Abstract

The thermal Bogoliubov transformation in thermo field dynamics is generalized in two respects. First, a generalization of the $\alpha$–degree of freedom to tilde non–conserving representations is considered. Secondly, the usual $2 \times 2$ Bogoliubov matrix is extended to a $4 \times 4$ matrix including mixing of modes with non–trivial multiparticle correlations. The analysis is carried out for both bosons and fermions.
1 Introduction

In recent years there have been two directions of development of the real time formulation of quantum field theory at finite temperature called thermo field dynamics (TFD). One problem has been to reconcile the calculations of vertex functions with the result from the imaginary time formalism [1, 2]. Another important issue has been to generalize the standard TFD to non–equilibrium systems, in particular to time dependent situations [3, 4, 5, 6]. In connection with the second problem one has been led to consider generalizations of the standard thermal Bogoliubov transformation. More precisely, there is a freedom of choosing the parameters in the Bogoliubov matrix corresponding to a given density matrix. That freedom was used in Ref.[7] to simplify the calculation of expectation values in the interaction picture. Only two choices give time and anti–time ordered products for the perturbation expansion. Furthermore, the Boltzmann equation in [5] gives increasing entropy only with the choice $\alpha = 1$ ($\alpha$ is one of the parameters in the Bogoliubov transformation), and when the thermal state is given at $t_0 = -\infty$. The choice $\alpha = 0$ and $t_0 = \infty$ leads to decreasing entropy. In the general case the density matrix, or the thermal state, may be given at some finite time. The corresponding Bogoliubov transformation can also be highly non–linear to include the initial correlation of particles.

In this paper we approach the problem by studying all possible choices of a linear Bogoliubov transformation for a given equilibrium density matrix, and discuss the properties under Hermitian and tilde conjugation for different choices (see Sec.2). Non–linear Bogoliubov transformations are in general very difficult to deal with but we can quite easily extend the usual $2 \times 2$ thermal matrix to a $4 \times 4$ matrix in several ways. In Sec.3 we study some relevant extensions for bosons. The whole discussion is repeated for fermions in Sec.4.

2 Generalizations of the $\alpha$–degree of freedom

There has recently been much discussion about the freedom of choosing the thermal vacuum in TFD corresponding to a given density matrix [3, 7, 8]. In particular the cyclicity of the trace gives the $\alpha$–degree of freedom where $\alpha$ is defined by $\langle A \rangle = \text{Tr}(\rho^{1-\alpha} A \rho^{\alpha}) = \langle \rho^{1-\alpha} | A | \rho^{\alpha} \rangle$. The last expectation value is calculated in the Hilbert space of density matrices and the scalar product is defined by the trace [10]. Note that $\langle \rho^{\alpha} \rangle$ is not the dual of $|\rho^{1-\alpha}\rangle$. In TFD the two vectors are constructed from the zero temperature vacuum $|0, \bar{0}\rangle$ as

$$|\rho^{\alpha}\rangle = \sum_{m,\bar{n}} \langle n| \rho^{\alpha} | m \rangle | m, \bar{n} \rangle, \quad \langle \rho^{1-\alpha} | = \sum_{m,\bar{n}} \langle m | \rho^{1-\alpha} | n \rangle \langle m, \bar{n} |. \quad (2.1)$$

In order to keep clear the meaning of Hermiticity, unitarity, bra– and ket–vectors, and
tilde conjugation etc., we define two distinct Hilbert (Fock) spaces \( \mathcal{F}_a \) and \( \mathcal{F}_\xi \). They are generated from vacuum vectors \(|\mathcal{O}_a\rangle\) and \(|\mathcal{O}_\xi\rangle\) by acting with the creation operators \((a^\dagger, \tilde{a}^\dagger)\) and \((\xi^\dagger, \tilde{\xi}^\dagger)\) respectively. The two spaces are trivially isomorphic. In each space Hermitian and tilde conjugation are defined in the usual way and when an operator is said to be e.g. unitary it is meant to be with respect to the structure in the space it is acting. The operators \((a, \tilde{a}^\dagger, a^\dagger, \tilde{a})\) and \((\xi, \tilde{\xi}^\dagger, \xi^\dagger, \tilde{\xi})\) satisfy the usual canonical commutation relations (CCR) and we call the algebras that they generate \(\mathcal{A}_a\) and \(\mathcal{A}_\xi\).

We are now interested in mappings \(\phi: \mathcal{A}_a \mapsto \mathcal{A}_\xi\) other than the trivial one. In particular, mappings that mix tilde and non–tilde operators are interesting since they represent mixed states. Then thermal expectation values of polynomials in \(a\) and \(a^\dagger\) (pol\((a, a^\dagger)\)) are computed by

\[
\text{Tr}(\rho \text{pol}(a, a^\dagger)) = \langle \mathcal{O}_\xi | \phi(\text{pol}(a, a^\dagger)) | \mathcal{O}_\xi \rangle. \tag{2.2}
\]

The two vacuum vectors \(|\mathcal{O}_a\rangle\) and \(|\mathcal{O}_\xi\rangle\) shall be thought of as the zero and finite temperature vacuum vectors. In this paper we only consider linear mappings though non–linear mappings are required if general density matrices should be represented in this way. Even in such cases the linear mappings are frequently useful when the non–linear effects can be treated by perturbation calculation.

