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On the relationship between thermo field dynamics and quantum statistical mechanics

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Abstract. The relationship between two approaches to the study of non-equilibrium field theories, namely quantum statistical mechanics and thermo field dynamics, is investigated. The formalism of superoperators acting in the Liouville space of density matrices is used to provide a detailed translation between the two approaches. It is found that thermo field dynamics is exactly equivalent to a restricted version of quantum statistical mechanics, in which the initial density matrix is constrained to be Gaussian. The dissipative perturbation theory developed within thermo field dynamics is translated into the language of statistical mechanics, and is found to be equivalent to that devised by the author using the statistical-mechanical closed-time-path method, except that the latter theory is not restricted to Gaussian initial states.

1. Introduction

Two apparently different mathematical structures have been developed over many years as means of estimating the real-time properties of thermally excited quantum field theories (see, for example, the review by Landsmann and van Weert [1]). One is standard quantum statistical mechanics, exemplified by the formula $\mathrm{Tr}[\rho A(t_1 \ldots t_n)]$ for the expectation value of a Heisenberg-picture operator A, which depends on several times $t_1 \ldots t_n$, in a state characterized at some initial time by the density operator ρ. The second, known as thermo field dynamics [2, 3], is most often presented as an axiomatic extension of ordinary quantum field theory, involving extra thermal degrees of freedom. Within statistical mechanics, a convenient method of undertaking perturbative calculations is afforded by the closed-time-path formalism [4–6]. As reviewed in section 2 below, this formalism is most easily constructed in terms of path integrals, and it turns out that two or more path integration variables are needed to represent each original quantum field. These extra variables are quite analogous to the thermal degrees of freedom introduced in thermo field dynamics, and the question naturally arises, to what extent the two mathematical structures are equivalent.

In the view of the present author, quantum statistical mechanics is the correct approach to describing thermally excited states. If the axioms of thermo field dynamics turned out to have physical implications different from those of statistical mechanics, it would perhaps be necessary to defend this view in detail. What is shown in this paper, however, is that thermo field dynamics is precisely equivalent to a restricted version of statistical mechanics, in which the density operator ρ is Gaussian. Thus, it is this restriction, implied by the use of thermo field dynamics, which actually stands in need of defence. It seems to the author that this restriction is not defensible. For example, it excludes all density operators

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of the form $\exp(-\beta H)$, where H is the Hamiltonian of any interacting field theory. Note, however, that in the Schrödinger picture one may consider a density operator which evolves with time, and this density operator is restricted to be Gaussian only at some initial time.

The foregoing remarks may seem curious, in view of the well known fact that thermo field dynamics and the closed-time-path formalism yield identical Feynman rules for perturbation theory when applied to systems in thermal equilibrium [1,7]. In thermal equilibrium, however, the state of the system is essentially determined by the Hamiltonian which governs the real-time evolution and can, for example, be envisaged as emerging adiabatically from a non-interacting state (described by a Gaussian density operator) which existed in the remote past. Thus, the questions studied here are of practical importance only in non-equilibrium situations, where one needs to specify an initial state at a time which is not infinitely remote. The non-equilibrium version of the closed-time-path formalism [8,9] involves three path-integration variables in an essential manner, whereas only two fields appear in the corresponding formalism of thermo field dynamics. The role of the third field is precisely to accommodate interaction terms in the initial density operator.

The relationship between thermo field dynamics and quantum statistical mechanics has been investigated in the past. In the case of thermal equilibrium, it can be discussed in terms of C^*-algebras [1,10]. At a somewhat less sophisticated level, this relationship can be described in terms of superoperators acting in the Liouville space of density operators [11–13], and the latter approach is adopted in the present work. Indeed, Arimitsu and Umezawa [14,15] have appealed to the superoperator formalism to reconstruct the axioms of thermo field dynamics, though they did not investigate the consequences of doing so as exhaustively as is done here.

The literature on thermo field dynamics being quite extensive, it is scarcely possible to do justice to the ingenuity which advocates of this theory have expended in developing their non-equilibrium formalism. For the purposes of this work, we regard the paper of Hardman *et al* [16] as representative, and our strategy will be to construct a detailed translation between their axiomatic formalism and the standard treatment of quantum statistical mechanics. In section 2 below, we briefly review the closed-time-path formalism, giving a formulation which, though unnecessarily general for all practical purposes, will facilitate our later discussions. Superoperators are introduced in section 3, where almost all of thermo field dynamics is reconstructed from statistical mechanics, without any need for special assumptions. The crucial restriction, known as a 'thermal state condition', which seems in practice to be an essential ingredient of thermo field dynamics, is discussed in section 4, where we establish the central result announced above, namely that this condition is equivalent to assuming a Gaussian density operator. In section 5, we discuss the description of dissipation in non-equilibrium theories, which has received more careful and widespread attention in the context of thermo field dynamics than within the closed-time-path formalism. We show in detail how the dissipative Feynman rules obtained by Hardman *et al* can be translated into closed-time-path terms, and find that the result is equivalent to the perturbation theory developed within the latter context by the present author [9,17,18]. Finally, our conclusions are summarized and discussed in section 6.

2. Quantum statistical mechanics and the closed-time-path formalism

We consider a quantum field theory defined in terms of a collection of fields denoted collectively by the vector $\phi(\boldsymbol{x}, t)$. At some initial time, say t_i, the state of the system is described by a density operator ρ. All information about the behaviour of the system

between t_i and a final time t_f is contained, according to quantum statistical mechanics, in the generating functional for time-ordered Green functions,

$$Z(\rho; j) = \mathrm{Tr}\left[\rho T \exp\left(\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x\; j(x,t)\cdot\phi_{\mathrm{H}}(x,t)\right)\right] \tag{2.1}$$

where T denotes latest-on-the-left time ordering and the subscript H denotes an operator in the Heisenberg picture. The Heisenberg and Schrödinger pictures will be taken to coincide at time t_i. When one attempts to evaluate the time-ordered Green functions in perturbation theory, one finds that anti-time-ordered propagators are required in addition to the time-ordered ones, so it becomes convenient to define a more general functional

$$\begin{aligned} Z(\rho; j_1, j_2) = \mathrm{Tr}\Bigg[&\rho\bar{T}\exp\left(\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x\; j_2(x,t)\cdot\phi_{\mathrm{H}}(x,t)\right) \\ &\times T\exp\left(\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x\; j_1(x,t)\cdot\phi_{\mathrm{H}}(x,t)\right)\Bigg] \end{aligned} \tag{2.2}$$

where $\bar{T}$ is the anti-time-ordering operator. For the purposes of the present work, it will be useful to generalize this further to

$$\begin{aligned} \hat{Z}(\rho_1, \rho_2; j_1, j_2) &= \mathrm{Tr}\Bigg[\rho_1\bar{T}\exp\left(\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x\; j_2(x,t)\cdot\phi_{\mathrm{H}}(x,t)\right) \\ &\quad\times \rho_2\, T\exp\left(\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x\; j_1(x,t)\cdot\phi_{\mathrm{H}}(x,t)\right)\Bigg] \\ &\equiv \mathrm{Tr}\left[\rho_1\bar{\mathcal{J}}_{\mathrm{H}}(j_2)\rho_2\mathcal{J}_{\mathrm{H}}(j_1)\right]. \end{aligned} \tag{2.3}$$

To the best of our knowledge, this generating functional has no particular physical meaning, though it obviously reduces to (2.1) if $j_2 = 0$ and $\rho_1\rho_2 = \rho$.

