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Free energy in thermo field dynamics

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A formula to obtain the free energy within the framework of thermo field dynamics (a real-time quantum field theory at finite temperature) is presented. The relation to the Matsubara method is discussed. Examples of a perturbation calculation are presented for the ϕ^4 model up to the two-loop order and are compared with the corresponding result obtained in the Matsubara formalism.

Recently, the relation between the thermo field dynamics (TFD),[1] a real-time quantum field theory at finite temperature, and the real-time path-ordered formulation of the statistical average has been extensively discussed and their equivalence has been examined with the context of perturbation theory.[2] However, since the free energy is not a thermal average, its calculation in TFD has not been formulated. Nevertheless, it was found in Ref. 3 that a summation over certain vacuum diagrams in TFD reproduces the familiar result for the free energy.

In this short paper, we present a formula for a systematic calculation of the free energy in the framework of TFD and show that the prescription taken in Ref. 3 is the right one. The relation between the result obtained in TFD and that obtained by means of the path-ordered formalism will be clarified.

Let us consider the following Hamiltonian:

$$H(s)=H_0+sH_I \ , \tag{1}$$

where s is a c-number parameter and $s=1$ leads to the Hamiltonian H under consideration. In the interaction representation, H_0 is the unperturbed Hamiltonian and H_I the interaction Hamiltonian. Corresponding to $H(s)$, the free energy $F(s)$ is given by

$$F(s)=-\beta^{-1}\ln \mathrm{tr}\{\exp[-\beta H(s)]\} \ , \tag{2}$$

where $\beta=1/(k_BT)$, with k_B being the Boltzmann constant and T the temperature. Since

$$dF(s)/ds=\mathrm{tr}(e^{-\beta H(s)}H_I)/\mathrm{tr}(e^{-\beta H(s)}) \ ,$$

we have, in TFD,

$$dF(s)/ds=\langle 0(\beta,s)|H_I|0(\beta,s)\rangle \ , \tag{3}$$

where $|0(\beta,s)\rangle$ is the thermal vacuum of TFD associated with the Hamiltonian $H(s)$. Equation (3) means that the change of the free energy induced by a small change in the strength of the interaction is proportional to the interaction energy. Integrating (3), we have

$$F\equiv F(1)=F(0)+\int_0^1 ds\,\langle 0(\beta,s)|H_I|0(\beta,s)\rangle \ . \tag{4}$$

In the interaction representation, (4) is given by

$$F=F(0)+\int_0^1 ds\left\langle 0,\beta\left|TH_I(t_0)\exp\left[-i\int_{-\infty}^{\infty}dt\,s\hat{H}_I(t)\right]\right|0,\beta\right\rangle \ , \tag{5}$$

where $|0,\beta\rangle$ is the thermal vacuum in the interaction representation with respect to H_0 and t_0 is some arbitrary time. The thermal interaction Hamiltonian $\hat{H}_I(t)$ is given by $\hat{H}_I(t)=H_I(t)-\tilde{H}_I(t)$, where $H_I(t)$ consists only of the first component of thermal doublet fields while $\tilde{H}_I(t)$ consists only of the second.

In Ref. 3 the free energy was calculated by means of a prescription such that one of the interaction vertices should be fixed to H_I. This prescription is now justified by the appearance of $H_I(t_0)$ in (5) as well as combinatorial factors which arise from the integration over s.

We can also see the relation between the formula given in (5) and one obtained by means of the path-ordered formalism as follows. The formula in the path ordered form may be rewritten as

$$\begin{aligned}F&=F(0)-\beta^{-1}\left\langle T_C\exp\left[-i\int_{\tau_0}^{\tau_0-i\beta}dzH_I(z)\right]-1\right\rangle_{\mathrm{con}}\\&=F(0)-\beta^{-1}\int_0^1 ds\frac{d}{ds}\left\langle T_C\exp\left[-is\int_{\tau_0}^{\tau_0-i\beta}dzH_I(z)\right]-1\right\rangle_{\mathrm{con}}\\&=F(0)-\beta^{-1}\int_0^1 ds(-i)\int_{\tau_0}^{\tau_0-i\beta}dz'\left\langle T_CH_I(z')\exp\left[-is\int_{\tau_0}^{\tau_0-i\beta}dzH_I(z)\right]\right\rangle_{\mathrm{con}} \ ,\end{aligned} \tag{6}$$

where $\langle\cdots\rangle_{\mathrm{con}}$ indicates the connected part of diagrams for the thermal average, T_C the path-ordering operator along a path C, and τ_0 an arbitrary complex number. Note that

