Prog. Theor. Phys. Vol. 70, No. 2, August 1983, Progress Letters

Thermo Field Dynamics in Interaction Representation

H. MATSUMOTO, Y. NAKANO, H. UMEZAWA, F. MANCINI* and M. MARINARO*

Department of Physics, University of Alberta, Edmonton, Alberta, Canada

**Instituto di Physica, Universite di Salerno, Salerno, Italy*

(Received April 18, 1983)

The relation between quantum field theory at finite temperature (thermo field dynamics) and a real time formulation in Matsubara's method is studied by comparing with the perturbation rules.

Thermo field dynamics was developed in Refs. 1)~3) as a field theory at finite temperature. It provides a straightforward method for the calculation of dynamical quantities. There, all of the machinery of the usual quantum field theory can be utilized. In particular, all of the operator techniques can be generalized to finite temperature and the causal time-ordered formulation of perturbation theory, the Feynman diagram method, is applicable with a real-time coordinate. Recently, it was shown that thermo field dynamics is equivalent to the so-called axiomatic statistical mechanics.[4)] It may also prove suitable in the study of gauge theories at finite temperature.[4),5)]

On the other hand, Matsubara's Green function method[6)] is commonly used for finite temperature calculation, especially for the calculation of static quantities. In this method, since the time variable is imaginary and restricted to a finite interval, the application of the Matsubara method to the calculation of dynamical quantities (i.e., frequency dependent amplitudes) ofen requires discrete frequency summations and a tedious process of analytical continuation. This paper aims at clarifying the relation between the field theoretical formulations (such as thermo field dynamics) and the Matsubara method.

In order to investigate the relationship, we use perturbation theory. A real-time extension of the perturbational rules in Matsubara's method has been obtained by the use of *the ordered products* along a path in complex time.[7)] From such rules, we construct a quantum field theory whose perturbational rules are expressed in terms of the *time ordered products*. A different choice of the path leads to a different quantum field theory at finite temperature. It will be shown that all of those theories lead to the same physical answer for equilibrium systems. The simplest one (the one with hermitian Hamiltonian consisting of the smallest number of fields) turns out to be the formalism of thermo field dynamics developed in Refs. 1)~3).

For simplicity, we consider a scalar field $\psi(\boldsymbol{x}, t)$, whose dynamics is determined by a Hamiltonian H. Since the space coordinates are irrelevant in the following argument, we retain only the time coordinate. The Heisenberg field with a complex time z is defined by

$$\psi(z)=\exp\{izH\}\psi(0)\exp\{-izH\}. \tag{1}$$

Consider a path C starting from a point τ and ending at $\tau-i\beta$ in the complex time plane. Assuming that $z_1, \cdots, z_n$ are on C, we define a statistical average of the path-ordering Heisenberg operator on C by

$$G(z_1, \cdots, z_n) =\mathrm{tr}[e^{-\beta H}T_c\psi(z_1)\cdots\psi(z_n)]/\,\mathrm{tr}[e^{-\beta H}], \tag{2}$$

where T_c is the path ordering operator and $\beta=1/k_BT$.

By separating H into an unperturbative part H_0 and an interaction part H_I, we can express (2) in the interaction representation as[7)]

$$G(z_1, \cdots, z_n) =\frac{\langle T_cU(\tau-i\beta, \tau)\varphi(z_1)\cdots\varphi(z_n)\rangle_0}{\langle T_cU(\tau-i\beta, \tau)\rangle_0}, \tag{3}$$

where $\varphi(z)$ is the free field whose Hamiltonian is H_0 and

$$U(\tau-i\beta, \tau)=\exp\left\{-i\int_\tau^{\tau-i\beta} dzH_I(z)\right\} \tag{4}$$

with the integration along the path C. Here $H_I(z)$ is the interaction Hamiltonian; $H_I(z)=e^{iH_0z}H_Ie^{-iH_0z}$. The symbol $\langle A\rangle_0$ means $\langle A\rangle_0\equiv\mathrm{tr}[e^{-\beta H_0}A]/\,\mathrm{tr}[e^{-\beta H_0}]$. Note that expression (3) is independent of τ because of the trace property and that the path C must be chosen with a monotonically decreasing imaginary part[7)] to ensure the simultaneous analyticity in $z_1, \cdots, z_n$.

