* = B_{22}{}^*B_{11} \in \mathbb{R}, \\ &E^2B_{12}B_{21}{}^* = E^{*2}B_{12}{}^*B_{21} \in \mathbb{R}. \end{aligned} \tag{11}$$

The invariance of $\hat{H}$ follows from the relationships between the elements of the matrices B and C and the anticommutation conditions of the single-particle operators, as can easily be seen by applying the transformations (6) and (7), i.e.

$$\hat{H} = \sum_{n=1}(E_n a_n^+ a_n - E_n^* \tilde{a}_n^+ \tilde{a}_n) = \sum_{n=1}(E_n \alpha_n^+ \alpha_n - E_n^* \tilde{\alpha}_n^+ \tilde{\alpha}_n) \tag{12}$$

and

$$\langle 0(\beta)|H|0(\beta)\rangle = \langle 0(\beta)|\tilde{H}|0(\beta)\rangle = -\sum_{n=1}(\bar{E}_n B_{21n} B_{12n}) \in \mathbb{R}, \tag{13}$$

where $\bar{E}_n = \lambda_n E_n$. Thus, if $\langle 0(\beta)|H|0(\beta)\rangle$ is real, from the equations which relate the elements of B, Eqs. (10) and (11), it is seen that B_{11n} and B_{22n} are real for all values of the eigenvalue index n.

It should be mentioned that, even for the adopted TFD representation, the operator a^+ is not the adjoint of a, except for states associated with real eigenvalues.

It can easily be shown that any operator $\hat{A}$ of the form

$$\hat{A} = A - \tilde{A} = \sum_n \bar{A}_n \left(\frac{a_n^+ a_n}{\lambda_n} - \frac{\tilde{a}_n^+ \tilde{a}_n}{\lambda_n^*} \right), \tag{14}$$

with $\bar{A}_n \in \mathbb{R}\ \forall n$, is invariant under complex thermal transformations and that the expectation value of A ($\tilde{A}$) is always real if the expectation value is considered on a state which is symmetric under the TFD "tilde" transformation [11,12,15,17]. This result is valid for the case of the Hamiltonian, as an operator, where $\bar{A}_n = \bar{E}_n$.

4. The generator of the thermal transformations

In the following we shall construct the generator G of the TFD transformations by applying the conditions described in the previous section. The TFD vacuum $|0(\beta)\rangle$ ($\langle 0(\beta)|$) is related to the corresponding one at zero temperature $|0\rangle$ ($\langle 0|$) by the operation

$$|0(\beta)\rangle = e^G|0\rangle \qquad (\langle 0(\beta)| = \langle 0|e^{-G}). \tag{15}$$

Since the vacuum must be invariant under both thermal and "tilde" transformations, one has $\widetilde{|0(\beta)\rangle} = |0(\beta)\rangle$ and $\widetilde{\langle 0(\beta)|} = \langle 0(\beta)|$, therefore $\tilde{G} = G$.

The transformations between single-particle operators can be written

$$\begin{aligned} &\alpha = e^G a e^{-G}, \qquad \alpha^+ = e^G a^+ e^{-G}, \\ &\tilde{\alpha} = e^G \tilde{a} e^{-G}, \qquad \tilde{\alpha}^+ = e^G \tilde{a}^+ e^{-G}. \end{aligned} \tag{16}$$

The transformed operators α and $\tilde{\alpha}$ (α^+ and $\tilde{\alpha}^+$) annihilate the thermal right (left) vacuum

$$\begin{aligned} &\alpha|0(\beta)\rangle = \tilde{\alpha}|0(\beta)\rangle = 0, \\ &\langle 0(\beta)|\alpha^+ = \langle 0(\beta)|\tilde{\alpha}^+ = 0. \end{aligned} \tag{17}$$

These are the so-called thermal state conditions [12]. Since $\hat{H}$ is invariant under these transformations

$$[\hat{H}, G] = 0. \tag{18}$$

The general form of G is

$$G = \sum_{n=1} \theta_n \left\{ B_{12n} \frac{a_n^+ \tilde{a}_n^+}{\lambda_n} + B_{21n} \frac{\tilde{a}_n a_n}{\lambda_n^*} + \frac{1}{2}(B_{11n} - B_{22n}) \left[\frac{a_n^+ a_n}{\lambda_n} + \frac{\tilde{a}_n^+ \tilde{a}_n}{\lambda_n^*} \right] \right\}, \tag{19}$$

where θ_n are parameters to be determined.