$$\left\langle T_CH_I(z')\exp\left[-is\int_{\tau_0}^{\tau_0-i\beta}dzH_I(z)\right]\right\rangle_{\mathrm{con}}$$

is independent of z' as long as z' lies on the path C. Then by performing the integration over z' in (6), we have

$$F=F(0)+\int_0^1 ds\left\langle T_C H_I(z_0)\exp\left(-is\int_{\tau_0}^{\tau_0-i\beta}dz\,H_I(z)\right)\right\rangle_{\text{con}} , \tag{7}$$

where z_0 is an arbitrary complex time on the path C. In the Matsubara method, the path C is chosen to lie along the imaginary axis in the complex time plane. In the present case, let us choose the path shown in Fig. 1

$$(\tau_0\rightarrow \mathrm{Re}\tau_0\rightarrow \tau_1\rightarrow \tau_1-i\beta/2\rightarrow \mathrm{Re}\tau_0-i\beta/2\rightarrow \tau_0-i\beta) ,$$

in which $\mathrm{Re}\tau_0\rightarrow -\infty$ and $\tau_1\rightarrow +\infty$, and take $z_0=t_0$ (real). With the usual prescription[2] by which we obtain the correspondence with TFD, (7) in the path-orderd formalism becomes (5) in TFD. [Note that the expression (5) automatically excludes diagrams disconnected from $H_I(t_0)$.]

As an example, we consider a system described by the Lagrangian density

$$\mathscr{L}=\tfrac{1}{2}\partial_\mu\phi\partial^\mu\phi-\tfrac{1}{2}m^2\phi^2-\frac{\lambda}{4!}\phi^4 . \tag{8}$$

Introducing the thermal expectation value v,

$$v=\langle 0(\beta,1)|\phi(x)|0(\beta,1)\rangle , \tag{9}$$

we rewrite (8) in terms of $\rho(x)=\phi(x)-v$:

$$\mathscr{L}=\tfrac{1}{2}\partial_\mu\rho\partial^\mu\rho-\frac{1}{2}\left(m^2+\frac{\lambda v^2}{2}\right)\rho^2-\frac{\lambda v}{3!}\rho^3-\frac{\lambda}{4!}\rho^4 -\left(mv+\frac{\lambda v^3}{3!}\right)\rho-\tfrac{1}{2}m^2v^2-\frac{\lambda}{4!}v^4 . \tag{10}$$

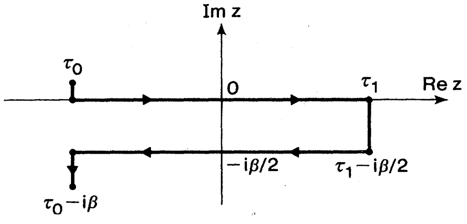

FIG. 1. The path C in the complex time plane, corresponding to TFD.

Hereafter we calculate the free energy as a function of the thermal expectation value v, instead of the strength of an external field which couples to ϕ. As is well known this kind of free energy is given by one-particle irreducible diagrams.

First, we apply the formula (5) to the calculation of the deviation of free energy induced by the change of the unperturbed Lagrangian density from

$$\mathscr{L}_0=\tfrac{1}{2}\partial_\mu\rho\partial^\mu\rho-\tfrac{1}{2}m^2\rho^2 \tag{11}$$

to

$$\mathscr{L}_0'=\tfrac{1}{2}\partial_\mu\rho\partial^\mu\rho-\frac{1}{2}\left(m^2+\frac{\lambda v^2}{2}\right)\rho^2 . \tag{12}$$

The term $-\frac{1}{4}\lambda v^2\rho^2$ is treated as an interaction. The deviation of free energy density, $F_0'-F_0$, is obtained from the series of one-loop diagrams given in Fig. 2. The lowest-order one-loop contribution to the effective potential considered in Ref. 4 is included here.

$$\begin{aligned}F_0'&=F_0+\int_0^1 ds\tfrac{1}{2}\,\mathrm{Tr}\int\frac{d^4k}{(2\pi)^4}\left[\left(\frac{\lambda v^2}{2}\tau_+\right)i\Delta_F(k,0)\sum_{n=0}^{\infty}\left(\tau\frac{s\lambda v^2}{2}\Delta_F(k,0)\right)^n\right]\\&=F_0+\int_0^1 ds\tfrac{1}{2}\,\mathrm{Tr}\int\frac{d^4k}{(2\pi)^4}\left[i\frac{\lambda v^2}{2}\tau_+\Delta_F(k,0)\left(1-\frac{s\lambda v^2}{2}\tau\Delta_F(k,0)\right)^{-1}\right]\\&=F_0+\int_0^1 ds\tfrac{1}{2}\,\mathrm{Tr}\int\frac{d^4k}{(2\pi)^4}\left(i\frac{\lambda v^2}{2}\tau_+\Delta_F(k,s)\right) ,\end{aligned} \tag{13}$$

