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## Liouville space description of thermofields and their generalisations

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**Abstract.** The thermofield representation of a thermal state by a pure-state wavefunction in a doubled Hilbert space is generalised to arbitrary mixed and pure states. We employ a Liouville space formalism to investigate the connection between these generalised thermofield wavefunctions and a generalised thermofield state vector in Liouville space which is valid for all cases of the quantum density operator. The system dynamics in the Schrödinger and Heisenberg pictures are discussed.

Quantum mechanical systems in mixed states are conventionally represented by density matrices and their evolution described by master equations. The so-called thermofield formalism (Takahashi and Umezawa 1975, Umezawa *et al* 1982, Barnett and Knight 1985) allows us to represent thermal mixed states by pure states in an enlarged Hilbert space consisting of the Hilbert space of the system and a duplicate 'fictitious' Hilbert space. In this paper we demonstrate the generalisation of the Takahashi-Umezawa thermofield formalism to the pure-state representation of arbitrary states of any quantum system. We demonstrate the connections between density matrix, Liouville space (Fiutak and Van Kranendonk 1962, Cohen-Tannoudji 1975, Dalton 1982) and thermofield representations of quantum states. We also discuss the dynamics in these representations.

The thermofield vacuum state representing a quantum mechanical system in a thermal state is given by the wavefunction

$$|0(\beta)\rangle = Z_{(\beta)}^{-1/2} \sum_n \exp(-\beta E_n/2) |n, \tilde{n}\rangle \quad (1)$$

where  $Z(\beta)$  is the partition function and  $\beta$  is the inverse temperature  $\beta = (k_B T)^{-1}$ . The quantum system has a Hamiltonian  $H$  and orthogonal energy states  $|n\rangle$  with energy eigenvalues  $E_n$

$$H|n\rangle = E_n|n\rangle. \quad (2)$$

Quantities associated with the duplicate Hilbert space are denoted by a tilde

$$\tilde{H}|\tilde{n}\rangle = E_n|\tilde{n}\rangle. \quad (3)$$

We see that for an operator  $A$  acting only in the original space, the thermofield vacuum state expectation value is

$$\begin{aligned} \langle 0(\beta) | A | 0(\beta) \rangle &= Z^{-1}(\beta) \sum_n \sum_m \exp[-\beta(E_n + E_m)/2] \langle n, \tilde{n} | A | m, \tilde{m} \rangle \\ &= Z^{-1}(\beta) \sum_n \exp(-\beta E_n) \langle n | A | n \rangle. \end{aligned} \quad (4)$$

This is the thermal state expectation value usually associated with mixed-state density matrices (see, for example, ter Haar 1961). The orthogonality of the energy eigenstates  $|\tilde{n}\rangle$  is responsible for destroying the off-diagonal density matrix elements usually associated with pure-state expectation values.

To generalise the thermofield representation to arbitrary states of any quantum system we require a pure-state wavefunction in a doubled Hilbert space

$$|\theta\rangle = \sum_{ij} \theta_{ij} |i, \tilde{j}\rangle. \quad (5)$$

This wavefunction must have the property that the expectation value of an operator  $A$ , acting only in the original space, is equal to that obtained when using a density matrix  $\rho$

$$\text{Tr}\{\rho A\} = \langle\theta|A|\theta\rangle. \quad (6)$$

In the discussion of the existence of  $|\theta\rangle$  and of its properties we find it convenient to employ the Liouville space formalism. There is a natural connection between density matrix, Liouville space and thermofield formalisms—the Liouville space formalism being intermediate between the density matrix and thermofield descriptions.

In Liouville space, each linear operator  $A$  corresponds to a vector  $|A\rangle\rangle$ . Particular operators in state space are associated with Liouville space vectors as follows:

$$A \leftrightarrow |A\rangle\rangle \quad (7a)$$

$$|i\rangle\langle j| \leftrightarrow |ij^+\rangle \quad (7b)$$

$$1 \leftrightarrow |1\rangle\rangle. \quad (7c)$$

For an orthonormal basis  $|i\rangle$  in state space we have

$$|1\rangle\rangle = \sum_i |ii^+\rangle \quad (8a)$$

$$A = \sum_{ij} A_{ij} |i\rangle\langle j| \leftrightarrow \sum_{ij} A_{ij} |ij^+\rangle. \quad (8b)$$