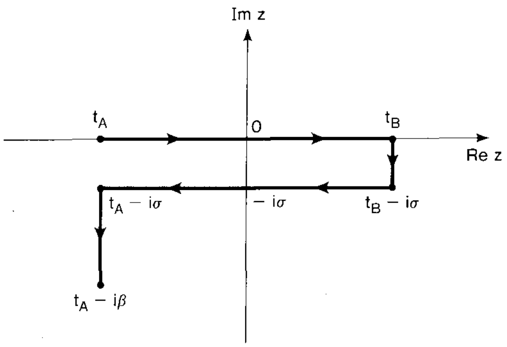

Fig. 1. The path C in the complex time plane.

When path C is chosen along the imaginary axis (and therefore $z_1, \cdots, z_n$ are also pure imaginary), (3) gives the perturbation formula in Matsubara's Green function method. In this sense (3) is considered as a generalization of the Matsubara formalism.

When we want to calculate the quantity in (3), with $\{z_1, \cdots, z_n\}$ being equal to a real-time set $\{t_1, \cdots, t_n\}$, the path C should contain a section of real axis which covers the set $\{t_1, \cdots, t_n\}$. One of the simplest paths is depicted in Fig. 1, in which the absolute values of t_A and t_B are sufficiently large ($t_A < t_1, \cdots, t_n < t_B$) and $0 < \sigma \leq \beta$. We might be tempted to assume that we can derive the Matsubara frequency method by making σ infinitesimally small. However, this is not the case since the contribution of the real-time axis is not eliminated even when σ is infinitesimal, while the Matsubara frequency method uses the imaginary path only.

We now consider the limits $t_A \to -\infty$, $t_B \to \infty$. In this limit the effect of the interaction Hamiltonian on the vertical portions of the contour C is disconnected from the fields $\varphi(t_1)\cdots\varphi(t_n)$ in (3). Then we get the following formula for the statistical average of the T_c-product:

$$G(t_1, \cdots, t_n) = \langle T_c \hat{U} \varphi(t_1) \cdots \varphi(t_n) \rangle_0 / \langle T_c U \rangle_0 \quad (5)$$

with

$$\hat{U} = \exp\left\{ -i \int_{-\infty}^{+\infty} dt [H_I(t) - H_I(t - i\sigma)] \right\}. \quad (6)$$

The perturbative expansion is obtained from (5), once the two-point functions are specified.

For simplicity, let us assume that the field is complex and the free Hamiltonian H_0 is given by

$$H_0 = \int d^3x \varphi^\dagger(x) \omega(i\nabla) \varphi(x). \quad (7)$$

Expanding $\varphi(x)$ as $\varphi(x) \equiv (2\pi)^{-3/2} \int d^3k a(\boldsymbol{k}) \exp\{i(\boldsymbol{k}\cdot\boldsymbol{x} - i\omega(\boldsymbol{k})t)\}$ and using the canonical commutation relation $[a(\boldsymbol{k}), a^\dagger(\boldsymbol{l})] = \delta(\boldsymbol{k} - \boldsymbol{l})$, we can obtain the two-point functions by calculating the thermal trace. We obtain the four types of two-point function which are summarized by the following 2×2 matrix formula:

$$\left\langle T_c \begin{pmatrix} \varphi(\boldsymbol{x}, t) \\ \varphi(\boldsymbol{x}, t - i\sigma) \end{pmatrix} (\varphi^\dagger(\boldsymbol{x}', t'), \varphi^\dagger(\boldsymbol{x}, t' - i\sigma)) \right\rangle_0 = \frac{i}{(2\pi)^4} \int d^4k e^{-ik(x-x')} \left\{ \frac{1}{k_0 - \omega(\boldsymbol{k}) + i\varepsilon} \frac{1}{e^{\beta\omega(\boldsymbol{k})} - 1} \right.$$
$$\left. \times \begin{pmatrix} e^{\beta\omega(\boldsymbol{k})} & e^{(\beta/2+\gamma)\omega(\boldsymbol{k})} \\ e^{(\beta/2-\gamma)\omega(\boldsymbol{k})} & 1 \end{pmatrix} - \frac{1}{k_0 - \omega(\boldsymbol{k}) - i\varepsilon} \frac{1}{e^{\beta\omega(\boldsymbol{k})} - 1} \begin{pmatrix} 1 & e^{(\beta/2+\gamma)\omega(\boldsymbol{k})} \\ e^{(\beta/2-\gamma)\omega(\boldsymbol{k})} & e^{\beta\omega(\boldsymbol{k})} \end{pmatrix} \right\}, \quad (8)$$

where $\gamma = \sigma - \beta/2 \,(-\beta/2 \leq \gamma < \beta/2)$. This two-point function reduces to the two-point function in thermo field dynamics[2),3)] when we choose $\gamma = 0$ (i.e. $\sigma = \beta/2$). The choice $\gamma = 0_+ - \beta/2$ (i.e. $\sigma = 0_+$) corresponds to the case in Ref. 7).