The condition $\tilde{G} = G$ restricts the value of these parameters and for each value of the index n one has

$$\theta^* B_{12}^*/\lambda^* = \theta B_{12}/\lambda \in \mathbb{R}, \qquad \theta^* B_{21}^*/\lambda = \theta B_{21}/\lambda^* \in \mathbb{R},$$
$$\theta^*(B_{11}^* - B_{22}^*) = \theta(B_{11} - B_{22}) \in \mathbb{R}. \tag{20}$$

Once the structure of G is determined one can evaluate $|0(\beta)\rangle$ and $\langle 0(\beta)|$. They are given by

$$|0(\beta)\rangle = e^G|0\rangle = \prod_{n=1} e^{\theta_n(B_{11n}-B_{22n})/2}[u_n + v_n a_n^+ \tilde{a}_n^+]|0\rangle, \tag{21}$$

$$\langle 0(\beta)| = \langle 0|e^{-G} = \langle 0|\prod_{n=1} e^{-\theta_n(B_{11n}-B_{22n})/2}[w_n + z_n \tilde{a}_n a_n], \tag{22}$$

where the coefficients u_n, v_n, w_n and z_n are determined by

$$u_n = \cosh(\theta_n q_n) - (B_{11n} - B_{22n})/(2q_n)\sinh(\theta_n q_n),$$
$$v_n = B_{12n}/(\lambda_n q_n)\sinh(\theta_n q_n),$$
$$w_n = \cosh(\theta_n q_n) + (B_{11n} - B_{22n})/(2q_n)\sinh(\theta_n q_n),$$
$$z_n = -B_{21n}/(\lambda_n^* q_n)\sinh(\theta_n q_n),$$
$$q_n = \tfrac{1}{2}[(B_{11n} - B_{22n})^2 + 4B_{12n}B_{21n}]^{1/2}. \tag{23}$$

From the above relations and from the thermal state conditions it follows that

$$B_{11}\sinh(\theta q) = -q\cosh(\theta q) + (B_{11} - B_{22})/2\sinh(\theta q),$$
$$B_{22}\sinh(\theta q) = -q\cosh(\theta q) - (B_{11} - B_{22})/2\sinh(\theta q). \tag{24}$$

These equations will be used to compute the thermal dependence of the elements of the matrix B, as shown below.

4.1. The partition function

We shall work in Fock's representation, which is equivalent to the grand canonical ensemble. In this representation the TFD vacuum can be written as

$$|0(\beta)\rangle = \rho^{1/2}\left\{\sum_{N=0}^{\infty}|N\rangle \otimes |\tilde{N}\rangle\right\},$$

$$\langle 0(\beta)| = \left\{\sum_{N=0}^{\infty}\langle\tilde{N}| \otimes \langle N|\right\}\rho^{1/2}, \tag{25}$$

where ρ is the statistical operator. Its TFD representation is defined by

$$\rho = Z^{-1}e^{-(\beta/2)(K+\tilde{K})}, \tag{26}$$

since $\tilde{\rho} = \rho$. $Z \in \mathbb{R}$ denotes the associated partition function and

$$K = H - \mu N = \sum_{n=1} (\bar{E}_n - \mu) \frac{a_n^+ a_n}{\lambda_n},$$
$$\tilde{K} = \tilde{H} - \mu \tilde{N} = \sum_{n=1} (\bar{E}_n - \mu) \frac{\tilde{a}_n^+ \tilde{a}_n}{\lambda_n^*}. \tag{27}$$

The Lagrange multiplier $\mu \in \mathbb{R}$ guarantees that $\langle 0(\beta)|N|0(\beta)\rangle = \langle 0(\beta)|\tilde{N}|0(\beta)\rangle = N_0$.