The Green functions generated by (2.3) may be evaluated perturbatively by means of the closed-time-path formalism, which is most easily constructed in terms of path integrals [6]. We first transform to the Schrödinger picture, denoting Schrödinger-picture operators by a subscript S. We obtain

$$\hat{Z}(\rho_1, \rho_2; j_1, j_2) = \mathrm{Tr}\left[\rho_1\bar{\mathcal{J}}_{\mathrm{S}}(j_2)U(t_i,t_f)\rho_2 U^{-1}(t_i,t_f)\mathcal{J}_{\mathrm{S}}(j_1)\right] \tag{2.4}$$

where

$$\mathcal{J}_{\mathrm{S}}(j) = T\exp\left\{-\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t\left[H(\phi_{\mathrm{S}},t) - \int \mathrm{d}^3x\; j(x,t)\cdot\phi_{\mathrm{S}}(x)\right]\right\} \tag{2.5}$$

$$\bar{\mathcal{J}}_{\mathrm{S}}(j) = \bar{T}\exp\left\{\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t\left[H(\phi_{\mathrm{S}},t) + \int \mathrm{d}^3x\; j(x,t)\cdot\phi_{\mathrm{S}}(x)\right]\right\} \tag{2.6}$$

and

$$U(t_i,t_f) = T\exp\left[-\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t\, H(\phi_{\mathrm{S}},t)\right]. \tag{2.7}$$

To accommodate non-equilibrium situations, we allow for explicit time dependence in the Hamiltonian $H(\phi, t)$, which will naturally also depend on the canonical momenta $\Pi(x,t)$, though we suppress these arguments in the interest of notational economy.

Next, we suppose that both of the density operators ρ_i are Hermitian and positive definite. They can therefore be written in the form

$$\rho_i(\phi_S) = \exp[-\beta_i H_i(\phi_S)] \tag{2.8}$$

and the Hermitian operators H_i can be regarded as generators of evolution in imaginary time, over intervals of length β_i. These operators are associated with the initial state of the system, and may in principle be quite unrelated to the Hamiltonian H which governs the subsequent evolution in real time. In practice, no doubt, the class of density operators which can usefully be represented in the form (2.8) may be quite restricted.

Each of the six operators in (2.4) has a path-integral representation, obtained in the usual way by splitting the real and imaginary time intervals into infinitesimal segments and making repeated insertions of the identity operator, resolved as

$$I = \int \mathcal{D}\phi \, |\phi\rangle\langle\phi| \tag{2.9}$$

where the vectors $|\phi\rangle$ are eigenvectors of ϕ_S. The six sets of integration variables which arise in this way can be envisaged as residing on segments of a contour in the complex time plane, as depicted in figure 1. To undertake perturbative calculations using $\hat{Z}$, one would introduce independent source terms into the operators ρ_1, ρ_2, U and U^{-1}. Then the path integral representation of $\hat{Z}$ has the form

$$\hat{Z}(\rho_1, \rho_2; \{j\}) = \int \mathcal{D}\phi_1 \cdots \mathcal{D}\phi_6 \exp\left[\sum_{i=1}^{6} iS_i(\phi_i) + \text{source terms}\right]. \tag{2.10}$$

If $S(\phi)$ is the action of the original field theory, then the exponent in (2.10) contains a term $iS(\phi_i)$ *for each time-ordered segment of the contour,* $-iS(\phi_i)$ *for each anti-time-ordered* segment and $-S_i(\phi_i)$ for each imaginary time segment, where S_i is the action associated with the 'Hamiltonian' H_i. The Feynman rules would involve a 6×6 matrix of propagators and six sets of interaction vertices.

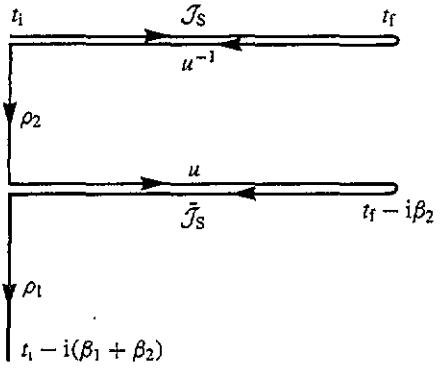

Figure 1. Path in the complex time plane corresponding to the generating functional (2.4).

Calculations of this sort would be quite unmanageable, and are also quite unnecessary. Within the closed-time-path formalism, only two special cases of the generating functional (2.4) are of any importance. In non-equilibrium situations, one may take $\rho_2 = 1$, in which case U and U^{-1} cancel out. Then $\hat{Z}$ reduces to the form (2.2), which is the

generating functional for expectation values of products of the quantum fields ϕ_H with a variety of time orderings. There is an irreducible set of three path integration variables, residing on the contour of figure 2 [8]. In the case of thermal equilibrium, which implies that the Hamiltonian is time independent, one may choose $\rho_1 = \exp(-\alpha\beta H)$ and $\rho_2 = \exp(-(1-\alpha)\beta H)$, where now β can be identified as the inverse temperature. Now U and U^{-1} commute with ρ_2 and again cancel, so that one obtains the contour shown in figure 3. If one takes the limits $t_i \to -\infty$ and $t_f \to +\infty$ in an appropriate manner, contributions from the vertical segments of the contour can be shown to factor out of $\hat{Z}$ [1, 6], so that only the two real-time segments need be considered. The Green functions generated by j_1 with $j_2 = 0$ correspond to the time-ordered Green functions of the original quantum field. However, other Green functions appear only in intermediate stages of perturbative calculations and have no clear physical meaning unless $\alpha = 1$, when we recover the contour of figure 2.

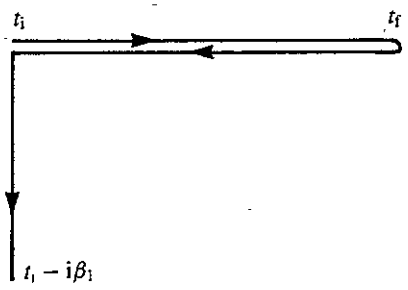

Figure 2. Path in the complex time plane corresponding to the generating functional (2.2).

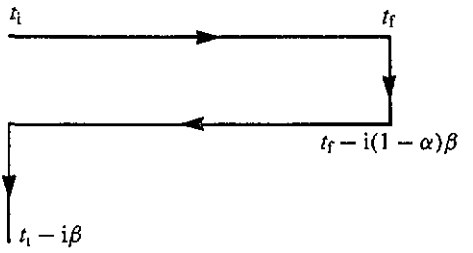

Figure 3. Path in the complex time plane corresponding to the generating functional (2.4) in the special case of a system in thermal equilibrium.

3. Superoperators and thermo field dynamics

For non-relativistic fields, which contain only positive frequencies, a perturbative formalism for dealing with non-equilibrium situations has been described in thermo field dynamics by Hardman *et al* [16] and further elaborated in several later papers [19–22]. Our object is to reconstruct this formalism by using the language of superoperators in Liouville space [11–15] to provide a detailed translation between thermo field dynamics and quantum statistical mechanics.