We shall see how the \(\alpha\)–degree of freedom emerges together with other parameters when we consider non–trivial mappings between \(\mathcal{F}_a\) and \(\mathcal{F}_\xi\). The most commonly used Bogoliubov transformation in TFD is

\[
\begin{pmatrix}
  a \\
  \tilde{a}^\dagger
\end{pmatrix}
\mapsto
\begin{pmatrix}
  \cosh \theta & \sinh \theta \\
  \sinh \theta & \cosh \theta
\end{pmatrix}
\begin{pmatrix}
  \xi \\
  \tilde{\xi}^\dagger
\end{pmatrix}
\equiv B_2(\theta)
\begin{pmatrix}
  \xi \\
  \tilde{\xi}^\dagger
\end{pmatrix}, \tag{2.3}
\]

and the Hermitian and tilde conjugates are defined anti–linearly. This represents the finite temperature density matrix

\[
\rho = \frac{\exp(-\beta \omega a^\dagger a)}{\text{Tr}(\exp(-\beta \omega a^\dagger a))}, \tag{2.4}
\]

where the inverse temperature \(\beta\) is related to \(\theta\) through

\[
\sinh^2 \theta = \frac{1}{e^{\beta \omega} - 1}. \tag{2.5}
\]

In this section we restrict ourselves to mappings that mix \(a\) and \(\tilde{a}^\dagger\), and their Hermitian conjugates. The most general linear mapping is

\[
\phi: a^\mu \mapsto B^{\mu \nu} \xi^\nu, \quad a^{\dagger \mu} \mapsto C^{\mu \nu} \xi^\nu. \tag{2.6}
\]
In the following we use the doublet notation, i.e. $a^\mu = (a, \tilde{a}^\dagger)$ and $a^{i\nu} = (a^i, \tilde{a})$. We require the CCR to be conserved under the mapping $\phi$ (we denote the Pauli matrices by $\tau_i$),

$$[a^\mu, a^{i\nu}] = \tau_3^{\mu\nu} = (B\tau_3C^T)^{\mu\nu} = [\xi^\mu, \xi^{i\nu}] ,$$

so the only condition on $B \in GL(2, \mathbb{C})$ is that it should be invertible to define $C$. This mapping leaves the free Hamiltonian invariant,

$$\hat{H}(a) = a^\dagger a - \tilde{a}^\dagger \tilde{a} \mapsto \hat{H}(\xi) = \xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi} .$$

(2.8)

There are eight independent real parameters in $B$ (except for the condition $\det(B) \neq 0$) but only one combination appears in the expectation values of observables. For example, the particle number $a^\dagger a$ is

$$\langle O_\xi | \phi(a^\dagger a) | O_\xi \rangle = \frac{\beta\gamma}{\zeta\delta - \beta\gamma} ,$$

if we parametrize $B$ by

$$B = \begin{pmatrix} \zeta & \beta \\ \gamma & \delta \end{pmatrix} .$$

(2.10)

It turns out that the only physical parameter is $\beta\gamma/\zeta\delta$, which should be chosen in $[0, 1] \in \mathbb{R}$ since the expectation value of the number operator must be real and positive.

The most general mapping conserves CCR but not Hermiticity and tilde conjugation in the sense that

$$\phi(a^\dagger) \neq \phi(a)^\dagger , \quad \phi(\tilde{a}) \neq \tilde{\phi}(a) .$$

(2.11)

Note that $\dagger$ and $\sim$ refer to different Hilbert spaces depending on which operator they act. In particular that means that the image of an Hermitian operator is not necessarily Hermitian. When the Hamiltonian is expressed in terms of $\xi$–operators it may be non–Hermitian and the time evolution non–unitary in $F_\xi$.

In many recent publications the mapping has been required to preserve the tilde but not Hermitian conjugation $[11, 12, 13, 3, 8]$. Since $a^\mu = \tau_1^{\mu\nu}a^{i\nu}$, the first relation in Eq.(2.6) leads to $\tilde{a}^\dagger \mu \mapsto (\tau_1 B\tau_1)^{\mu\nu} \tilde{\xi}^{i\nu}$. On the other hand the tilde conjugation of the second relation in Eq.(2.6) gives $a^{i\nu} \mapsto (C^*)^{\mu\nu} \tilde{\xi}^{i\nu}$. The invariance under tilde conjugation means $C^* = \tau_1 B\tau_1$. This, together with Eq.(2.7), gives

$$B\tau_2 B^\dagger = \tau_2 .$$

(2.12)
The solution is

\[ B = e^{i\psi} \begin{pmatrix} \zeta & \beta \\ \gamma & \delta \end{pmatrix}, \]  

(2.13)

where \( \zeta, \beta, \gamma, \delta, \psi \in \mathbb{R}, \psi \) is an arbitrary phase and \( \zeta\delta - \beta\gamma = 1 \). Thus \( B \in SL(2, \mathbb{R}) \times U(1) \).

The commonly used tilde–preserving Bogoliubov transformation is \([8, 9]\)

\[ B = \frac{1}{\sqrt{1 - f}} \begin{pmatrix} e^{-s} & f^\alpha e^s \\ f^{1-\alpha} e^{-s} & e^s \end{pmatrix}. \]  

(2.14)

(Note that in Refs.[8, 9] this matrix is called \( B^{-1} \).) Then the relation between \( (\zeta, \beta, \gamma, \delta) \) and the parameters \( (\alpha, s, f) \) is

\[ f = \frac{\beta\gamma}{\zeta\delta}, \quad s = \frac{1}{2} \log\left(\frac{\delta}{\zeta}\right), \quad \alpha = \frac{\log(\beta\zeta)}{\log(\beta\gamma) - \log(\zeta\delta)}. \]  

(2.15)

The only combination that occurs in physical expectation values is

\[ n = \frac{f}{1 - f} = \beta\gamma. \]  

(2.16)

It is also possible to preserve the Hermitian conjugation but not tilde conjugation and that imposes the condition

\[ B\tau_3 B^\dagger = \tau_3. \]  

(2.17)

The solution is

\[ B = e^{i\phi} \begin{pmatrix} \zeta e^{i\phi} & \beta e^{i\phi} \\ \beta e^{-i\phi} & \zeta e^{-i\phi} \end{pmatrix}, \]  

(2.18)

where \( \zeta, \beta, \phi, \varphi, \psi \in \mathbb{R} \) and \( \zeta^2 - \beta^2 = 1 \). This mapping leaves the Hamiltonian Hermitian so the time evolution in \( \mathcal{F}_\xi \) is unitary.

Finally we can consider mappings that preserve both Hermiticity and tilde conjugation. The Bogoliubov transformation is then reduced to the usual

\[ B \equiv e^{i\psi} B_2(\theta) = e^{i\psi} \begin{pmatrix} \cosh \theta & \sinh \theta \\ \sinh \theta & \cosh \theta \end{pmatrix}. \]  

(2.19)

The phase \( e^{i\psi} \) is just the arbitrary of the phase of a state in \( \mathcal{F}_\xi \).