The same perturbative expansions can be obtained from the following quantum field theoretical formulation, which will be called thermo field dynamics. (As will be shown later, the formulation in Refs. 1)~3) is a particular case of this.) To show this, we introduce *two mutually commuting fields* $\phi(x, \gamma)$ and $\tilde{\phi}(x, \gamma)$ which satisfy the usual equal time commutation relations $[\phi(x, \gamma), \phi^\dagger(y, \gamma)] = \delta(\boldsymbol{x} - \boldsymbol{y})$, $[\tilde{\phi}(x, \gamma), \tilde{\phi}(y, \gamma)] = \delta(\boldsymbol{x} - \boldsymbol{y})$ and we make the following correspondence:

$$\varphi(t) \to \phi(t, \gamma), \quad \varphi^\dagger(t) \to \phi^\dagger(t, \gamma),$$
$$\varphi(t - i\sigma) \to \tilde{\phi}^\dagger(t, \gamma), \quad \varphi^\dagger(t - i\sigma) \to \tilde{\phi}(t, \gamma). \quad (9)$$

We require that the statistical averages are given by the vacuum expectation values. The temperature dependent vacuum $|0(\beta)\rangle$ is introduced and creation and annihilation operators of physical particles are denoted by $a_\beta{}^\dagger(\boldsymbol{k})$,

$\tilde{a}_\beta{}^\dagger(\boldsymbol{k})$ and $a_\beta(\boldsymbol{k})$, $\tilde{a}_\beta(\boldsymbol{k})$: $a_\beta(\boldsymbol{k})|0(\beta)\rangle = \tilde{a}_\beta(\boldsymbol{k})|0(\beta)\rangle = 0$. In terms of those physical operators, the Fourier components $a(\boldsymbol{k},\gamma)$ defined by $\phi(x,\gamma)=(2\pi)^{-3/2}\int d^3k a(\boldsymbol{k},\gamma)\times\exp\{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega(\boldsymbol{k})t)\}$ etc. are given by

$$a(\boldsymbol{k},\gamma)=e^{\gamma\omega(\boldsymbol{k})/2}a(\boldsymbol{k}),$$
$$a^\dagger(\boldsymbol{k},\gamma)=e^{-\gamma\omega(\boldsymbol{k})/2}a^\dagger(\boldsymbol{k}),$$
$$\tilde{a}(\boldsymbol{k},\gamma)=e^{\gamma\omega(\boldsymbol{k})/2}\tilde{a}(\boldsymbol{k}),$$
$$\tilde{a}^\dagger(\boldsymbol{k},\gamma)=e^{-\gamma\omega(\boldsymbol{k})/2}\tilde{a}^\dagger(\boldsymbol{k}), \tag{10}$$

where $a(\boldsymbol{k})$ and $\tilde{a}^\dagger(\boldsymbol{k})$ are defined by

$$\begin{pmatrix}a(\boldsymbol{k})\\ \tilde{a}^\dagger(\boldsymbol{k})\end{pmatrix}=\begin{pmatrix}\cosh\theta(\boldsymbol{k}), & \sinh\theta(\boldsymbol{k})\\ \sinh\theta(\boldsymbol{k}), & \cosh\theta(\boldsymbol{k})\end{pmatrix}\begin{pmatrix}a_\beta(\boldsymbol{k})\\ \tilde{a}_\beta{}^\dagger(\boldsymbol{k})\end{pmatrix}. \tag{11}$$

Here $\sinh^2\theta(\boldsymbol{k})=(e^{\beta\omega(\boldsymbol{k})}-1)^{-1}$, $\cosh^2\theta(\boldsymbol{k})=(1-e^{-\beta\omega(\boldsymbol{k})})^{-1}$. Note that $a(\boldsymbol{k})$ and $a^\dagger(\boldsymbol{k})$ ($\tilde{a}(\boldsymbol{k})$ and $\tilde{a}^\dagger(\boldsymbol{k})$) are hermitian conjugate to each other, but $a(\boldsymbol{k},\gamma)$ and $a^\dagger(\boldsymbol{k},\gamma)$ are not (unless $\gamma=0$). Now it is easy to show that the left-hand side of Eq. (8) becomes

$$\langle 0(\beta)|T\begin{pmatrix}\phi(\boldsymbol{x},t,\gamma)\\ \tilde{\phi}^\dagger(\boldsymbol{x},t,\gamma)\end{pmatrix}(\phi^\dagger(\boldsymbol{x}',t',\gamma),\ \tilde{\phi}(\boldsymbol{x}',t',\gamma))|0(\beta)\rangle, \tag{12}$$

where T is the *time ordered* product. It should be noted that the original $\varphi(t)$ and $\varphi^\dagger(t-i\sigma)$ do not commute with each other. After correspondence (9) is made with the commuting $\phi(t,\gamma)$ and $\tilde{\phi}(t,\gamma)$, the T_c-product (the path-ordered product) is rewritten in terms of the T-product (the time-ordered product).