Suppose that the Hilbert space $\mathcal{H}$ of states available to our system is spanned by a set of basis vectors $|n\rangle$. An operator A in $\mathcal{H}$ can be written in the form $\sum_{n,n'} A_{n,n'}|n\rangle\langle n'|$ and these operators themselves form a linear vector space, which is spanned by the basis $|n\rangle\langle n'|$. (These bases are depicted as being countable only for notational simplicity. In particular, we do not envisage that the states of interest are restricted to a Fock subspace of $\mathcal{H}$. On the other hand, our discussion does not by any means aim at complete mathematical rigour; the various restrictions, e.g. on boundedness of operators, which might be required for a fully rigorous construction will not be examined.) Thus, we may consider a linear mapping ket$(\cdot)$ from operators in $\mathcal{H}$ to vectors $|\cdot\rangle\rangle$ in a vector space, called the Liouville space, which we denote by

$$\text{ket}(A) = |A\rangle\rangle \tag{3.1}$$

with the property

$$\mathrm{ket}(\lambda A + \mu B) = \lambda|A\rangle\rangle + \mu|B\rangle\rangle \tag{3.2}$$

for any two operators A and B and complex numbers λ and μ. An inner product on the Liouville space may be defined by

$$\langle\langle A|B\rangle\rangle = \mathrm{Tr}[A^\dagger B] \tag{3.3}$$

and this induces an antilinear mapping $\mathrm{bra}(\cdot) = \langle\langle\cdot|$, such that

$$\mathrm{bra}(\lambda A + \mu B) = \lambda^*\langle\langle A| + \mu^*\langle\langle B|. \tag{3.4}$$

Products of operators in $\mathcal{H}$ may now be represented in terms of *superoperators* in the Liouville space. Thus, we may define a linear mapping $L(\cdot)$, with $L(A) = A^{\mathrm{L}}$, and an antilinear mapping $R(\cdot)$, with $R(A) = A^{\mathrm{R}}$, by

$$|A\rho\rangle\rangle = A^{\mathrm{L}}|\rho\rangle\rangle \tag{3.5}$$

and

$$|\rho A^\dagger\rangle\rangle = A^{\mathrm{R}}|\rho\rangle\rangle. \tag{3.6}$$

For our purposes, there is no particular distinction between the operators A and ρ in these definitions. The notation merely indicates that it will be convenient to represent density operators in $\mathcal{H}$ as vectors in the Liouville space and other operators as superoperators. We shall refer to A^{L} and A^{R} as left- and right-handed superoperators respectively. In view of the definition (3.3) of the inner product, we also have

$$\langle\langle A^\dagger\rho| = \langle\langle\rho|A^{\mathrm{L}} \tag{3.7}$$

$$\langle\langle\rho A| = \langle\langle\rho|A^{\mathrm{R}} \tag{3.8}$$

and it is straightforward to show that, for any two operators A and B,

$$L(AB) = A^{\mathrm{L}}B^{\mathrm{L}} \tag{3.9}$$

$$R(AB) = A^{\mathrm{R}}B^{\mathrm{R}} \tag{3.10}$$

$$[A^{\mathrm{L}}, B^{\mathrm{R}}] = 0. \tag{3.11}$$

For theories which involve fermionic fields, these mappings may be generalized in such a way that left- and right-handed superoperators anticommute [13–15], but we shall deal only with bosonic fields in this work. Moreover, if Hermitian conjugation in the Liouville space is defined by $|\rho\rangle\rangle^\dagger = \langle\langle\rho|$, $\langle\langle\rho|^\dagger = |\rho\rangle\rangle$ and $(C|\rho\rangle\rangle)^\dagger = \langle\langle\rho|C^\dagger$, where C is any superoperator, then it is easily seen that $(A^\dagger)^{\mathrm{L}} = (A^{\mathrm{L}})^\dagger$ and $(A^\dagger)^{\mathrm{R}} = (A^{\mathrm{R}})^\dagger$, and so Hermitian conjugation in $\mathcal{H}$ and in the Liouville space may be represented by the same symbol. The identity operator is unique:

$$I^{\mathrm{L}} = I^{\mathrm{R}}. \tag{3.12}$$

An antilinear operation tilde(·) (with the notation tilde(C) = $\tilde{C}$) plays an important role in thermo field dynamics. In the language used here, it may be defined by

$$|\rho)\rangle\tilde{} = |\rho^\dagger)\rangle \tag{3.13}$$

$$(C|\rho)\rangle)\tilde{} = \tilde{C}|\rho)\rangle\tilde{} \tag{3.14}$$

where C is any superoperator. This implies

$$(\lambda C + \mu D)\tilde{} = \lambda^* \tilde{C} + \mu^* \tilde{D} \tag{3.15}$$

$$\widetilde{A^{\mathrm{L}}} = A^{\mathrm{R}} \tag{3.16}$$

$$\widetilde{A^{\mathrm{R}}} = A^{\mathrm{L}} \tag{3.17}$$

$$(CD)\tilde{} = \tilde{C}\tilde{D} \tag{3.18}$$

where A is any operator in $\mathcal{H}$ and C and D are any superoperators. It is customary in thermo field dynamics to denote our left-handed operators by A and the right-handed operators by $\tilde{A}$, but we do not adopt this convention here. Superoperators which have no L or R superscript are, in general, composed of sums and products of both left- and right-handed operators. The distinction between these superoperators and operators in $\mathcal{H}$ is one for which we have not found an economical notation, and will be indicated explicitly in the rare cases in which it is not evident from the context.

The model field theory studied by Hardman *et al* [16] is defined by a Lagrangian density of the form

$$\mathcal{L} = \mathrm{i}\psi_{\mathrm{H}}^\dagger(x,t)\frac{\partial}{\partial t}\psi_{\mathrm{H}}(x,t) - \psi_{\mathrm{H}}^\dagger(x,t)\omega(-\mathrm{i}\nabla,t)\psi_{\mathrm{H}}(x,t) - gW(\psi_{\mathrm{H}}^\dagger\psi_{\mathrm{H}},t). \tag{3.19}$$

The canonical momentum conjugate to ψ_{H} is

$$\Pi_{\mathrm{H}}(x,t) = \mathrm{i}\psi_{\mathrm{H}}^\dagger(x,t) \tag{3.20}$$

and the Hamiltonian is

$$H = \int \mathrm{d}^3x \left[\Pi_{\mathrm{H}}(x,t)\omega(-\mathrm{i}\nabla,t)\psi_{\mathrm{H}}(x,t) + gW(-\mathrm{i}\Pi_{\mathrm{H}}\psi_{\mathrm{H}},t)\right]. \tag{3.21}$$

For this model, we wish to obtain an expression in superoperator language for the generating functional (2.3), where we now identify

$$j_{\mathrm{i}}(x,t)\cdot\phi_{\mathrm{H}}(x,t) = j_{\mathrm{i}}(x,t)\psi_{\mathrm{H}}(x,t) + j_{\mathrm{i}}^*(x,t)\psi_{\mathrm{H}}^\dagger(x,t). \tag{3.22}$$