Among all the parameters only one combination has physical meaning for each mapping \( \phi \), the others being similar to the \( \alpha \)–degree of freedom. For a given value of e.g.
\[ \langle O_\xi | \phi(a^\dagger a) | O_\xi \rangle, \] which fixes the physical parameter, all mappings considered so far represent the same density matrix.

The fact that we only consider linear mappings from \((a, a^\dagger)\) to \((\xi, \xi^\dagger)\) implies that multiparticle expectation values are given in a simple way from the single particle number. For example, with the transformation in Eq.(2.19) we have

\[ \langle O_\xi | \phi(a^\dagger a) | O_\xi \rangle = \sinh^2 \theta, \]
\[ \langle O_\xi | \phi((a^\dagger)^2(a)^2) | O_\xi \rangle = 2 \sinh^4 \theta. \] (2.20)

These expectation values probe different components of the thermal vacuum belonging to different \(n\)–particle subspaces of the Fock space and their values need not be related for a general density matrix.

In all cases above the free Hamiltonian is left invariant and satisfies the usual conditions under Hermitian and tilde conjugation in \(F_\xi\). However, when interactions are included new terms appear that destroy these properties.

The free propagator for a real field

\[ \phi(x) = \int \frac{d^3k}{\sqrt{(2\pi)^3 2\omega_k}} \left( a^\dagger_k e^{i(\omega_k t - kx)} + a_k e^{-i(\omega_k t - kx)} \right), \] (2.21)
in the state \(|O_\xi\rangle\) can be calculated in a straightforward manner. We find

\[ D^{ab}(k_0, \vec{k}) = \begin{pmatrix} \Delta_F & 0 \\ 0 & -\Delta_F^* \end{pmatrix} \]
\[ -\frac{2\pi i \delta(k_0^2 - \omega^2_k)}{\zeta \delta - \beta \gamma} \begin{pmatrix} \beta \gamma & \beta \delta \theta(k_0) + \zeta \gamma \theta(-k_0) \\ \zeta \gamma \theta(k_0) + \beta \delta \theta(-k_0) & \beta \gamma \end{pmatrix} \] (2.22)

where

\[ \Delta_F = \frac{1}{k_0^2 - \omega^2_k + i\epsilon}. \] (2.23)

It reduces to the well–known expression when the parameters \((\zeta, \beta, \gamma, \delta)\) are constrained by preservation of \(\dagger\) and \(\sim\) (Eq.(2.19)).

### 2.1 Another way of describing the non–standard Bogoliubov transformations

It is often convenient to formally think of \(|O_a\rangle\) and \(|O_\xi\rangle\) as vectors in the same Hilbert space \(F_a\). This is not mathematically rigorous in field theory since the Hilbert spaces
\( \mathcal{F}_a \) and \( \mathcal{F}_\xi \) are unitarily inequivalent. Any density matrix \( \rho \) can be represented by a vector \( |\mathcal{O}_\xi\rangle \in \mathcal{F}_a \) that is obtained by a unitary transformation of \( |\mathcal{O}_a\rangle \). It is usually written

\[
|\mathcal{O}_\xi\rangle = e^{iG}|\mathcal{O}_a\rangle = U|\mathcal{O}_a\rangle ,
\]  

(2.24)

where \( G \) is Hermitian and \( U \) is unitary. It is also possible to choose \( U \) to be tilde invariant \( \tilde{U} = U \) which fixes \( U \) completely. The \( \xi \) operators that annihilates \( |\mathcal{O}_\xi\rangle \) is obtained by the corresponding transformation

\[
\xi = UaU^{-1} = Ua^\dagger.
\]  

(2.25)

Since since \( U \) is both unitary and tilde invariant we also have

\[
\tilde{\xi} = U\tilde{a}U^\dagger, \quad \text{and} \quad \xi^\dagger = Ua^\dagger U^\dagger.
\]  

(2.26)

In the particular case of a linear transformation between \( a \) and \( \xi \), \( G \) takes the form

\[
G = \psi(a^\dagger a - \tilde{a}^\dagger \tilde{a}) + i\theta(aa\tilde{a} - a^\dagger \tilde{a}^\dagger),
\]  

(2.27)

where \( \psi \) and \( \theta \) are the parameters occuring in Eq.(2.19).

The generalizations of the thermal Bogoliubov transformation considered so far amounts to replacing \( U \) by an another invertible operator \( V \) which may be non–unitary and non–tilde invariant. Let us first say a few words about the tilde conjugation. It can be described by the Tomita–Takesaki modular operator \( J_a \) [14] which is defined relative to the vacuum \( |\mathcal{O}_a\rangle \) and the algebras generated by \( \{a, a^\dagger\} \) and \( \{\tilde{a}, \tilde{a}^\dagger\} \). It leaves \( |\mathcal{O}_a\rangle \) invariant and maps \( \{a, a^\dagger\} \) to \( \{\tilde{a}, \tilde{a}^\dagger\} \) by \( J_a a J_a = \tilde{a} \) etc. Given another vacuum \( |\mathcal{O}_\xi\rangle \) there is another \( J_\xi \) defined by \( J_\xi = VJ_a V^{-1} \). If \( V \) is tilde invariant we have \( J_\xi = J_a \), otherwise the tilde conjugation is not preserved. It is however replaced by a new tilde conjugation rule relative to the \( \xi \)–operators and \( |\mathcal{O}_\xi\rangle \).

In more physical terms we can say that there is a tilde conjugation defined for the zero temperature vacuum. If the transformation to the thermal vacuum commutes with that tilde conjugation we will have the same tilde conjugation operator for the thermal vacuum. Otherwise we have to define a new tilde conjugation with respect to the thermal vacuum. Note that we can always find such a new tilde conjugation rule.