The scalar product in Liouville space is defined via association with the trace operation in state space

$$\langle\langle B|A\rangle\rangle = \text{Tr}\{B^\dagger A\}. \quad (9)$$

Linear operators in Liouville space (superoperators) are defined by their action on the Liouville space vectors. As an example of a superoperator consider the operator relation

$$B = F_1 A F_2^\dagger. \quad (10)$$

We define the superoperator

$$F = F_1 \times F_2^\dagger \quad (11)$$

and its action on a Liouville space vector

$$\begin{aligned} |B\rangle\rangle &= F|A\rangle\rangle \\ &= |(F_1 A F_2^\dagger)\rangle\rangle. \end{aligned} \quad (12)$$

A particularly important superoperator is the Liouville superoperator which is defined in terms of the Hermitian Hamiltonian operator in state space ( $H$ )

$$\mathcal{L} \equiv H \times 1 - 1 \times H. \quad (13)$$

A more complete discussion of Liouville space is given by Dalton (1982, appendix 1).

We proceed by introducing the Liouville representation of the thermofield vacuum state (which we will later identify as a specific case of the generalised thermofield state vector  $|\theta\rangle\rangle$ )

$$|0(\beta)\rangle\rangle = Z^{-1/2}(\beta) \sum_n \exp(-\beta E_n/2) |nn^\dagger\rangle. \quad (14)$$

Consider a Hilbert space operator  $A$  and the related superoperator in Liouville space

$$A_s = A \times 1. \quad (15)$$

The expectation value of  $A_s$  in the Liouville thermofield vacuum state is

$$\begin{aligned} \langle\langle 0(\beta)|A \times 1|0(\beta)\rangle\rangle &= Z^{-1}(\beta) \sum_n \sum_m \exp[-\beta(E_n - E_m)/2] \langle\langle nn^\dagger|A \times 1|mm^\dagger\rangle\rangle \\ &= Z^{-1}(\beta) \sum_n \exp(-\beta E_n) \langle n|A|n\rangle \\ &= \langle\langle \rho|A\rangle\rangle \end{aligned} \quad (16)$$

$$= \langle A \rangle. \quad (17)$$

Thus, both  $\langle\langle 0(\beta)|A \times 1|0(\beta)\rangle\rangle$  and  $\langle\langle \rho|A\rangle\rangle$  give the thermal-state expectation value of the operator  $A$ . In the case where  $A$  is Hermitian we also have  $\langle\langle \rho|A\rangle\rangle = \langle\langle A|\rho\rangle\rangle$ . The expectation values  $\text{Tr}\{\rho A\}$ ,  $\langle\langle \rho|A\rangle\rangle$ ,  $\langle\langle 0(\beta)|A \times 1|0(\beta)\rangle\rangle$  and  $\langle 0(\beta)|A|0(\beta)\rangle$  are identical. Moreover, because  $A$  is an arbitrary operator,  $\rho$ ,  $|\rho\rangle\rangle$ ,  $|0(\beta)\rangle\rangle$  and  $|0(\beta)\rangle$  all provide a complete (and equivalent) description of the thermal state.

The Liouville space vector may be represented as a pure state in a doubled Hilbert space with a double set of operators (Crawford 1958, Schmutz 1978, Arimitsu and Umezawa 1985) if we make the identifications

$$|nm^\dagger\rangle\rangle \leftrightarrow |n\rangle|\tilde{m}\rangle \quad (18a)$$

$$A \times 1 \leftrightarrow A \quad (18b)$$

$$1 \times A \leftrightarrow \tilde{A}^\dagger. \quad (18c)$$

We now consider whether the relation (16) can be generalised to arbitrary density matrices  $\rho$ . That is, given a density matrix  $\rho$  with Liouville space representation

$$|\rho\rangle\rangle = \sum_{n,m} \rho_{nm} |nm^\dagger\rangle\rangle \quad (19)$$

we need to show that there is a Liouville space vector representing a generalised thermofield state

$$|\theta\rangle\rangle = \sum_{ij} \theta_{ij} |ij^\dagger\rangle\rangle \quad (20)$$

such that

$$\begin{aligned} \langle A \rangle &= \langle\langle \rho|A\rangle\rangle \\ &= \langle\langle \theta|A \times 1|\theta\rangle\rangle. \end{aligned} \quad (21)$$