where

$$\begin{aligned}\Delta_F(k,s)&=U_B(|k^0|)\Delta_0(k,s)\,U_B^\dagger(|k^0|)\\&=U_B(|k^0|)\tau[(k^0)^2-\omega(\mathbf{k},s)^2+i\tau\epsilon]^{-1}U_B^\dagger(|k^0|) &&(14a)\\&=U_B[\omega(\mathbf{k},s)]\tau[(k^0)^2-\omega(\mathbf{k},s)^2+i\tau\epsilon]^{-1}U_B^\dagger[\omega(\mathbf{k},s)] &&(14b)\end{aligned}$$

and

$$U_B(\omega)=\begin{pmatrix}c(\omega)&s(\omega)\\s(\omega)&c(\omega)\end{pmatrix},\quad c(\omega)=(1-e^{-\beta\omega})^{-1/2},\quad s(\omega)=(e^{\beta\omega}-1)^{-1/2} , \tag{15}$$

$$\omega(\mathbf{k},s)=(\mathbf{k}^2+m^2+s\lambda v^2/2)^{1/2} , \tag{16}$$

with

$$\tau=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad \tau_+=\frac{1+\tau}{2}=\begin{pmatrix}1&0\\0&0\end{pmatrix} . \tag{17}$$

Although the trace is taken with respect to the thermal indices, the matrix τ_+ picks up only the (1,1) component of $\Delta(k,s)$ in (13). The free energy density F_0 obtained has

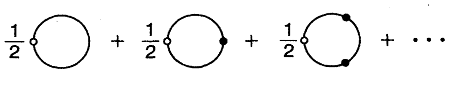

FIG. 2. Diagrams contributing to $F_0'-F_0$. A solid line denotes the propagator $i\Delta_F(k,0)$, a small open circle is assigned by H_I, and a dot is by $s\hat{H}_I$.

the familiar form

$$F_0=\beta^{-1}\int \frac{d^3\mathbf{k}}{(2\pi)^3}[\ln(1-e^{-\beta\omega(\mathbf{k},0)})+\tfrac{1}{2}\beta\omega(\mathbf{k},0)] \ . \tag{18}$$

After a simple calculation, we have

$$\begin{aligned}F_0' &= F_0+\int_0^1 ds\tfrac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(\mathbf{k},s)}\frac{\lambda v^2}{2}\coth\frac{\beta\omega(\mathbf{k},s)}{2}\\ &= F_0+\int_0^1 ds\tfrac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{2}{\beta}\frac{d}{ds}\ln\left|\sinh\frac{\beta\omega(\mathbf{k},s)}{2}\right|\\ &= F_0+\beta^{-1}\int \frac{d^3\mathbf{k}}{(2\pi)^3}[\ln(1-e^{-\beta\omega(\mathbf{k},1)})+\tfrac{1}{2}\beta\omega(\mathbf{k},1)\\ &\qquad -\ln(1-e^{-\beta\omega(\mathbf{k},0)})-\tfrac{1}{2}\beta\omega(\mathbf{k},0)]\\ &= \beta^{-1}\int \frac{d^3\mathbf{k}}{(2\pi)^3}[\ln(1-e^{-\beta\omega(\mathbf{k},1)})+\tfrac{1}{2}\beta\omega(\mathbf{k},1)] \ . \end{aligned}\tag{19}$$

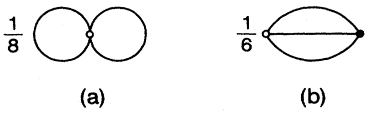

FIG. 3. Diagrams contributing to $F_2^{(a)}$ and $F_2^{(b)}$. A solid line denotes the propagator $i\Delta_F(k,1)$.

As expected, the result (19) corresponds simply to the replacement of m^2 appearing in (8) by $m^2+\lambda v^2/2$.