Let us consider some general transformation of \( |\mathcal{O}_a\rangle \)

\[
|\mathcal{O}_\xi\rangle = V|\mathcal{O}_a\rangle.
\]  

(2.28)

In order that \( \xi \) annihilates \( |\mathcal{O}_\xi\rangle \) we take \( \xi = VaV^{-1} \). To preserve the CCR we define \( \xi^\dagger = Va^\dagger V^{-1} \) to be the canonical conjugate of \( \xi \). Note that \( \xi^\dagger \neq \xi^\dagger \) if \( V \) is non–unitary.
The bra state annihilated by $\xi^\dagger$ is $\langle \mathcal{O}_\xi | = \langle \mathcal{O}_a | V^{-1}$ which is not the dual of $| \mathcal{O}_\xi \rangle$ if $V$ is non–unitary. We also want to define a tilde conjugate of $\xi$, call it $\tilde{\xi}$, such that $\xi$ and $\tilde{\xi}$ commute. The obvious choice is $\tilde{\xi} = V \xi V^{-1} = J_\xi \xi J_\xi$, but we note that $\tilde{\xi} \neq \tilde{\xi}$ if $V \neq \tilde{V}$.

The idea with the usual thermal Bogoliubov transformation is that thermal expectation values of observables like polynomials in $a$ and $a^\dagger$ ($\text{pol}(a, a^\dagger)$) are obtained as vacuum expectation values in the thermal vacuum $| \mathcal{O}_\xi \rangle$. With the transformation $V$ the thermal expectation value is instead computed as

$$\text{Tr}(\rho \text{pol}(a, a^\dagger)) = \langle \mathcal{O}_\xi | \text{pol}(a, a^\dagger) | \mathcal{O}_\xi \rangle .$$

(2.29)

We also notice that $| \mathcal{O}_\xi \rangle$ is no longer normalized if $V \neq V^\dagger$ but satisfies $\langle \mathcal{O}_\xi | \mathcal{O}_\xi \rangle = 1$. In particular, in the $\alpha = 1$ representation of a single oscillator [7, 8] at equilibrium we have

$$\langle \mathcal{O}_\xi | = \sum_n \langle n, \bar{n} | ,$$

(2.30)

which is not normalizable. The linear mapping in Eq.(2.10) is still well–defined if, for instance, $\zeta = \gamma = \delta$ for which $s = 0$, $\alpha = 1$ and $f = (\zeta^2 - 1)/\zeta$.

The freedom of choosing different rules for tilde conjugation arises from the independence of the unitary operator $U$ in the expectation value $\text{Tr}(U^\dagger \rho^{1/2} A \rho^{1/2} U) = \langle A \rangle$. It has been studied in detail as a gauge degree of freedom when representing $\rho$ in as states in $\mathcal{F}_a$ [15, 16].

3 Thermal and particle mixing Bogoliubov transformations

The equilibrium state of a harmonic oscillator can be represented by the simple mapping in Eq.(2.19). It describes independent particles with all multiparticle correlations determined in terms of the number expectation value $\langle \mathcal{O}_\xi | a^\dagger a | \mathcal{O}_\xi \rangle$. This is clearly a very particular state.

In field theory the system is often assumed to be at equilibrium with respect to the interacting Hamiltonian at $t = -\infty$ and the vacuum $| \mathcal{O}(\beta) \rangle$ satisfies $\hat{H} | \mathcal{O}(\beta) \rangle = 0$. To do perturbation theory we rather want to use the thermal vacuum of the free Hamiltonian $| \mathcal{O}(\beta) \rangle_0$ satisfying $\hat{H}_0 | \mathcal{O}(\beta) \rangle_0 = 0$. The difference between the two states is related to the vertical integration paths in the path integral formulation of TFD. These paths can often (but not always [17]) be neglected when $t \to \pm \infty$, due to clustering properties of QFT.  

\footnote{In the rest of the paper we shall write $\langle \mathcal{O}_\xi | a^\dagger a | \mathcal{O}_\xi \rangle$ as a simplified notation for $\langle \mathcal{O}_\xi | \phi(a^\dagger a) | \mathcal{O}_\xi \rangle$.}
If, on the other hand, the initial state is given at some finite time one may have to deal with non-trivial correlations. The thermal Bogoliubov transformation is then non-linear in general.

To do simple things first we shall consider the kind of states that can be described by generalizing the Bogoliubov transformation to a mixing of four operators while still being linear. Common to these transformations is that the free Hamiltonian is no longer invariant. But there is no reason why the initial correlation of particles should be constrained by the Hamiltonian which governs the dynamics of the particles.

We shall consider three different kinds of particle mixing. They are all combinations of some zero and finite temperature transformation.

First, the simple mixing of $a$ and $\tilde{a}^\dagger$ can be extended to include $\tilde{a}$ and $a^\dagger$ as well. This is a toy model for a state out of equilibrium where the time dependence of correlation function can be calculated explicitly for a free Hamiltonian.

Secondly, we study a mixing of two modes, $a$ and $b$, which can be different momentum modes for instance. Such a mixing occurs naturally at local equilibrium where not only two but all modes mix [18, 6].

As a third example a mixing of the superfluidity type between $a$ and $b^\dagger$ is considered.

The two last cases have in common that the most general transformation respecting $\dagger$– and $\sim$–conjugation has more parameters than a simple tensor product of zero and finite temperature transformations. The parameters can be interpreted as different temperatures for the different modes and a rotation, but there is also a fourth parameter that has not been discussed earlier.