Evaluating  $\langle\langle \theta|A \times 1|\theta\rangle\rangle$  we find

$$\begin{aligned} \langle\langle \theta|A \times 1|\theta\rangle\rangle &= \sum_{n,j,m,l} \langle\langle nj^\dagger|A \times 1|ml^\dagger\rangle\rangle \\ &= \sum_{n,j,m} A_{nm} \theta_{nj}^* \theta_{mj}. \end{aligned} \quad (22)$$

The expectation value of  $A$  calculated from the density matrix  $\rho$  is

$$\langle\langle \rho | A \rangle\rangle = \sum_{n,m} \rho_{nm}^* A_{nm}. \quad (23)$$

Since  $A$  is arbitrary, equality between expressions (22) and (23) requires that

$$\rho_{nm} = \sum_j \theta_{nj} \theta_{mj}^*. \quad (24)$$

In matrix form, this condition reduces to

$$\rho = \theta \theta^\dagger. \quad (25)$$

Factorisation of the density matrix into a product of two square roots of the density matrix has been considered before by Crawford (1958) and Schmutz (1978). We shall see that the Liouville description ties together the descriptions afforded by the square root of the density matrix and the pure state in an expanded Hilbert space. We now have to prove that the density matrix can always be factorised in the form of equation (25). The density operator is Hermitian, and can therefore be diagonalised in the form

$$\rho = \sum_\lambda \rho_\lambda P_\lambda \quad (26)$$

where  $P_\lambda$  is the projector  $|\lambda\rangle\langle\lambda|$  and  $|\lambda\rangle$  are the orthogonal eigenstates of  $\rho$  with eigenvalues  $\rho_\lambda$  obeying the condition

$$0 \leq \rho_\lambda \leq 1. \quad (27)$$

Using the orthonormality of the states  $|\lambda\rangle$  the projectors satisfy  $P_\lambda P_\mu = \delta_{\lambda\mu} P_\lambda$ . We can write the density operator in the factorised form

$$\begin{aligned} \rho &= \left( \sum_\lambda \rho_\lambda^{1/2} \exp(i\phi_\lambda) P_\lambda \right) \left( \sum_\mu \rho_\mu^{1/2} \exp(-i\phi_\mu) P_\mu \right) \\ &= \theta \theta^\dagger. \end{aligned} \quad (28)$$

This result is independent of the diagonal basis used to derive it. Taking matrix elements in an arbitrary basis  $|n\rangle$  yields the required result, equation (24). Note that the phase factors  $\phi_\lambda$  are undetermined and therefore  $\theta$  is not unique. Thus the density matrix can always be factorised into a product of a matrix with its Hermitian conjugate. Therefore we can always find a Liouville space vector  $|\theta\rangle$  to represent the state of a quantum mechanical system associated with the density matrix  $\rho$ . That is, we can write the expectation value of any operator acting in the system Hilbert space as

$$\begin{aligned} \langle A \rangle &= \langle\langle \rho | A \rangle\rangle \\ &= \langle\langle \theta | A \times 1 | \theta \rangle\rangle. \end{aligned} \quad (29)$$

Making the identifications (18) we can associate  $|\theta\rangle$  with a pure-state wavefunction in a doubled Hilbert space

$$|\theta\rangle = \sum_{ij} \theta_{ij} |ij^+\rangle \leftrightarrow |\theta\rangle = \sum_{ij} \theta_{ij} |i, \tilde{j}\rangle. \quad (30)$$

The Hermitian character of the density matrix implies the existence of the equivalent representations  $\rho$ ,  $|\rho\rangle$ ,  $|\theta\rangle$  and  $|\theta\rangle$  for an arbitrary state of any quantum system.