The index N of (25) labels the set of different configurations of N fermions, which are obtained by occupying N one-particle states from all possible states belonging to the Fock space. More explicitly, for the case of $N \geqslant 1$ one has

$$|N\rangle = \prod_{j=1}^{N} \lambda_{p_j}^{-1/2} a_{p_j}^+ |0\rangle, \qquad |\tilde{N}\rangle = \prod_{j=1}^{N} (\lambda_{p_j}^*)^{-1/2} \tilde{a}_{p_j}^+ |0\rangle, \tag{28}$$

where $p_j (j = 1, \dots, N) \equiv P_N$ is the Pth configuration of N fermions defined in Fock's space. Since we are dealing with fermions we shall assume that these configurations are different. By definition $|0\rangle \equiv |0\rangle \otimes |\tilde{0}\rangle$ is the TFD vacuum at $T = 0$.

The notation $|N\rangle \equiv |N, P_N\rangle$ will be adopted to denote all possible different configurations of N fermions. In this notation the one-body term of ρ can be written

$$K|N\rangle = \sum_{j=1}^{N} (\bar{E}_{p_j} - \mu)|N\rangle, \qquad \tilde{K}|\tilde{N}\rangle = \sum_{j=1}^{N} (\bar{E}_{p_j} - \mu)|\tilde{N}\rangle. \tag{29}$$

Replacing the TFD vacuum by its definition and writing the states of N particles explicitly, one has

$$|0(\beta)\rangle = Z^{-1/2} \left\{ |0\rangle \otimes \widetilde{|0\rangle} + \sum_{N>0, P_N} e^{-(\beta/2)\sum_{j=1}^{N} (\bar{E}_{p_j} - \mu)} |N, P_N\rangle \otimes \widetilde{|N, P_N\rangle} \right\} \tag{30}$$

and

$$\langle 0(\beta)| = Z^{-1/2} \left\{ \widetilde{\langle 0|} \otimes \langle 0| + \sum_{N>0, P_N} e^{-(\beta/2)\sum_{j=1}^{N} (\bar{E}_{p_j} - \mu)} \widetilde{\langle N, P_N|} \otimes \langle N, P_N| \right\}. \tag{31}$$

Since the vacuum is normalized ($\langle 0(\beta)|0(\beta)\rangle = 1$) the partition function Z can be expressed as

$$Z = 1 + \sum_{N>0, P_N} e^{-\beta \sum_{j=1}^{N} (\bar{E}_{p_j} - \mu)} \tag{32}$$

up to an overall factor given by the vacuum expectation value of the operator K.

These results should coincide with those obtained in terms of the complex thermal Bogoliubov transformations. By writing $|0(\beta)\rangle$ ($\langle 0(\beta)|$) as a power series of the operators $[a^+\tilde{a}^+]$ $([\tilde{a}a])$ and comparing term by term with the previous equations one obtains

$$Z^{-1/2} = \prod_{n=1} e^{\theta_n(B_{11n}-B_{22n})/2} u_n = \prod_{n=1} e^{-\theta_n(B_{11n}-B_{22n})/2} w_n, \tag{33}$$

$$\begin{aligned} Z^{-1/2}\frac{e^{-(\beta/2)(\bar{E}_m-\mu)}}{|\lambda_m|} &= \left(\prod_{n\neq m} e^{\theta_n(B_{11n}-B_{22n})/2} u_n\right) e^{\theta_m(B_{11m}-B_{22m})/2} v_m \\ &= \left(\prod_{n\neq m} e^{-\theta_n(B_{11n}-B_{22n})/2} w_n\right) e^{-\theta_m(B_{11m}-B_{22m})/2} z_m. \end{aligned} \tag{34}$$