**Case I**

We introduce a quadruple notation for the operators

$$\xi^\mu = (\xi, \tilde{\xi}^\dagger, \xi^\dagger, \tilde{\xi}), \quad a^\mu = (a, \tilde{a}^\dagger, a^\dagger, \tilde{a}) ,$$

with which we can write the CCR as

$$[\xi^\mu, \xi^\nu] = (\tau_2 \otimes \tau_3)^{\mu\nu} .$$

With this notation the Bogoliubov transformation is $a = B_4 \xi$, where $B_4$ is a $4 \times 4$ matrix. The conditions that CCR, $\dagger$– and $\sim$–conjugations are preserved are

$$\begin{align*}
\text{CCR} : \quad B_4(\tau_2 \otimes \tau_3)B_4^T &= (\tau_2 \otimes \tau_3) , \\
\dagger : \quad B_4^*(\tau_1 \otimes \mathbb{1}) &= (\tau_1 \otimes \mathbb{1})B_4 , \\
\sim : \quad B_4^*(\tau_1 \otimes \tau_1) &= (\tau_1 \otimes \tau_1)B_4 .
\end{align*}$$
The solution is of the form

$$B_4 = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}, \quad (3.4)$$

where $\alpha$ and $\beta$ are $2 \times 2$ matrices

$$\alpha = \begin{pmatrix} \rho_1 & \rho_2 \\ \rho_2 & \rho_1 \end{pmatrix} e^{i\psi_1}, \quad \beta = \begin{pmatrix} r_1 & r_2 \\ r_2 & r_1 \end{pmatrix} e^{i\psi_2}, \quad (3.5)$$

with the conditions that ($r_i, \rho_i, \psi_i \in \mathbb{R}$)

$$(r_1^2 + r_2^2) - (\rho_1^2 + \rho_2^2) = 1, \quad \rho_1 r_2 - \rho_2 r_1 = 0. \quad (3.6)$$

If we assume that $\rho_1^2 - \rho_2^2 \geq 1$ we can satisfy the conditions by parametrizing $B_4$ as a simple tensor product

$$B_4 = \begin{pmatrix} e^{i\psi_1} \cosh \phi e^{i\psi_2} \sinh \phi \\ e^{-i\psi_2} \sinh \phi e^{-i\psi_1} \cosh \phi \end{pmatrix} \otimes B_2(\theta). \quad (3.7)$$

The free Hamiltonian, expressed in terms of $\xi$–operators, is not invariant under this transformation and it does not annihilate the vacuum.

$$\hat{H}_0(a) = \omega (a^\dagger a - \tilde{a}^\dagger \tilde{a}) \mapsto \hat{H}(\xi) = \omega (1 + 2 \sinh^2 \phi)(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi})$$

$$+ \omega \frac{\sinh 2\phi}{2} [e^{i(\psi_1 - \psi_2)}(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi}) + e^{-i(\psi_1 - \psi_2)}(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi})]. \quad (3.8)$$

This means that the thermal vacuum is not stationary. We note that $\hat{H}(\xi)$ satisfy the usual conditions

$$\hat{H}^\dagger = \hat{H}, \quad \tilde{\hat{H}} = -\hat{H}. \quad (3.9)$$

The expectation value of the number operator is given by

$$\langle \mathcal{O}_\xi | a^\dagger a | \mathcal{O}_\xi \rangle = \cosh^2 \theta \sinh^2 \phi + \sinh^2 \theta \cosh^2 \phi, \quad (3.10)$$

and

$$\langle \mathcal{O}_\xi | (a^\dagger)^2 (a)^2 | \mathcal{O}_\xi \rangle = 2 \langle \mathcal{O}_\xi | a^\dagger a | \mathcal{O}_\xi \rangle^2 + \cosh^2 \phi \sinh^2 \phi (\sinh^2 \theta + \cosh^2 \theta)^2, \quad (3.11)$$

which, by comparing with Eq.(2.20), clearly shows that there is a non–trivial multiparticle correlation.
Case II

In the case of mode mixing we include two independent operators $a$ and $b$ in the quadruple

$$a^\mu = (a, \tilde{a}^\dagger, b, \tilde{b}^\dagger), \quad \xi^\mu = (\xi, \tilde{\xi}^\dagger, \eta, \tilde{\eta}^\dagger). \quad (3.12)$$

They can, for instance, be modes of different momenta [18, 6]. The Bogoliubov transformation $a = B_4 \xi$ preserves CCR, $\dagger$– and $\sim$–conjugation if it satisfies

$$B_4(\mathbb{1} \otimes \tau_3)B_4^\dagger = (\mathbb{1} \otimes \tau_3),$$
$$B_4(\mathbb{1} \otimes \tau_1) = (\mathbb{1} \otimes \tau_1)B_4. \quad (3.13)$$

A tensor product of a $SU(2)$ and a $SO(1, 1)$ rotation satisfies Eq.(3.13) but it is not the most general solution. The most general complex matrix satisfying Eq.(3.13) is rather complicated so we restrict it to be real for simplicity. We then have

$$B_4 = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad \alpha = \begin{pmatrix} \alpha_1 & \alpha_2 \\ \alpha_2 & \alpha_1 \end{pmatrix} \text{ etc. for } \beta, \gamma \text{ and } \delta, \quad (3.14)$$

with the conditions

$$(\alpha_1^2 - \alpha_2^2) + (\beta_1^2 - \beta_2^2) = 1,$$
$$(\gamma_1^2 - \gamma_2^2) + (\delta_1^2 - \delta_2^2) = 1,$$
$$\alpha_1 \gamma_1 - \alpha_2 \gamma_2 + \beta_1 \delta_1 - \beta_2 \delta_2 = 0,$$
$$\alpha_2 \gamma_1 - \alpha_1 \gamma_2 + \beta_1 \delta_2 - \beta_2 \delta_1 = 0. \quad (3.15)$$

If we assume that $(\alpha_1^2 - \alpha_2^2), (\beta_1^2 - \beta_2^2), (\gamma_1^2 - \gamma_2^2), (\delta_1^2 - \delta_2^2) \geq 0$ it is easy to parametrize the solutions as

$$B_4 = \begin{pmatrix} B_2(\theta_1) \cos \phi & B_2(\theta_2 - \delta) \sin \phi \\ \mp B_2(\theta_1 + \delta) \sin \phi & \pm B_2(\theta_2) \cos \phi \end{pmatrix}. \quad (3.16)$$

The two parameters $\theta_1$ and $\theta_2$ are interpreted as the Bogoliubov parameters referring to the temperatures of the $a$ and $b$ particles, which may be different. The $\phi$ parameter is the mixing angle between $a$ and $b$. Finally, there is fourth parameter $\delta$ which only exist when the particle and thermal mixing occur simultaneously.