A special case of this relation (29) occurs for a pure-state density matrix, where  $\rho$  can be written in the form

$$\rho = |\psi\rangle\langle\psi| \quad (31)$$

so that  $|\psi\rangle$  is an eigenvector of  $\rho$  with eigenvalue 1. The corresponding  $\theta$  is therefore

$$\theta = e^{i\phi} |\psi\rangle\langle\psi| \quad (32)$$

so that in an arbitrary basis  $|n\rangle$  we have

$$\theta_{nm} = e^{i\phi} c_n c_m^* \quad (33)$$

with  $c_n = \langle n | \psi \rangle$  the expansion coefficients for a pure state  $|\psi\rangle$ . Thus

$$|\theta\rangle\rangle = \sum_{n,m} e^{i\phi} c_n c_m^* |nm\rangle\rangle = e^{i\phi} ||\psi\rangle\langle\psi||. \quad (34)$$

In the Schrödinger picture, the density matrix evolves according to the equation of motion

$$i\hbar d\rho/dt = [H, \rho]. \quad (35)$$

In Liouville space, this equation becomes (Fiutak and Van Kranendonk 1962, Cohen-Tannoudji 1975, Dalton 1982)

$$i\hbar(d/dt)|\rho\rangle\rangle = \mathcal{L}|\rho\rangle\rangle. \quad (36)$$

Integrating the density matrix equation of motion (35) we find

$$\begin{aligned} \rho(t) &= u(t)\rho(0)u^\dagger(t) \\ &= u(t)\theta(0)u^\dagger(t)u(t)\theta^\dagger(0)u^\dagger(t) \end{aligned} \quad (37)$$

where  $u(t) = \exp(-iHt/\hbar)$  is the unitary time evolution operator and we have used the density matrix factorisation (28). From equation (37) we see that we can choose the density matrix factors such that at time  $t$

$$\theta(t) = u(t)\theta(0)u^\dagger(t). \quad (38)$$

Differentiating this equation we find the equation of motion for  $\theta$

$$i\hbar d\theta/dt = [H, \theta]. \quad (39)$$

A similar equation of motion has been derived for the square root of the density matrix by Crawford (1958) and Schmutz (1978). In Liouville space, equation (39) becomes

$$i\hbar(d/dt)|\theta\rangle\rangle = \mathcal{L}|\theta\rangle\rangle. \quad (40)$$

Making the identifications (18), we can associate the Liouville space vector  $|\theta\rangle\rangle$  with a pure-state wavefunction in a doubled Hilbert space. With this identification, the Liouville superoperator becomes the Hamiltonian for the pure-state thermofield wavefunction

$$\mathcal{L} \leftrightarrow H - \tilde{H} \quad (41)$$

where we have used the fact that the Hamiltonian is an Hermitian operator. This is the Hamiltonian associated with the free field evolution of the thermofield vacuum state (Takahashi and Umezawa 1975, Umezawa *et al* 1982, Barnett and Knight 1985). Here we see the significance of the form adopted by Takahashi and Umezawa (1975) for the thermofield free field Hamiltonian. The real Hamiltonian ( $H$ ) is associated with the ket dynamics of the density matrix while the fictitious Hamiltonian ( $-\tilde{H}$ ) is associated with the bra dynamics. Equivalently,  $H(-\tilde{H})$  is associated with  $H \times 1(-1 \times H)$  in the Liouville superoperator  $\mathcal{L}$ .

In the Heisenberg picture  $\rho$  and  $\theta$  are independent of time and an operator  $A$  satisfies the equation

$$i\hbar(d/dt)A = [A, H]. \quad (42)$$

Thus in Liouville space

$$i\hbar(d/dt)|A\rangle\rangle = -\mathcal{L}|A\rangle\rangle. \quad (43)$$

In the thermofield representation, where operators act in either the real or fictitious spaces (Takahashi and Umezawa 1985, Umezawa *et al* 1982) or in both spaces (Barnett and Knight 1985), the Heisenberg equation of motion for an arbitrary operator  $A$  is

$$i\hbar dA/dt = [A, H - \tilde{H}]. \quad (44)$$

The mean value of a physical quantity  $\langle A \rangle$  is, of course, the same in the Schrödinger and Heisenberg pictures for each of the formalisms discussed here.