Using the cyclic property of the trace, we find

$$\begin{aligned}\hat{Z}(\rho_1,\rho_2;j_1,j_2) &= \langle(\rho_2|\mathcal{J}(j_1)\rho_1\bar{\mathcal{J}}(j_2)\rangle) \\ &= \langle(\rho_2|\mathcal{J}^{\mathrm{L}}(j_1)\bar{\mathcal{J}}^{\dagger R}(j_2)|\rho_1)\rangle).\end{aligned} \tag{3.23}$$

Since the adjoint of an anti-time-ordered expression is time-ordered, since left-handed operators commute with right-handed ones, and in view of the antilinearity of R(·), we have

$$\begin{aligned}\hat{\mathcal{J}}(j_1,j_2) &\equiv \mathcal{J}^{\mathrm{L}}(j_1)\bar{\mathcal{J}}^{\dagger R}(j_2) \\ &= T\exp\left[\mathrm{i}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}}\mathrm{d}t\left(j_1(t)\cdot\psi_{\mathrm{H}}^{\mathrm{L}}(t) + j_2^*(t)\cdot\psi_{\mathrm{H}}^{\mathrm{R}}(t)\right)\right]\end{aligned} \tag{3.24}$$

where, for brevity, spatial arguments and integrations have been suppressed. Similarly, we find that time evolution of superoperators is described by the evolution operator

$$\hat{U}(t_i, t) \equiv U^{\mathrm{L}}(t_i, t)U^{\mathrm{R}}(t_i, t) = T \exp\left[-\mathrm{i}\int_{t_i}^{t} \hat{H}(\psi_{\mathrm{S}}^{\mathrm{L}}, \psi_{\mathrm{S}}^{\mathrm{R}}, t')\mathrm{d}t'\right] \tag{3.25}$$

where

$$\hat{H}(\psi_{\mathrm{S}}^{\mathrm{L}}, \psi_{\mathrm{S}}^{\mathrm{R}}, t) = H(\psi_{\mathrm{S}}^{\mathrm{L}}, t) - H(\psi_{\mathrm{S}}^{\mathrm{R}}, t). \tag{3.26}$$

The Schrödinger-picture field operators may be expressed in terms of annihilation operators a_k and $a_k^\dagger$, with the usual commutation relation

$$[a_k, a_{k'}^\dagger] = \delta(k - k') \tag{3.27}$$

as

$$\psi_{\mathrm{S}}(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \mathrm{e}^{\mathrm{i}k\cdot x} a_k. \tag{3.28}$$

The corresponding superoperators are

$$\psi_{\mathrm{S}}^{\mathrm{L}}(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \mathrm{e}^{\mathrm{i}k\cdot x} a_k^{\mathrm{L}} \tag{3.29}$$

and, again taking account of the antilinearity of $R(\cdot)$,

$$\psi_{\mathrm{S}}^{\mathrm{R}}(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^{3/2}} \mathrm{e}^{-\mathrm{i}k\cdot x} a_k^{\mathrm{R}} \tag{3.30}$$

with

$$[a_k^{\mathrm{L}}, a_{k'}^{\dagger\mathrm{L}}] = [a_k^{\mathrm{R}}, a_{k'}^{\dagger\mathrm{R}}] = \delta(k - k') \tag{3.31}$$

and all other commutators equal to zero.

Within this canonical framework, perturbative calculations are accomplished using the interaction picture. Splitting the total Hamiltonian into an unperturbed part and an interaction,

$$\hat{H}(\psi, t) = \hat{H}_0(\psi, t) + \hat{H}_{\mathrm{int}}(\psi, t) \tag{3.32}$$

we define interaction-picture superoperators $A_{\mathrm{I}}(t)$ by

$$A_{\mathrm{I}}(t) = U_0^{-1}(t) A_{\mathrm{S}} U_0(t) \tag{3.33}$$

where

$$U_0(t) = T \exp\left[-\mathrm{i}\int_{t_i}^{t} \hat{H}_0(\psi_{\mathrm{S}}, t')\mathrm{d}t'\right] = \bar{T} \exp\left[-\mathrm{i}\int_{t_i}^{t} \hat{H}_0(\psi_{\mathrm{I}}(t'), t')\mathrm{d}t'\right]. \tag{3.34}$$

A convenient matrix notation, called the thermal doublet notation in thermo field dynamics, introduces a row vector $\bar{\psi} = (\bar{\psi}^1 \bar{\psi}^2)$ and a column vector ψ, whose transpose is $(\psi^1 \psi^2)$, where

$$\psi_I^1(x,t) = U_0^{-1}(t)\psi_S^L(x)U_0(t) \tag{3.35}$$

$$\psi_I^2(x,t) = U_0^{-1}(t)\psi_S^{R\dagger}(x)U_0(t) \tag{3.36}$$

$$\bar{\psi}_I^1(x,t) = U_0^{-1}(t)\psi_S^{L\dagger}(x)U_0(t) \tag{3.37}$$

$$\bar{\psi}_I^2(x,t) = -U_0^{-1}(t)\psi_S^R(x)U_0(t). \tag{3.38}$$

The fields thus defined have the equal-time commutation relation

$$[\psi_I^\mu(x,t), \bar{\psi}_I^\nu(x',t)] = \delta^{\mu\nu}\delta(x-x'). \tag{3.39}$$

However, the unperturbed evolution operator $U_0(t)$ used by Hardman *et al* is neither unitary, nor expressible in the form (3.25) as the product of a left- and a right-handed operator. In that case, $\bar{\psi}_I^1(x,t)$, for example, is not the adjoint of $\psi_I^1(x,t)$ and none of the operators (3.35)–(3.38) is purely left- or right-handed, except at $t = t_i$. If we define a corresponding set of sources by

$$J^1(x,t) = j_1^*(x,t) \tag{3.40}$$

$$J^2(x,t) = -j_2^*(x,t) \tag{3.41}$$

$$\bar{J}^1(x,t) = j_1(x,t) \tag{3.42}$$

$$\bar{J}^2(x,t) = j_2(x,t) \tag{3.43}$$

then the lowest-order approximation to the generating functional (3.23) may be written as

$$\hat{Z}_0(\rho_1, \rho_2; j_1, j_2) = \langle\langle \rho_2 | T \exp\left[i \int_{t_i}^{t_f} dt \left(\bar{J}(t)\psi_I(t) + \bar{\psi}_I(t)J(t) \right) \right] | \rho_1 \rangle\rangle. \tag{3.44}$$

The strategy adopted by Hardman *et al* [16] is now to specify *a priori* the time dependence of the interaction-picture fields and then to construct the unperturbed Hamiltonian $\hat{H}_0$ which generates this time dependence. In terms of the time-dependent creation and annihilation operators

$$a_k(t) = \int \frac{d^3x}{(2\pi)^{3/2}} e^{-ik\cdot x}\psi_I(x,t) \tag{3.45}$$

$$\bar{a}_k(t) = \int \frac{d^3x}{(2\pi)^{3/2}} e^{ik\cdot x}\bar{\psi}_I(x,t) \tag{3.46}$$

this time dependence has the form

$$a_k(t) = C_k^{-1}(t)\xi_k \tag{3.47}$$

$$\bar{a}_k(t) = \bar{\xi}_k C_k(t) \tag{3.48}$$

in which the real matrix $C_k(t)$ can be decomposed as

$$C_k(t) = E_k^{-1}(t) \begin{pmatrix} 1+n_k(t) & -n_k(t) \\ -1 & 1 \end{pmatrix} \begin{pmatrix} b_k(t) & 0 \\ 0 & 1/b_k(t) \end{pmatrix}. \tag{3.49}$$