The free Hamiltonian for two modes, when the upper sign in Eq.(3.16) is chosen, is transformed into

$$\hat{H}_0(a, b) = \omega_a (a^\dagger a - \tilde{a}^\dagger \tilde{a}) + \omega_b (b^\dagger b - \tilde{b}^\dagger \tilde{b})$$

$$\mapsto \hat{H}(\xi, \eta) = (\omega_a \cos^2 \phi + \omega_b \sin^2 \phi)(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi}) + (\omega_b \cos^2 \phi + \omega_a \sin^2 \phi)(\eta^\dagger \eta - \tilde{\eta}^\dagger \tilde{\eta})$$

$$+ \frac{\sin 2\phi}{2} (\omega_a - \omega_b) \{ \cosh(\theta_1 - \theta_2 + \delta)[\xi^\dagger \eta + \eta^\dagger \xi - \tilde{\xi}^\dagger \tilde{\eta} - \tilde{\eta}^\dagger \tilde{\xi}] \}$$

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\[
+ \sinh(\theta_1 - \theta_2 + \delta)[\eta \tilde{\xi} + \eta^{\dagger} \tilde{\xi}^{\dagger} - \xi \tilde{\eta} - \xi^{\dagger} \tilde{\eta}^{\dagger}] \right) .
\]

(3.17)

It turns out that the Hamiltonian depends only on \( \phi \) and the combination \( \theta_1 - \theta_2 + \delta \). Other operators may depend on other combinations and, for instance, the number expectation values for the two modes are

\[
\langle O_\xi | a^{\dagger} a | O_\xi \rangle = \cos^2 \phi \sinh^2 \theta_1 + \sin^2 \phi \sinh^2 (\theta_2 - \delta)
\]

(3.18)

Case III
A mixing between \( a \) and \( b^{\dagger} \) is interesting in the theory of superfluid bosons where \( a = a_k \) and \( b^{\dagger} = a^{\dagger}_{-k} \) are particles of opposite momentum forming a pair that constitutes the elementary excitations. Using the quadruple notation

\[
a^\mu = (a, \tilde{a}^{\dagger}, b^{\dagger}, \tilde{b}) , \quad \xi^\mu = (\xi, \tilde{\xi}^{\dagger}, \eta, \tilde{\eta}) ,
\]

(3.19)

the preservation of CCR, \( \dagger \) and \( \sim \) gives the conditions

\[
B_4 (\tau_3 \otimes \tau_3) B_4^{\dagger} = (\tau_3 \otimes \tau_3) ,
\]

\[
B_4 (\mathbb{I} \otimes \tau_1) = (\mathbb{I} \otimes \tau_1) B_4 .
\]

(3.20)

Similarly to the case II a tensor product of a \( SU(1,1) \) and a \( SO(1,1) \) rotations would satisfy the conditions but we look for more general solutions. For a real \( B_4 \) we find similarly

\[
B_4 = \left( \begin{array}{cc}
B_2(\theta_1) \cosh \phi & B_2(\theta_2 - \delta) \sinh \phi \\
B_2(\theta_1 + \delta) \sinh \phi & B_2(\theta_2) \cosh \phi
\end{array} \right) ,
\]

(3.21)

with the same interpretation as in case II. Again, we give the free Hamiltonian

\[
\hat{H}(\xi, \eta) = (\omega_a \cosh^2 \phi + \omega_b \sinh^2 \phi) (\xi^{\dagger} \xi - \tilde{\xi}^{\dagger} \tilde{\xi}) + (\omega_b \cosh^2 \phi + \omega_a \sinh^2 \phi) (\eta^{\dagger} \eta - \tilde{\eta}^{\dagger} \tilde{\eta})
\]

\[
+ \frac{\sinh 2\phi}{2} (\omega_a + \omega_b) \left\{ \cosh(\theta_1 - \theta_2 + \delta) [\xi^{\dagger} \eta^{\dagger} + \eta^{\dagger} \xi^{\dagger} - \xi \tilde{\eta}^{\dagger} - \tilde{\xi} \eta] \\
- \sinh(\theta_1 - \theta_2 + \delta) [\xi^{\dagger} \tilde{\eta} + \tilde{\eta}^{\dagger} \xi - \xi^{\dagger} \eta - \eta^{\dagger} \tilde{\xi}] \right\}
\]

(3.22)

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and the number expectation values

\[ \langle O_\xi | a^\dagger a | O_\xi \rangle = \cosh^2 \phi \sinh^2 \theta_1 + \sinh^2 \phi \cosh^2 (\theta_2 - \delta) , \]

\[ \langle O_\xi | b^\dagger b | O_\xi \rangle = \cosh^2 \phi \sinh^2 \theta_2 + \sinh^2 \phi \cosh^2 (\theta_1 + \delta) . \] (3.23)

4 Extension to fermions

The analysis of Sec.2 and Sec.3 can be repeated for fermions. Since we want the fermions to anti–commute we need to define the thermal doublet like \( a^\mu = (a, i\tilde{a}^\dagger) , \) \( a^{\dagger \mu} = (a^\dagger, -i\tilde{a}) \) and we use the convention \( \tilde{a} = a \) [19]. Differences in signs in the canonical anti–commutation relation (CAR) and the factors of \( i \) lead to slightly different conditions compared to Sec.3, but they can all be solved in a similar manner.

4.1 2 × 2 Bogoliubov matrices

We start with the extension of the thermal 2 × 2 Bogoliubov transformation to the cases when Hermitian and tilde conjugation are not preserved. Defining \( a^\mu = F_2^{\mu \nu} \xi^\nu \) and \( a^{\dagger \mu} = G_2^{\mu \nu} \xi^{\dagger \nu} \) the CAR gives

\[ F_2^{-1} = G_2^T . \] (4.1)

The only restriction on \( F_2 \) is that it should be invertible. When we require \( \sim \) invariance we get the extra condition

\[ F_2 \tau_2 F_2^\dagger = \tau_2 , \] (4.2)

just as for bosons. The condition for preserving Hermiticity is however

\[ F_2 F_2^\dagger = 1 . \] (4.3)