The interaction Hamiltonian is given by $H_I=\int d^3x\,\mathcal{H}_I(\varphi^\dagger(x),\varphi(x))$. Thus $\mathcal{H}_I(\varphi^\dagger(\boldsymbol{x},t),\varphi(\boldsymbol{x},t))$ is $\mathcal{H}_I(\phi^\dagger(\boldsymbol{x},t,\gamma),\phi(\boldsymbol{x},t,\gamma))$, while $\mathcal{H}_I(\varphi^\dagger(\boldsymbol{x},t-i\sigma),\varphi(\boldsymbol{x},t-i\sigma))$ is $\mathcal{H}_I(\tilde{\phi}(\boldsymbol{x},t,\gamma),\tilde{\phi}^\dagger(\boldsymbol{x},t,\gamma))$. Because of the hermiticity of $\mathcal{H}((\varphi^\dagger,\varphi)$, the operator relation $\mathcal{H}_I{}^*(\varphi,\varphi^\dagger)=\mathcal{H}_I(\varphi^\dagger,\varphi)$ is satisfied, where the symbol * indicates the complex conjugate for c-numbers in $\mathcal{H}_I$. Then we have

$$H_I(t)\to H_I(t,\gamma)\equiv\int d^3x\,\mathcal{H}_I(\phi^\dagger(x,\gamma),\phi(x,\gamma)), \tag{13a}$$

$$H_I(t-i\sigma)\to\widetilde{H_I(t,\gamma)}\equiv\int d^3x\,\mathcal{H}_I{}^*(\tilde{\phi}^\dagger(x,\gamma),\tilde{\phi}(x,\gamma)). \tag{13b}$$

(For fermion fields, a careful treatment of operator ordering is required.) Note that relations (10), (11) and (13) are consistent with rules of tilde operation.[1)~4)] In summary we have

$$\langle T_cU\varphi(x_1)\cdots\varphi(x_n)\rangle_0/\langle T_cU\rangle_0=\frac{\langle 0(\beta)|TS(\gamma)\phi(x_1,\gamma)\cdots\phi(x_n,\gamma)|0(\beta)\rangle}{\langle 0(\beta)|TS(\gamma)|0(\beta)\rangle}, \tag{14}$$

where $S(\gamma)=\exp\{-i\int dt\hat{H}_I(t,\gamma)\}$ with $\hat{H}_I=H_I(t,\gamma)-\tilde{H}_I(t,\gamma)$.

When $\phi(x)=(2\pi)^{-3/2}\int d^3k a(\boldsymbol{k})\exp\{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega(\boldsymbol{k})t)\}$ is introduced, we have from (10)

$$\phi(x,\gamma)=\eta_\gamma\phi(x)\eta_\gamma{}^{-1},\quad \phi^\dagger(x,\gamma)=\eta_\gamma\phi^\dagger(x)\eta_\gamma{}^{-1}, \tag{15}$$

where $\eta_\gamma=e^{-\gamma H_0/2}$ with $H_0=\int d^3k\omega(\boldsymbol{k})a^\dagger(\boldsymbol{k})a(\boldsymbol{k})$. A similar relation holds for the tilde operators. When $\gamma\neq 0$, because of the presence of the metric operators η_γ, $\phi^\dagger(x,\gamma)$ is not the hermitian conjugate of $\phi(x,\gamma)$, although $\phi^\dagger(x)$ is the hermitian conjugate of $\phi(x)$. Indeed, we have, for the hermitian conjugate of $\phi(x,\gamma)$, $\{\phi(x,\gamma)\}_{\text{h.c.}}=\eta_\gamma{}^{-2}\phi^\dagger(x,\gamma)\eta_\gamma{}^2$. Therefore, $H_I(t,\gamma)$ is not self-adjoint unless $\gamma=0$. The case $\gamma=0$ is of particular significance; in this case, since $\eta_\gamma=\tilde{\eta}_\gamma=1$, the dagger operation reduces to hermitian conjugation and $\hat{H}_I$ becomes self-adjoint. This is the formalism of thermo field dynamics given in Refs. 1)~4).