The matrix $E_k(t)$ is composed of mode functions which describe single quasi-particle modes, and may be written as

$$E_k(t) = \begin{pmatrix} f_k^-(t) & 0 \\ 0 & f_k^+(t) \end{pmatrix} \tag{3.50}$$

where

$$f_k^{\pm}(t) = \exp\left[-\mathrm{i}\int_{t_1}^{t} \mathrm{d}t' \left(\omega_k(t') \pm \mathrm{i}\kappa_k(t')\right)\right]. \tag{3.51}$$

The function $\kappa_k(t)$ represents a quasi-particle decay width, while $\omega_k(t)$ is a renormalized frequency. In principle, this frequency may differ from the one which appears in (3.19), but we shall not be concerned with details of the renormalization process in this paper. The function $n_k(t)$ will turn out to represent the occupation number of the quasi-particle mode of momentum k, while $b_k(t)$ is arbitrary at this point. This prescription for the time dependence of the interaction-picture fields is designed so that the unperturbed propagator matrix $\langle\langle\rho_2|\psi_{\mathrm{I}}^{\mu}(x,t)\bar{\psi}_{\mathrm{I}}^{\nu}(x',t')|\rho_1\rangle\rangle$ has the same structure as the full propagator matrix. Consequently, the functions $\omega_k(t)$, $\kappa_k(t)$ and $n_k(t)$ can be specified self-consistently by a suitable renormalization prescription, together with a knowledge of the initial state.

The time-independent operators ξ_k and $\bar{\xi}_k$ which appear in (3.47) and (3.48) are respectively a column vector, whose transpose is $(\xi_k\ \bar{\xi}_k^{\ddagger})$, and a row vector $(\xi_k^{\ddagger}\ -\bar{\xi}_k)$. The non-tilde operators are related to the Schrödinger-picture creation and annihilation operators by

$$\xi_k = b_{k0}(1+n_{k0})a_k^{\mathrm{L}} - (n_{k0}/b_{k0})a_k^{\dagger\mathrm{R}} \tag{3.52}$$

$$\xi_k^{\ddagger} = (1/b_{k0})a_k^{\dagger\mathrm{L}} - b_{k0}a_k^{\mathrm{R}} \tag{3.53}$$

where b_{k0} and n_{k0} denote $b_k(0)$ and $n_k(0)$ respectively, and the tilde operators are obtained from these by using (3.15)–(3.17). It is easily verified that these operators satisfy the commutation rule

$$[\xi_k, \bar{\xi}_{k'}] = \delta^{\mu\nu}\delta(k-k') \tag{3.54}$$

although $\xi^{\ddagger}$ is not equal to $\xi^{\dagger}$ in general. Correspondingly, the operators $a_k(t)$ and $\bar{a}_k(t)$ satisfy the equal-time commutation relations

$$[a_k^{\mu}(t), \bar{a}_{k'}^{\nu}(t)] = \delta^{\mu\nu}\delta(k-k'). \tag{3.55}$$

It is straightforward to find that the Hamiltonian which generates this time dependence is

$$\begin{aligned}\hat{H}_0(\psi_{\mathrm{I}}, t) &= \int \mathrm{d}^3k\, \bar{a}_k(t)H_k(t)a_k(t) \\ &= \int \mathrm{d}^3x\, \bar{\psi}_{\mathrm{I}}(x,t)H(-\mathrm{i}\nabla, t)\psi_{\mathrm{I}}(x,t)\end{aligned} \tag{3.56}$$

where

$$\begin{aligned}H_k(t) &= \mathrm{i}\frac{\mathrm{d}C_k^{-1}(t)}{\mathrm{d}t}C_k(t) \\ &= \omega_k(t)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - \mathrm{i}\kappa_k(t)\begin{pmatrix}1+2n_k(t) & -2n_k(t)/b_k^2(t)\\ 2b_k^2(t)(1+n_k(t)) & -(1+2n_k(t))\end{pmatrix} \\ &\quad + \mathrm{i}\dot{n}_k(t)\begin{pmatrix}-1 & 1/b_k^2(t)\\ -b_k^2(t) & 1\end{pmatrix} - \mathrm{i}\frac{\dot{b}_k(t)}{b_k(t)}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\end{aligned} \tag{3.57}$$

and $H(-i\nabla, t)$ is found by making the replacement $k \to -i\nabla$ in this expression.

At this point, we have been able to reproduce most of the formalism constructed by Hardman *et al* [16] without any need for special assumptions. Thus, if Green functions generated by (3.23) can be calculated within the superoperator formalism, they should be precisely equivalent to those generated by (2.3). In particular, the functional $Z(\rho_1\rho_2; j_1) = \hat{Z}(\rho_1, \rho_2; j_1, 0)$, which coincides with (2.1), generates the physical expectation values that are of interest in quantum statistical mechanics. However, the perturbative evaluation of these Green functions, using (3.44) as the unperturbed theory, is accomplished in thermo field dynamics by introducing a crucial assumption, known as the thermal state condition, which we discuss in the following section. In all presentations of thermo field dynamics known to the present author, this assumption is introduced as a fundamental postulate. As we shall see, it restricts the class of initial states of the system which can be dealt with. This restriction distinguishes thermo field dynamics proper from the more general superoperator formalism we have studied up to now, and therefore also from quantum statistical mechanics.

4. Thermal states

The aim of thermo field dynamics is to offer a canonical, operator-based treatment of thermal field theory. In particular, it seeks to apply Wick's theorem to develop a perturbation series similar to that used to study scattering processes in the vacuum. For this reason, the vectors $|\rho_1\rangle\rangle$ and $\langle\langle\rho_2|$ are known in thermo field dynamics as 'thermal vacua'—a term which we avoid as being inappropriate to a description of highly excited thermal states. First of all, it is assumed that

$$|\rho_1\rangle\rangle^{\sim} = |\rho_1\rangle\rangle \qquad \text{and} \qquad \langle\langle\rho_2|^{\sim} = \langle\langle\rho_2|. \tag{4.1}$$

According to (3.13), this implies that the density operators ρ_1 and ρ_2 are Hermitian, as they should be. The crucial feature is that normal-ordered products of the operators ξ_k^μ and $\tilde{\xi}_k^\mu$ (in which $\xi_k^\dagger$ and $\tilde{\xi}_k^\dagger$ stand to the left of ξ_k and $\tilde{\xi}_k$) must have vanishing matrix elements between $\langle\langle\rho_2|$ and $|\rho_1\rangle\rangle$. To this end, one imposes the conditions

$$\xi_k|\rho_1\rangle\rangle = \tilde{\xi}_k|\rho_1\rangle\rangle = 0 \tag{4.2}$$

$$\langle\langle\rho_2|\xi_k^\dagger = \langle\langle\rho_2|\tilde{\xi}_k^\dagger = 0. \tag{4.3}$$

Assuming that $\langle\langle\rho_2|\rho_1\rangle\rangle = \mathrm{Tr}[\rho_2\rho_1] = 1$, a consequence of these conditions, together with (3.47)–(3.51) is that

$$\langle\langle\rho_2|\bar{a}_k^1(t)a_{k'}^1(t)|\rho_1\rangle\rangle = \delta(k-k')n_k(t) \tag{4.4}$$

and it is in this sense that $n_k(t)$ are occupation numbers for the quasiparticle modes described by $\psi_1(x, t)$.