We summarize the various possibilities for fermions and bosons in Tab.1.
<table>
<thead>
<tr>
<th>preserve</th>
<th>~ yes</th>
<th>~ no</th>
</tr>
</thead>
<tbody>
<tr>
<td>† yes [\beta \in \mathbb{R}] bosons</td>
<td>[e^{i\theta} \left( \begin{pmatrix} \pm \sqrt{1 + \beta^2} &amp; \beta \ \beta &amp; \pm \sqrt{1 + \beta^2} \end{pmatrix} \right)]</td>
<td>[e^{i\theta} \left( \begin{pmatrix} \sqrt{1 + \beta^2} e^{i\phi} &amp; \beta e^{i\varphi} \ \beta e^{-i\varphi} &amp; \sqrt{1 + \beta^2} e^{-i\phi} \end{pmatrix} \right)]</td>
</tr>
<tr>
<td>† yes [\alpha \in [-1, 1]] fermions</td>
<td>[e^{i\theta} \left( \begin{pmatrix} \pm \sqrt{1 - \alpha^2} &amp; \alpha \ -\alpha &amp; \pm \sqrt{1 - \alpha^2} \end{pmatrix} \right)]</td>
<td>[e^{i\theta} \left( \begin{pmatrix} \sqrt{1 - \alpha^2} e^{i\phi} &amp; \alpha e^{i\varphi} \ -\alpha e^{-i\varphi} &amp; \sqrt{1 - \alpha^2} e^{-i\phi} \end{pmatrix} \right)]</td>
</tr>
<tr>
<td>† no</td>
<td>[e^{i\theta} \left( \begin{pmatrix} \zeta &amp; \beta \ \gamma &amp; 1 + \beta \gamma \zeta \end{pmatrix} \right) \in U(1) \times SL(2, \mathbb{R})]</td>
<td>[\left( \begin{pmatrix} \zeta &amp; \beta \ \gamma &amp; \delta \end{pmatrix} \right) \in GL(2, \mathbb{C})]</td>
</tr>
</tbody>
</table>

Table 1. The 2 × 2 Bogoliubov matrices for bosons and fermions.

### 4.2 4 × 4 Bogoliubov matrices

It is straightforward to determine what kind of 4 × 4 Bogoliubov transformations are possible for fermions along the lines of Sec.3.

**Case I**

The fermionic cases are quite different from the bosonic ones. At zero temperature a transformation like \[\xi = \alpha a + \beta a^\dagger\] can only satisfy the CAR if \[\alpha \beta = 0\] (and \[|\alpha|^2 + |\beta|^2 = 1\]), i.e. if one of \(\alpha\) and \(\beta\) is zero. This kind of constraint survives also at finite temperature.

Using the quadruple notation

\[
a^\mu = (a, i\tilde{a}^\dagger, a^\dagger, -i\tilde{a}) \; , \; \xi^\mu = (\xi, i\tilde{\xi}^\dagger, \xi^\dagger, -i\tilde{\xi}) \; ,
\]

(4.4)
the condition for preserving CAR, † and ∼ are

\[
\begin{align*}
\text{CAR} : \quad F_4(\tau_1 \otimes \mathbb{1})F_4^T &= (\tau_1 \otimes \mathbb{1}) , \\
† : \quad F_4^†(\tau_1 \otimes \mathbb{1}) &= (\tau_1 \otimes \mathbb{1})F_4 , \\
∼ : \quad F_4^*(\tau_2 \otimes \tau_2) &= (\tau_2 \otimes \tau_2)F_4 .
\end{align*}
\]

The only solution which is continuously connected to the identity is in fact

\[
\begin{pmatrix}
a \\
i\tilde{a}^†
\end{pmatrix}
= \begin{pmatrix}
e^{i\psi_1} \cos \theta & e^{i\psi_2} \sin \theta \\
-e^{i\psi_2} \sin \theta & e^{i\psi_1} \cos \theta
\end{pmatrix}
\begin{pmatrix}
\xi \\
i\tilde{\xi}^†
\end{pmatrix},
\]

and its Hermitian conjugate. We conclude that it is only the usual thermal mixing that is possible for a single fermionic mode.

In connection with the observation that there is no non–trivial mixing of fermions as described above we want to comment on another convention for tilde conjugation of fermions. In many places in the literature it is postulated that \( \tilde{a} = -a \) for fermions and the thermal doublet \((a, \tilde{a}^†)\) is used. This notation gives the same possible 2×2 Bogoliubov matrices at equilibrium, and no physical difference between the two conventions is known so far. For the 4×4 mixing considered here in case I the conditions for preservation of CAR, †– and ∼–conjugation allows for non–trivial transformations using this alternative convention. To be more precise, if we define

\[
a = \alpha \xi + \beta \tilde{\xi}^† + \gamma \xi^† + \delta \tilde{\xi},
\]

and extend it through †– and the altered ∼–conjugation, the CAR can be satisfied even when all \(\alpha, \beta, \gamma\) and \(\delta\) are non–zero. For example we can take

\[
\begin{align*}
\alpha &= \cos \phi \cos \theta , \quad \gamma = -\sin \phi \sin \theta , \\
\beta &= \cos \phi \sin \theta , \quad \delta = \sin \phi \cos \theta ,
\end{align*}
\]