These equations should be satisfied for an arbitrary value of θ_n and n, therefore

$$\begin{aligned} &B_{11n} = B_{22n}, \\ &\lambda_n B_{21n} = -\lambda_n^* B_{12n}, \\ &u_n = w_n = \cosh(\theta_n\sqrt{B_{12n}B_{21n}}), \\ &v_n = z_n = \cosh(\theta_n\sqrt{B_{12n}B_{21n}})\frac{e^{-(\beta/2)\bar{E}_n}}{|\lambda_n|}, \\ &Z^{-1/2} = \prod_{n=1}\cosh(\theta_n\sqrt{B_{12n}B_{21n}}). \end{aligned} \tag{35}$$

4.2. *The occupation numbers*

The coefficients of the complex thermal transformation B of Section 2 can be determined from the results obtained in the previous subsection. For real values of B_{11n} and θ_n and after some algebra one obtains

$$\begin{aligned} B_{11n} &= [1 + e^{-\beta(\bar{E}_n-\mu)}]^{-1/2}, \\ B_{12n} &= -\frac{\lambda_n}{|\lambda_n|} e^{-(\beta/2)(\bar{E}_n-\mu)} B_{11n}, \\ B_{21n} &= \frac{\lambda_n^*}{|\lambda_n|} e^{-(\beta/2)(\bar{E}_n-\mu)} B_{11n}, \end{aligned} \tag{36}$$

up to a global multiplicative factor of unitary modulus. In consequence, the fermion occupation numbers n_F can be written as

$$\begin{aligned} n_F &= \langle 0(\beta)|\frac{a_n^+ a_n}{\lambda_n}|0(\beta)\rangle = -B_{12n}B_{21n} = v_n{}^2 \\ &= -[\sinh(\theta_n\sqrt{B_{12n}B_{21n}})]^2 = -[\sinh(\theta_n\sqrt{-n_F})]^2. \end{aligned} \tag{37}$$

By introducing the definition $\varphi_n = \theta_n\sqrt{n_F}$ the occupation numbers n_F can be written as

$$n_F = [\sin(\varphi_n)]^2,$$

$$
\begin{aligned}
B_{11n} = B_{22n} &= \cos(\varphi_n) = \sqrt{1-n_F}, \\
B_{12n} &= -\frac{|E_n|}{E_n}\sin(\varphi_n) = -\frac{|E_n|}{E_n}\sqrt{n_F}, \\
B_{21n} &= \frac{|E_n|}{E_n^*}\sin(\varphi_n) = \frac{|E_n|}{E_n^*}\sqrt{n_F}.
\end{aligned} \tag{38}
$$

These equalities lead to the following form for G, which is the generator of the thermal transformations:

$$
G = \sum_{n=1} \frac{\varphi_n}{|\lambda_n|}\{\tilde{a}_n a_n - a_n^+ \tilde{a}_n^+\}. \tag{39}
$$

Mean values of the energy and particle number on the ensemble and their deviations can be defined, as usual, as derivatives of the partition function Z

$$
Z = \prod_{m=1}[1 + e^{-\beta(\bar{E}_m - \mu)}] = \prod_{m=1} B_{11m}^{-2}. \tag{40}
$$

The factors λ_n, appearing in the anticommutators of Eqs. (2) and (3) and in G of Eq. (39), are complex factors which are determined from the definition of the creation and annihilation operators

$$
a_n a_n^+|0\rangle = \zeta_n|0\rangle, \tag{41}
$$

so that $|\zeta_n| = 1\ \forall n$. Thus

$$
\langle 0|a_n a_n^+|0\rangle = \zeta_n = \langle n|n\rangle = \lambda_n, \tag{42}
$$

and in consequence

$$
|\lambda_n| = 1, \qquad \bar{E}_n = |E_n| = \sqrt{\varepsilon_n^2 + \gamma_n^2/4}, \tag{43}
$$

where $E_n = \varepsilon_n - i\gamma_n/2$, $\gamma_n \geqslant 0\ \forall n$.