The restrictions which (4.2) and (4.3) place on the density operators is easily determined from (3.52) and (3.53), which relate the ξ operators to a_k^{L} and a_k^{R}, together with the mapping rules (3.7) and (3.8). Translating (4.2), we find

$$a_k\rho_1 = \mathrm{e}^{-\nu_1(k)}\rho_1 a_k \tag{4.5}$$

where

$$e^{-\gamma_1(k)} = \frac{n_{k0}}{b_{k0}^2(1+n_{k0})} \tag{4.6}$$

and the adjoint of the same equation. This implies that ρ_1 is of the form

$$\rho_1 = \mathcal{N}_1 \exp\left[-\int d^3k\, a_k^\dagger \gamma_1(k) a_k\right] \tag{4.7}$$

where $\mathcal{N}_1$ is a normalizing constant. Similarly, (4.3) implies

$$\rho_2 = \mathcal{N}_2 \exp\left[-\int d^3k\, a_k^\dagger \gamma_2(k) a_k\right] \tag{4.8}$$

with

$$e^{-\gamma_2(k)} = b_{k0}^2. \tag{4.9}$$

According to the discussion of section 2, the initial state of the system is specified by the density operator

$$\rho = \rho_1\rho_2 = \mathcal{N} \exp\left[-\int d^3k\, a_k^\dagger \gamma(k) a_k\right] \tag{4.10}$$

where $\mathcal{N} = \mathcal{N}_1\mathcal{N}_2$ and

$$e^{-\gamma(k)} = e^{-(\gamma_1(k)+\gamma_2(k))} = \frac{n_{k0}}{(1+n_{k0})} \tag{4.11}$$

and we see that this is independent of the arbitrary quantity b_{k0}. Thus, the physical expectation values generated by (2.1) should also be independent of b_{k0}, as is confirmed by calculations within thermo field dynamics [16]. Evidently, a special choice [16] of this quantity, namely

$$b_{k0} = \left(\frac{n_{k0}}{(1+n_{k0})}\right)^{(1-\alpha)/2} \tag{4.12}$$

gives $\rho_1 = \rho^\alpha$ and $\rho_2 = \rho^{1-\alpha}$.

In thermo field dynamics, the initial state will be specified by a choice of the initial occupation numbers n_{k0}. In particular, the choice

$$n_{k0} = \left[e^{\beta\omega_k} - 1\right]^{-1} \tag{4.13}$$

corresponding to the Bose–Einstein distribution for an ideal gas, implies

$$\rho = \mathcal{N} \exp\left[-\beta \int d^3k\, a_k^\dagger \omega_k a_k\right] \equiv \mathcal{N} e^{-\beta H_{ig}} \tag{4.14}$$

which is the equilibrium density operator for such a gas. Clearly, more general choices are possible, but we see that thermo field dynamics permits only Gaussian initial density operators. These correspond to the canonical ensemble for a gas of particles which do

not interact, but have an arbitrary dispersion relation, specified by $\gamma(k)$. This explains why, even in the non-equilibrium formalism, only two copies of the original quantum fields appear in thermo field dynamics, compared with the three copies which are required in the closed-time-path formalism [8]. In the latter formalism, the third copy, which inhabits the imaginary-time segment of the contour of figure 2, is required to describe the initial density operator. When this is Gaussian, the information it contains can be completely absorbed in the unperturbed real-time propagators. In the case of a system in thermal equilibrium, it makes sense to take the limits $t_i \to -\infty$ and $t_f \to +\infty$. In that case, the equilibrium state of the interacting system can be treated as growing adiabatically from that of a non-interacting system, represented by a Gaussian density operator. Then, as is well known [1,7], the two formalisms become equivalent.

Having specified the initial state, it is still necessary to construct a perturbation theory for the generating functional (3.23), starting from its unperturbed version (3.44). This generating functional may be expressed in the interaction picture as

$$\hat{Z}(\rho_1, \rho_2; j_1, j_2) = \langle\langle \rho_2 | \hat{S} T \exp\left[-\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t \left(\hat{H}_{\mathrm{int}}(\psi_{\mathrm{I}}(t), t) - \bar{J}(t)\psi_{\mathrm{I}}(t) - \bar{\psi}_{\mathrm{I}}(t)J(t)\right)\right] | \rho_1 \rangle\rangle \tag{4.15}$$

where

$$\hat{S} = \bar{T} \exp\left[\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t\ \hat{H}_{\mathrm{int}}(\psi_{\mathrm{I}}(t), t)\right]. \tag{4.16}$$

This expression does not lead directly to a perturbation expansion of the form used in vacuum field theory because one cannot appeal to the Gell-Mann–Low theorem and vacuum stability to eliminate $\hat{S}$. As emphasized by Evans *et al* [23], it is perfectly possible to evaluate (4.15) perturbatively as it stands, but the extra terms arising from $\hat{S}$ have to be included. We see that these extra terms correspond, in the closed-time-path formalism, to the extra real-time segments of the contour shown in figure 1 and, correspondingly, to the extra integration variables in (2.10). As explained above, the role of the imaginary-time segments and their integration variables is invisible in (4.15) because of the Gaussian nature of the density operators.

It turns out that these extra complications can be eliminated by making a special choice for the arbitrary function $b_k(t)$, namely

$$b_k(t) = 1. \tag{4.17}$$

In particular, this means that $b_{k0} = 1$, or to $\alpha = 1$ in (4.12), so that ρ_2 is the identity operator, and $\hat{Z}$ reduces to the form (2.2) associated with the contour of figure 2. With this choice of $b_k(t)$, it is not difficult to show [21,22] that both $\hat{H}_0$ and $\hat{H}_{\mathrm{int}}$ annihilate $\langle\langle \rho_2|$, provided that they are normal-ordered with respect to the ξ operators. Thus we have $\langle\langle \rho_2 | \hat{S} = \langle\langle \rho_2|$ and a perturbation series of the standard form can be developed.

We are now able to see that thermo field dynamics is completely equivalent to quantum statistical mechanics and, indeed, to the closed-time-path formalism, except that it deals only with those situations described by Gaussian initial density matrices. However, this equivalence exists at the level of the complete generating functional (2.3) or (3.23). The final point we wish to examine is whether the perturbation series constructed in thermo field dynamics is equivalent to an approximation scheme which can also be applied in the closed-time-path formalism, and this is discussed in the next section.