which is not possible with the convention \( \tilde{a} = a \). The relations between the different conventions for non–equilibrium states is not yet clear and we continue to use \( \tilde{a} = a \) since the construction of such anti–commuting tilde operators is possible from the basic Tomita-Takesaki modular theory [19].
Case II
Mixing of two species of fermions is important e.g. for massive neutrinos in connection with the solar neutrino problem. When we write the quadruple like
\[ a^\mu = (a, i\tilde{a}^\dagger, b, i\tilde{b}^\dagger) , \quad \xi^\mu = (\xi, i\tilde{\xi}^\dagger, \eta, i\tilde{\eta}^\dagger) , \] (4.9)
the condition for CAR, \( \dagger \) and \( \sim \) are
\[
F_4 F_4^\dagger = \mathbb{1} \otimes \mathbb{1} , \\
F_4 (\mathbb{1} \otimes \tau_2) = (\mathbb{1} \otimes \tau_2) F_4 .
\] (4.10)
A tensor product of the particle and thermal mixing fulfills Eq.(4.10), but more general solutions are allowed. Assuming that \( F_4 \) is real we get
\[
F_4 = \begin{pmatrix}
F_2(\theta_1) \cos \phi & F_2(\theta_2 - \delta) \sin \phi \\
-F_2(\theta_1 + \delta) \sin \phi & F_2(\theta_2) \cos \phi
\end{pmatrix},
\] (4.11)
where
\[
F_2(\theta) = \begin{pmatrix}
\cos \theta & \sin \theta \\
-\sin \theta & \cos \theta
\end{pmatrix}.
\] (4.12)
The free Hamiltonian and the number expectation values are in this case
\[
\hat{H}(\xi, \eta) = (\omega_a \cos^2 \phi + \omega_b \sin^2 \phi)(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi}) + (\omega_b \cos^2 \phi + \omega_a \sin^2 \phi)(\eta^\dagger \eta - \tilde{\eta}^\dagger \tilde{\eta})
+ \frac{\sin 2\phi}{2}(\omega_a - \omega_b) \left\{ \cos(\theta_1 - \theta_2 + \delta)[\xi^\dagger \eta + \eta^\dagger \xi - \tilde{\xi}^\dagger \tilde{\eta} - \tilde{\eta}^\dagger \tilde{\xi}] \\
- i \sin(\theta_1 - \theta_2 + \delta)[\xi^\dagger \tilde{\eta} + \tilde{\xi}^\dagger \eta]\right\} ,
\] (4.13)
\[
\langle O_\xi| a^\dagger a | O_\xi \rangle = \cos^2 \phi \sin^2 \theta_1 + \sin^2 \phi \sin^2(\theta_2 - \delta) ,
\]
\[
\langle O_\xi| b^\dagger b | O_\xi \rangle = \cos^2 \phi \sin^2 \theta_2 + \sin^2 \phi \sin^2(\theta_1 + \delta) .
\] (4.14)
Case III
In the BCS theory of superconductivity there is a mixing between $a_{k,\uparrow}$ and $a_{-k,\downarrow}$. Thermo field dynamics was first invented as an operator formalism to deal with superconductivity at finite temperature [20] and this application is still of current interest [21]. A general mixing of the BCS type preserving CAR, $\dagger$- and $\sim$-conjugation must satisfy

$$F_4 F_4^\dagger = \mathbb{1} \otimes \mathbb{1} ,$$
$$F_4 (\tau_3 \otimes \tau_2) = (\tau_3 \otimes \tau_2) F_4^* ,$$ (4.15)

if we use the notation $a^\mu = (a, i \tilde{a}^\dagger, b^\dagger, -i \tilde{b})$. The solution is

$$F_4 = \begin{pmatrix}
F_2(\theta_1) \cos \phi & \tau_3 F_2(\theta_2 - \delta) \sin \phi \\
-\tau_3 F_2(\theta_2 - \delta) \sin \phi & F_2(\theta_1) \cos \phi
\end{pmatrix} .$$ (4.16)

The transformed Hamiltonian and the number expectation values are

$$\hat{H}(\xi, \eta) = (\omega_a \cos^2 \phi - \omega_b \sin^2 \phi)(\xi^\dagger \xi - \tilde{\xi}^\dagger \tilde{\xi}) + (\omega_a \cos^2 \phi - \omega_b \sin^2 \phi)(\eta^\dagger \eta - \tilde{\eta}^\dagger \tilde{\eta})$$

$$+ \frac{\sin 2 \phi}{2} (\omega_a - \omega_b) \left\{ \cos(\theta_1 + \theta_2 - \delta)[\xi^\dagger \eta + \eta^\dagger \xi - \tilde{\xi}^\dagger \tilde{\eta} - \tilde{\eta}^\dagger \tilde{\xi}] \right\} ,$$ (4.17)

$$\langle O_\xi | a^\dagger a | O_\xi \rangle = \cos^2 \phi \sin^2 \theta_1 + \sin^2 \phi \cos^2(\theta_2 - \delta) ,$$

$$\langle O_\xi | b^\dagger b | O_\xi \rangle = \cos^2 \phi \sin^2 \theta_2 + \sin^2 \phi \cos^2(\theta_1 - \delta) .$$ (4.18)

5 Conclusions
We have generalized the $\alpha$–degree of freedom and discussed the relation to Hermitian and tilde conjugation. Depending on which algebraic properties one wishes to preserve when representing the operators in the thermal Hilbert space different parametrizations of the thermal Bogoliubov transformation are possible. Some of the parameters have been used earlier to simplify time dependent non–equilibrium calculations in TFD and we hope that the extensions considered here will also turn out to be useful.

Mixing of modes occurs in several systems at zero temperature. We have combined particle mixing and thermal mixing for a number of cases for bosons and fermions. The
essential result is that the number of physical parameters increases when we consider both mixings at the same time. Even when Hermitian and tilde conjugation are preserved, so that the corresponding \( \alpha \)-degree of freedom is eliminated, there remains a new parameter which we call \( \delta \). One can, for instance, imagine a system that undergoes a phase transition acquires a value of \( \delta \) which is determined by the dynamics. Quite generally we would like to stress that the set of all Bogoliubov transformations is very rich when one leaves the simple equilibrium case, mostly considered in the literature so far.

The meaning of the parameter \( \delta \) has yet to be clarified in greater detail but we can speculate about its role in the thermal states. Let us take the bosonic case II as an example and let \( \theta_1 = \theta_2 \) for simplicity. The usual way of determining the value of the mixing parameter \( \phi \) is to diagonalize the quadratic part of the interacting Hamiltonian \([20, 21]\).

In Eq.(3.17) we start out from a diagonal Hamiltonian but we can see what kind of terms the non–zero \( \delta \) generates. The term with a factor \( \cosh(\delta) \) contains no mixing of tilde and non–tilde modes, they are only in the \( \sinh(\delta) \) term. The mixing of tilde and non–tilde operators is usually related to dissipation so we may expect that the \( \delta \) parameter is also related to dissipation. These are only speculations that have to be substantiated by further research.

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References