Secondly, in (10) considering $\mathscr{L}_0'$ as the unperturbed part and regarding $\mathscr{L}_I=-(\lambda v/3!)\rho^3-(\lambda/4!)\rho^4$ as the perturbation, we calculate the two-loop approximation. As it was pointed out previously, the one-loop contribution considered in Ref. 4 is included in F_0' through the effect of $\frac{1}{4}\lambda v^2\rho^2$ term in $\mathscr{L}_0'$. The two-loop contributions $F_2^{(a)}$ and $F_2^{(b)}$ are given by the diagrams in Figs. 3(a) and 3(b). The diagram 3(a) gives

$$\begin{aligned}F_2^{(a)} &= \int_0^1 ds\frac{i^2}{8}\int\frac{d^4k_1}{(2\pi)^4}\int\frac{d^4k_2}{(2\pi)^4}\lambda\Delta_F^{11}(k_1,1)\Delta_F^{11}(k_2,1)\\ &= \frac{\lambda}{8}\left[i\int\frac{d^4k}{(2\pi)^4}\left(\frac{c[\omega(\mathbf{k},1)]^2}{(k^0)^2-\omega(\mathbf{k},1)^2+i\epsilon}-\frac{s[\omega(\mathbf{k},1)]^2}{(k^0)^2-\omega(\mathbf{k},1)^2-i\epsilon}\right)\right]^2\\ &= \frac{\lambda}{8}\left(\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{1}{2\omega(\mathbf{k},1)}\coth\frac{\beta\omega(\mathbf{k},1)}{2}\right)^2 , \end{aligned}\tag{20}$$

and the diagram 3(b) gives

$$F_2^{(b)}=\int_0^1 ds\frac{i^2}{6}\int\frac{d^4k_1}{(2\pi)^4}\int\frac{d^4k_2}{(2\pi)^4}\int\frac{d^4k_3}{(2\pi)^4}(2\pi)^4\delta^{(4)}(k_1+k_2+k_3)\lambda v\sum_{\alpha=1}^{2}\Delta_F^{1\alpha}(k_1,1)\Delta_F^{1\alpha}(k_2,1)\Delta_F^{1\alpha}(k_3,1)\tau^{\alpha\alpha}s\lambda v \ . \tag{21}$$

Since $\Delta_F^{12}(k_i,1)$ does not contribute to the integration because of the on-shell condition in $\Delta_F^{12}(k_i,1)$, we obtain

$$\begin{aligned}F_2^{(b)} &= -\frac{\lambda^2v^2}{12}\int\frac{d^4k_1}{(2\pi)^4}\int\frac{d^4k_2}{(2\pi)^4}\int\frac{d^3\mathbf{k}_3}{(2\pi)^3}(2\pi)^3\delta^{(3)}(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)\left(\frac{c_1{}^2}{(k_1^0)^2-\omega_1{}^2+i\epsilon}-\frac{s_1{}^2}{(k_1^0)^2-\omega_1{}^2-i\epsilon}\right)\\ &\quad\times\left(\frac{c_2{}^2}{(k_2^0)^2-\omega_2{}^2+i\epsilon}-\frac{s_2{}^2}{(k_2^0)^2-\omega_2{}^2-i\epsilon}\right)\\ &\quad\times\left(\frac{c_3{}^2}{(-k_1^0-k_2^0)^2-\omega_3{}^2+i\epsilon}-\frac{s_3{}^2}{(-k_1^0-k_2^0)^2-\omega_3{}^2-i\epsilon}\right)\\ &= -\frac{\lambda^2v^2}{6}\int\frac{d^3\mathbf{k}_1}{(2\pi)^3 2\omega_1}\int\frac{d^3\mathbf{k}_2}{(2\pi)^3 2\omega_2}\int\frac{d\mathbf{k}_3}{(2\pi)^3 2\omega_3}(2\pi)^3\delta^{(3)}(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)\\ &\quad\times\left(\frac{c_1{}^2c_2{}^2c_3{}^2}{\omega_1+\omega_2+\omega_3}+\frac{c_1{}^2c_2{}^2s_3{}^2}{\omega_1+\omega_2-\omega_3}+\frac{c_1{}^2s_2{}^2c_3{}^2}{\omega_1-\omega_2+\omega_3}+\frac{c_1{}^2s_2{}^2s_3{}^2}{\omega_1-\omega_2-\omega_3}\right.\\ &\qquad\left.+\frac{s_1{}^2c_2{}^2c_3{}^2}{-\omega_1+\omega_2+\omega_3}+\frac{s_1{}^2c_2{}^2s_3{}^2}{-\omega_1+\omega_2-\omega_3}+\frac{s_1{}^2s_2{}^2c_3{}^2}{-\omega_1-\omega_2+\omega_3}+\frac{s_1{}^2s_2{}^2s_3{}^2}{-\omega_1-\omega_2-\omega_3}\right) , \end{aligned}\tag{22}$$

where

$$\omega_i=\omega(\mathbf{k}_i,1)=(\mathbf{k}_i^2-m^2+\lambda v^2/2)^{1/2} \ , \quad c_i=c(\omega_i) \ , \quad s_i=s(\omega_i) \ .$$

One can easily check that the results (19), (20), and (22) are identical with those obtained by the use of the Matsubara frequency method.

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