5. Dissipative perturbation theory

If a system is disturbed slightly from an equilibrium state, and subsequently left undisturbed, it will decay back towards equilibrium, provided that there are interactions which permit the necessary redistribution of energy. Consequently, the elementary excitations of the equilibrium state, or quasi-particles, may be expected to have decaying modes. For a system in a non-equilibrium state, the evolution of the state with time is governed by similar dissipative processes, and it is essential to have an approximation scheme which takes adequate account of these. Conventional perturbation theory, which takes a non-interacting system as its lowest-order approximation, is unable to do this, and this is a problem to which Hardman *et al* [16], following earlier authors [14, 15, 24–27], have rightly given close attention. (We do not subscribe to the qualitative explanation of dissipation offered by these authors, in terms of unobserved 'tilde particles' carrying negative energy, which seems to us to misinterpret the superoperator formalism, but we do not consider it worthwhile to quibble about words.)

In the 'semi-free' Hamiltonian (3.56) with (3.57), dissipative effects appear in the terms involving the quasi-particle decay widths $\kappa_k(t)$ and the time derivative of the occupation numbers $\dot{n}_k(t)$. We see that the matrix coefficients of these quantities have off-diagonal elements which couple ψ^1 and $\bar{\psi}^1$ with ψ^2 and $\bar{\psi}^2$. Now, any field theory defined initially in terms of quantum fields acting in a Hilbert space $\mathcal{H}$ will translate into a Liouville-space theory with a Hamiltonian of the form (3.26), where no such couplings appear. Consequently, the semi-free Hamiltonian does not correspond to any *bona fide* quantum field theory with a Hilbert space of states available to it. It must be emphasized, however, that the off-diagonal terms in $\hat{H}_0$ by no means constitute an arbitrary mutilation of the original theory. Their role is to mimic, in the unperturbed self-energy, the absorptive parts of higher-order contributions to the full self-energy, and a well conceived renormalization scheme, of the kind considered by the authors cited above, will ensure that they do so with reasonable fidelity.

It might seem, then, that thermo field dynamics is able to give a description of dissipative processes which is not available in other approaches to thermal field theory. This is not so, however. The present author has developed an approximation scheme within the closed-time-path formalism which achieves the same end [9, 17, 18], and we wish to show here that the two schemes are equivalent (except that the closed-time-path method encompasses more general initial states, as discussed above). Indeed, the path integral form of $\hat{Z}$ shown in (2.10) shares with the Hamiltonian (3.26) the feature that the total action contains no terms coupling the various sets of integration variables. However, the effective action (the Legendre transform of $-\mathrm{i}\ln\hat{Z}$) does contain such coupling terms, again arising from higher-order contributions to the self-energy, and an unperturbed action which mimics these can be used to develop a dissipative perturbation theory.

We use the mapping rules (3.5)–(3.8) to translate the unperturbed generating functional (3.44) into the form discussed in section 2. It will be convenient to work in the Schrödinger picture and, if the time-ordered operator in (3.44) is denoted by $\hat{\mathcal{J}}_0(j_1, j_2)$, we have

$$\hat{\mathcal{J}}_0 = U_0^{-1}(t_f)T\exp\left[-\mathrm{i}\int_{t_i}^{t_f}\mathrm{d}t\left(\hat{H}_0(\psi_S, t) - \tilde{J}(t)\psi_S - \bar{\psi}_S J(t)\right)\right] \tag{5.1}$$

where $U_0(t)$ was defined in (3.34). We consider only the case $b_k(t) = 1$, so that U_0^{-1} can be dropped from (5.1) and the last term of (3.57) vanishes. The density operator ρ_2 is now just the identity. According to (3.3), we have

$$\hat{Z}_0(\rho_1, \mathcal{I}; j_1, j_2) = \mathrm{Tr}\left[\mathcal{R}^\dagger(t_i, t_f)\rho_1\right] \tag{5.2}$$

where $\mathcal{R}(t_i, t_f)$ is defined by

$$\langle(\mathcal{R}(t_i, t_f)| = \langle(\mathcal{I}|T\exp\left[-\mathrm{i}\int_{t_i}^{t_f} \mathrm{d}t\left(\hat{H}_0(\psi_S, t) - \bar{J}(t)\psi_S - \bar{\psi}_S J(t)\right)\right]. \tag{5.3}$$

This operator is difficult to write down in terms of field operators, but we shall derive a path-integral representation for it. Define the kernel $\mathcal{R}(\psi_{1t}, \psi_{2t}, t, t_f)$ by

$$\mathcal{R}(t, t_f) = \int \mathcal{D}\psi_{1t}\,\mathcal{D}\psi_{2t}\;|\psi_{1t})\,\mathcal{R}(\psi_{1t}, \psi_{2t}, t, t_f)(\psi_{2t}|. \tag{5.4}$$

Then we have

$$\hat{Z}_0(\rho_1, \mathcal{I}; j_1, j_2) = \int \mathcal{D}\psi_1\,\mathcal{D}\psi_2\,\mathcal{R}^*(\psi_1, \psi_2, t_i, t_f)\langle\psi_2|\rho_1|\psi_1\rangle. \tag{5.5}$$

Now, using (3.35)–(3.38) in (3.56), we find

$$\hat{H}_0(\psi_S, t) = \int \mathrm{d}^3x\left[\psi_S^{L\dagger}H^{11}\psi_S^L + \psi_S^{L\dagger}H^{12}\psi_S^{R\dagger} - \psi_S^R H^{21}\psi_S^L - \psi_S^R H^{22}\psi_S^{R\dagger}\right]. \tag{5.6}$$

Strictly, this expression should be normal-ordered so that it annihilates $\langle(\mathcal{I}|$. However, since it is quadratic in the fields, normal ordering introduces only an additive constant, which can be taken into account by the normalization condition $\hat{Z}_0(\rho_1, \mathcal{I}; 0, 0) = 1$, and need not be considered explicitly.

The standard heuristic procedure can now be employed to derive the path-integral representation. In (5.3), operators at the latest times act first on $\langle(\mathcal{I}|$ and we build up $\mathcal{R}(t_i, t_f)$ by moving the earlier time backwards from t_f to t_i in infinitesimal steps Δt. At each step, $\mathcal{R}(t - \Delta t, t_f)$ involves operators acting on $\mathcal{R}(t, t_f)$ both from the left and from the right. Schematically, we have

$$\mathcal{R}(t - \Delta t, t_f) = \mathcal{R}(t, t_f) + \mathrm{i}\Delta t\left[H^{11*}\psi^\dagger\psi\mathcal{R}(t, t_f) + H^{12*}\psi\mathcal{R}(t, t_f)\psi^\dagger + \cdots\right]. \tag{5.7}$$