We are now in a position to show that the operators H and $\tilde{H}$ are indeed hermitian operators. The demonstration holds in general for any operator which is invariant under thermal transformations, as defined in Eq. (14). In order to illustrate the concepts we shall introduce creation operators a'^+_n and $\tilde{a}'^+_n$, which differ from the adjoints of a_n and $\tilde{a}_n$. Starting from the anticommutator between a and a'^+, Eq. (2), and demanding that for states with real eigenvalues the $^+$ symbol represents hermitian conjugation (†), it can be shown that

$$
\begin{aligned}
a^\dagger &= (\lambda^*/\lambda)^{1/2} a'^+, \\
(a'^+)^\dagger &= (\lambda^*/\lambda)^{1/2} a.
\end{aligned} \tag{44}
$$

Similar relations hold for the "tilde" partners.

We can define the renormalized operators b, b'^+ ($\tilde{b}$, $\tilde{b}'^+$) by

$$b = a/\lambda^{1/2}, \qquad \tilde{b} = \tilde{a}/\lambda^{*1/2},$$
$$b'^{+} = a'^{+}/\lambda^{1/2}, \qquad \tilde{b}'^{+} = \tilde{a}'^{+}/\lambda^{*1/2}. \tag{45}$$

These operators satisfy the usual anticommutation relations, i.e. $\{b_n, b'^{+}_m\} = \delta_{nm}$, $\{\tilde{b}_n, \tilde{b}'^{+}_m\} = \delta_{nm}$, and the remaining anticommutators vanish. In addition, in the (b, b'^{+}) basis, the operations $^{+}$ and † coincide, in consequence

$$b'^{+} = b^{\dagger}, \qquad b = (b'^{+})^{\dagger}. \tag{46}$$

Hence, when H and $\tilde{H}$ are written in the (b, b^{+}), $(\tilde{b}, \tilde{b}^{+})$ basis they exhibit their hermitian character

$$H = \sum_{n=1} |E_n| b_n^{+} b_n \tag{47}$$

and

$$\tilde{H} = \sum_{n=1} |E_n| \tilde{b}_n^{+} \tilde{b}_n. \tag{48}$$

The (b_n, b_n^{+}) basis, where all the eigenvalues are real, is equivalent to a basis which includes Gamow states, e.g. Berggren's basis [13].

As described in Refs. [9,10] the Hamiltonian eigenvalue density distribution can include resonances, which are added to the bound states as broad states with a distribution on the real energy axis. That is to say that the full spectrum is treated as a set of states with purely real eigenvalues, some of them having a width. This procedure seems to be correct for very narrow resonances but the question about its validity at high temperatures remains to be investigated. The procedure of Refs. [9,10] was constructed to include the concept of a resonance, i.e. a decaying state, in the context of the conventional statistical mechanics. The TFD description of physical states in the presence of resonances, as described above, gives support to the treatment of Refs. [9,10]. By definition [2], the TFD quasi-particles are always stable states, in spite of the fact that the original physical states can, in general, have a finite lifetime. This is obviously true if one is working in a Fock space, as we have done.

5. Conclusions

In this work we have shown that the rules of the TFD can be applied to a basis including states of complex energies. The invariance of the total Hamiltonian, under thermal transformations, and the structure of the corresponding partition functions have been obtained by using generalized commutation relations and complex Bogoliubov transformations. It is shown that this assumption does not contradict the basic rules of the TFD and that it leads to a description where states with complex energies are included as broad states on the real axis. This result is central in the application of statistical concepts in a basis with complex eigenvalues, i.e. in Berggren's basis [13].

To conclude, we think that the use of TFD together with the use of Berggren's basis to account for the continuum may be the suitable theoretical framework to describe temperature-dependent nuclear structure effects. As we have shown in this work, the already known approximations based on the use of effective Hamiltonian density distributions of eigenvalues [9,10] seem to be justified in a rigorous way.

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