The observable quantities are given by the vacuum expectation value of certain *non-tilde* operators. We now show that the vacuum expectation values of non-tilde operators in the perturbation theory given by (14) are independent of γ. At first glance, this γ-independence is not obvious in the *field theoretical formulation* because in the latter formulation, the concept of the complex path (and, therefore, deformation of the path) is lost. The γ-dependence appears only through the presence of the two-point functions consisting of a tilde and a non-tilde field; $\langle T\phi\tilde{\phi}\rangle$ contains $e^{\gamma\omega(\boldsymbol{k})}$ while $\langle T\tilde{\phi}^\dagger\phi^\dagger\rangle$ contains $e^{-\gamma\omega(\boldsymbol{k})}$. These two-point functions will be referred to as "cross propagators". The fact that the interaction Hamiltonian $\hat{H}_I$ contains both H_I and $\tilde{H}_I$ means that the typical diagrammatic contribution to a multipoint Green function will contain two types of vertices. One corresponding to the H_I term and the other corresponding to the $\tilde{H}_I$ term. We can thus subdivide any diagram into several subdiagrams consisting of sets of all the connected vertices of only one particular type. Obviously such subdiagrams will not contain any cross propagators and are thus independent of the parameter γ. The γ-dependence therefore arises from the lines joining the various subdiagrams to each other or to the external lines. In other words the γ-dependence can be attributed to the *cross propagator lines* attached to each subdiagram consisting of only those vertices arising from the $\tilde{H}_I$ term in $\hat{H}_I$. (We will refer to those subdiagrams as $\tilde{H}_I$ subdiagrams.) These terms will give rise to a factor $\exp\{\gamma[\sum_i\omega_i-\sum_j\omega_j]\}$ for each $\tilde{H}_I$-subdiagram, the positive signs and negative signs arising from $\langle T\phi\tilde{\phi}\rangle$ and the $\langle T\tilde{\phi}^\dagger\phi^\dagger\rangle$ terms respectively. Since all the four-momenta of the cross propagators are on-shell, as is seen in (8), the energy conservation law for the $\tilde{H}_I$-subdiagram requires that those factors are equal to the identity, implying the γ-independence.

The present analysis demonstrates the presence of a variety of the quantum field theories at finite temperature. Even when we restrict ourselves to the choice of the path illustrated in Fig. 1, the variety is exhibited by the parameter γ. (This is consistent with the result of Ref. 8) in which the construction of $|0(\beta)\rangle\rangle$ in Ref. 1) was extended.) The field on the returning path in the path ordering formalism becomes the tilde field in the field theoretical formulation, which results in the doubling of the number of degrees of freedom and the tilde operation rules. Only for the special case ($\gamma=0$), the hermiticity of interaction Hamiltonian density is preserved; this is the formalism of thermo field dynamics discussed in 1)~4). The physical equivalence among quantum field theoretical formulations, (i.e., γ-independence) is based on the energy conservation which holds separately for the tilde and non-tilde fields. It is therefore extremely interesting to see how the present theory should be modified when there exists an energy flow to/from the thermal bath as in the case of an *inequilibrium* phenomena. Our study in this direction is in progress.

1) Y. Takahashi and H. Umezawa, Collect. Phen. **2** (1975), 55.
A preliminary form of the thermo field dynamics was presented in F. Mancini, L. Leplae and H. Umezawa, Phys. Rep. **10C** (1974), 151.
2) H. Matsumoto, Fortschr. Phys. **25** (1977), 1.
3) Elaborate presentation of the thermo field dynamics and many applications are found in H. Umezawa, H. Matsumoto and M. Tachiki, *Thermo Field Dynamics and Condensed States* (North-Holland, Amsterdam-New York-Oxford, 1982).
4) I. Ojima, Ann. of Phys. **137** (1981), 1.
5) H. Matsumoto, Y. Nakano and H. Umezawa, Preprint, University of Alberta, 1983.
6) T. Matsubara, Prog. Theor. Phys. **14** (1955), 351.
A. A. Abrikosov, L. Gor'kov and I. Dyzaloshinski, *Method of Quantum Field Theory in Statistical Physics* (Pergamon, Oxford, 1965).
D. A. Kirzhnits, *Field Theoretical Methods in Many Body Systems* (Pergamon, Oxford, 1965).
7) R. A. Craig, J. Math. Phys. **9** (1968), 605.
L. V. Keldysh, Zh. Eksp. Theor. Fiz. **47** (1964), 1515 [Sov. Phys. -JETP **20** (1965), 1018].
R. Mills, *Propagators for Many-Particle Systems* (Gordon and Breach Science Publishers, N. Y., 1965).
8) M. Schmutz, Z. Phys. **B30** (1978), 97.