Thus, we build the kernel $\mathcal{R}(\psi_{1t-\Delta t}, \psi_{2t-\Delta t}, t - \Delta t, t_f)$ by acting on the left and right of (5.7) with two copies of the identity operator (2.9) and estimating the resulting matrix elements in the usual way. The result we obtain is

$$\mathcal{R}^*(\psi_1, \psi_2, t_i, t_f) = \int \mathcal{D}\psi_1(t)\,\mathcal{D}\psi_1^*(t)\,\mathcal{D}\psi_2(t)\,\mathcal{D}\psi_2^*(t)\,\mathrm{e}^{\mathrm{i}S_0(\psi, j)} \tag{5.8}$$

where

$$S_0(\psi, j) = \int_{t_i}^{t_f}\mathrm{d}t\int \mathrm{d}^3x\left[\mathrm{i}\psi_1^*\frac{\mathrm{d}\psi_1}{\mathrm{d}t} - \mathrm{i}\psi_2^*\frac{\mathrm{d}\psi_2}{\mathrm{d}t} - \psi_1^*H^{11}\psi_1 - \psi_1^*H^{12}\psi_2\right.$$
$$\left. + \psi_2^*H^{21}\psi_1 + \psi_2^*H^{22}\psi_2 + j_1\cdot\psi_1 + j_2\cdot\psi_2\right]. \tag{5.9}$$

The complete path-integral form of $\hat{Z}_0(\rho_1, \mathcal{I}; j_1, j_2)$ is obtained by constructing the path-integral representation of $\langle\psi_2|\rho_1|\psi_1\rangle$ in (5.5). This adds to $\mathrm{i}S_0$ a term of the form $-S_E(\psi_3)$, where S_E is the Euclidean action associated with ρ_1. We described in [9, 17, 18] how an analogous unperturbed action may be constructed within the closed-time-path formalism for a relativistic scalar field (known as a 'type 2' field in the thermo field dynamics literature). For the non-relativistic theory considered by Hardman *et al*, we have checked that the same construction leads to a real-time action of exactly the form of (5.9), with $H^{\mu\nu}$ given by (3.57), but we shall not reproduce the details here.

It is not hard to see what would have happened if we had not made the choice $b_k(t) = 1$. The non-trivial density operator ρ_2 and the factor U_0^{-1} in (5.1) would have led to an extra component in $\mathcal{R}$ corresponding to the contour segments labelled by ρ_2, U^{-1} and U in figure 1. If $b_k(0) = 1$, then the length of the ρ_2 segment would be zero, but the contributions from U and U^{-1} cancel only if $b_k(t) = 1$ at later times also.

6. Discussion

It frequently appears from the literature that thermo field dynamics is thought by its proponents to offer a more general description of thermal phenomena than quantum statistical mechanics, although categorical assertions to this effect are hard to find. Certainly, Evans *et al* [23] claim that thermo field dynamics is more general than the closed-time-path formalism, to the extent that it involves the arbitrary function $b_k(t)$ or, more restrictively, the parameter α introduced in (4.12), while Henning and Umezawa [28] suggest that the closed-time-path method is unsuited to the analysis of non-equilibrium phenomena.

In this work, we have used the superoperator formalism to provide a detailed translation between thermo field dynamics and statistical mechanics, and this shows that in fact the reverse is true. In fact, every feature of thermo field dynamics can be expressed in closed-time-path terms. Contrary to the assertion of Evans *et al*, that the α degree of freedom exists in the closed-time-path formalism only when it is applied to equilibrium situations, we have shown that it and, indeed, the more general freedom represented by $b_k(t)$, correspond quite generally to contours of the kind shown in figure 1. This, however, is a trivial detail. By and large, it is agreed on all sides that Green functions associated with fields of index 1 contain all the physical information, while fields of index 2 (or greater) have a direct physical interpretation only when they are associated with the contour of figure 2. (Somewhat exceptionally, Umezawa [29] has speculated that it might be possible to detect 'thermal quanta' associated with the tilde fields of thermo field dynamics which, presumably, would be different from normal physical particles. Such speculations seem to the present author to be quite misguided.) This being so, the freedom to choose different time paths, or different functions $b_k(t)$ is a purely mathematical one. Except in thermal equilibrium, indeed, any choice other than the contour of figure 2 ($b_k(t) = 1$) leads to unnecessary mathematical complications, so the generality is neither physically meaningful nor mathematically advantageous.

Actually, there is a second choice of b_k, corresponding to $\alpha = 0$ in (4.12) which, as discussed by Evans *et al* [23], has the same advantages as $b_k = 1$ when the Schrödinger and Heisenberg pictures are taken to coincide at t_f rather than at t_i as we have done. This choice corresponds to the time-reversed version of figure 2, with the imaginary-time segment at t_f. The point here is that the density operators are time-independent functions of the Schrödinger-picture field operators. Thus, in the time-reversed situation, one specifies what the state of the system will be at the time t_f, which is later than all the other times of interest. While this anti-causal procedure is possible mathematically, it would seem to have limited physical applications and, as remarked by Evans *et al*, has received little attention.

A much more important conclusion of this work is that thermo field dynamics deals only with thermal states which are initially described by Gaussian density matrices. In thermal equilibrium, this is of no importance, since the equilibrium state of an interacting system can be represented as growing adiabatically from that of a non-interacting system in the remote past. In non-equilibrium situations, however, this is a highly restrictive feature of thermo field dynamics, since one generally wants to study the evolution of the system at times shortly after the initial state was set up. In particular, several authors have suggested that thermo field dynamics is particularly suitable for studying the early universe [16, 21, 27, 30]. We disagree with this view, on the grounds that the early universe possesses no remote past! In the closed-time-path formalism, by contrast, the class of initial density matrices is restricted in principle only by considerations such as renormalizability. In practice, though, it is probably difficult to deal with initial states which differ greatly from an equilibrium state.

Quite probably, the postulates of thermo field dynamics could be modified to accommodate more general states, for example, by translating the density operator into a superoperator. This would presumably entail promoting the thermal doublet to a thermal triplet of fields, in precise analogy to those of the closed-time-path formalism. Alternatively, one might allow the ξ operators (3.52), (3.53) to become nonlinear functions of the original fields. The nonlinearity would, presumably, have to be treated perturbatively, leading to extra terms in the perturbation series, which must reproduce the corresponding terms obtained in the closed-time-path method. Indeed, we see no point in pursuing these possibilities, since the resulting theory would necessarily be equivalent to the path-integral formalism which already exists. Moreover, it is apparently difficult to construct a non-equilibrium theory of relativistic ('type 2') fields within thermo field dynamics, except in the case of stationary states [16, 23], whereas this presents no difficulty of principle in the closed-time-path approach [8, 9, 17, 18].

Finally, we remark that there is a mathematical sense in which both thermo field dynamics and the closed-time-path formalism are more general than quantum statistical mechanics. Thus, in both approaches, it seems fairly natural to consider expressions of the form $\mathrm{Tr}\left[\rho_1 A_1(t_1)\cdots A_n(t_n)\rho_2 A_{n+1}(t_{n+1})\cdots A_N(t_N)\right]$, whereas quantum statistical mechanics assigns physical meaning only to expectation values of the form $\mathrm{Tr}\left[\rho A_1(t_1)\cdots A_N(t_N)\right]$. Indeed, an indefinite multiplicity of density operators might be considered in terms of closed-time-paths, though not, in any natural way, in thermo field dynamics. There is some temptation to speculate on a generalization of quantum theory in which these more general 'expectation values' would acquire a physical significance. In such a theory, the right- and left-handed superoperators might have independent physical meanings, rather than merely giving a redundant representation of the single set of original operators. There are hints of such speculation both in the work of Crawford [11] and in the thermo field dynamics literature, but we know of no physical motivation for them.

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