In conclusion, we illustrate our results with two simple examples. Our first example is the well known case of a simple harmonic oscillator in a thermal (thermofield) state (Takahashi and Umezawa 1975, Umezawa *et al* 1982, Barnett and Knight 1985). The thermal density matrix may be written as (ter Haar 1961)

$$\rho_{\text{th}} = Z^{-1}(\beta) \exp(-\beta H) \quad (45)$$

where  $H$  is the free Hamiltonian

$$H = \hbar\omega a^\dagger a. \quad (46)$$

The evolution of the density matrix is governed by equation (35). The Liouville space equation for the generalised thermofield state vector  $|\theta\rangle\rangle$  is

$$i\hbar(d/dt)|\theta\rangle\rangle = \mathcal{L}|\theta\rangle\rangle. \quad (47)$$

Making the identifications (18) we arrive at the following form for the pure-state thermofield vacuum wavefunction:

$$|0(\beta)\rangle\rangle = Z^{-1/2}(\beta) \sum_n \exp(-\beta n\hbar\omega/2) \exp(i\phi_n) |n, \tilde{n}\rangle. \quad (48)$$

Setting the arbitrary phases  $\phi_n$  to zero we arrive at the form of the thermofield vacuum state for a simple harmonic oscillator

$$|0(\beta)\rangle\rangle = Z^{-1/2}(\beta) \exp[\exp(-\beta\hbar\omega/2) a^\dagger \tilde{a}^\dagger] |0, \tilde{0}\rangle \quad (49)$$

which we identify with the corresponding Liouville space expression

$$|0(\beta)\rangle\rangle = Z^{-1/2}(\beta) \exp[\exp(-\beta\hbar\omega/2) a^\dagger \times a] |00^\dagger\rangle\rangle. \quad (50)$$

Our second example is the state of a two-level quantum system which, for simplicity, we take to have equal probability of being in the excited state  $|+\rangle$  or de-excited state  $|-\rangle$ . In matrix form, the density matrix has the form

$$\rho = \begin{pmatrix} \frac{1}{2} & C e^{-i\phi} \\ C e^{i\phi} & \frac{1}{2} \end{pmatrix}. \quad (51)$$

If  $C = \frac{1}{2}$ , the system is in a pure superposition state of  $|+\rangle$  and  $|-\rangle$ . If  $C = 0$ , the system is in a statistical mixture of  $|+\rangle$  and  $|-\rangle$ . Values of  $C$  that are intermediate between

0 and  $\frac{1}{2}$  are also possible and describe the existence of partial coherence between the levels. The expectation value of an operator  $A$  with matrix representation

$$A = \begin{pmatrix} A_{++} & A_{+-} \\ A_{-+} & A_{--} \end{pmatrix} \quad (52)$$

is given by

$$\begin{aligned} \langle A \rangle &= \text{Tr}\{\rho A\} \\ &= \frac{1}{2}A_{++} + C e^{i\phi}A_{+-} + C e^{-i\phi}A_{-+} + \frac{1}{2}A_{--}. \end{aligned} \quad (53)$$

The thermofield state

$$|\theta\rangle = a|+, \tilde{+}\rangle + b e^{-i\phi}|+, \tilde{-}\rangle + b e^{i\phi}|-, \tilde{+}\rangle + a|-, \tilde{-}\rangle \quad (54)$$

where

$$a = \frac{1}{2}[(\frac{1}{2} + C)^{1/2} + (\frac{1}{2} - C)^{1/2}] \quad (55)$$

$$b = \frac{1}{2}[(\frac{1}{2} + C)^{1/2} - (\frac{1}{2} - C)^{1/2}] \quad (56)$$

provides an equivalent representation of the state, for

$$\langle \theta | A | \theta \rangle = \frac{1}{2}A_{++} + C e^{i\phi}A_{+-} + C e^{-i\phi}A_{-+} + \frac{1}{2}A_{--}. \quad (57)$$

We can identify the thermofield wavefunction  $|\theta\rangle$  with the Liouville space expression

$$|\theta\rangle\rangle = a|++\rangle\rangle + b e^{-i\phi}|+-\rangle\rangle + b e^{i\phi}|-+\rangle\rangle + a|--\rangle\rangle. \quad (58)$$

In this paper we have generalised the thermofield formalism to the representation of arbitrary states of any quantum system. We have shown that all quantum states may be represented by a wavefunction in a doubled Hilbert space. The density matrix  $\rho$ , its Liouville space representation  $|\rho\rangle\rangle$ , the thermofield wavefunction  $|\theta\rangle$  and its Liouville space representation  $|\theta\rangle\rangle$  form equivalent representations of a state. We have demonstrated the natural connection between the density matrix and thermofield representations by employing the Liouville space formalism. In particular we have demonstrated the relationship between the Liouville superoperator and the Hamiltonian for the generalised thermofield wavefunction. We have also discussed the system dynamics in the Schrödinger and Heisenberg pictures.

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