2.3. Evaluation of thermal sums

Due to the previously established equality between Eqs. (2.19), (2.20), we have arrived at two different representations for the free energy density of free scalar field theory, Eqs. (2.24), (2.26). The purpose of this section is to take the step from Eq. (2.24) to (2.26) directly, and learn on the way how to carry out thermal sums such as those in Eq. (2.24) also in more general cases.

In fact, the very sum in Eq. (2.24) is a somewhat special case: it includes a "physical term", the first one, which depends on the energy (and thus on the mass of the scalar particle); as well as "unphysical" subtractions, the second and third terms, which are independent of the energy, but are needed in order to make the sum convergent. Only the result from energy-dependent term "survives" in Eq. (2.26). In order not to lose focus on the peculiarities of this special case, we will mostly concentrate on another, convergent sum:

$$i(E) \equiv \frac{1}{E} \frac{\mathrm{d}j(E)}{\mathrm{d}E} = T \sum_{\omega_n} \frac{1}{\omega_n^2 + E^2} , \qquad (2.27)$$

from which the first term appearing in Eq. (2.24),

$$j(E) \equiv T \sum_{\omega_n} \frac{1}{2} \ln(\omega_n^2 + E^2) ,$$
 (2.28)

can be obtained by integration with respect to E, apart from an integration constant, which should be chosen according to the 2nd and 3rd terms in Eq. (2.24).

To begin with, we want to be completely general. Let f(p) be a function which is analytic in the complex plane, and regular on the real axis. We then consider the sum

$$S \equiv T \sum_{\omega_n} f(\omega_n) .$$
(2.29)

Consider now the auxiliary function

$$i n_{\rm B}(ip) \equiv \frac{i}{\exp(i\beta p) - 1} \,. \tag{2.30}$$

This function has poles at $i\beta p = 2\pi n$, $n \in \mathbb{Z}$, i.e. $p = \omega_n$. Expanding in Laurent series around any pole we get

$$i n_{\rm B}(i[\omega_n + z]) = \frac{i}{\exp(i\beta[\omega_n + z]) - 1} = \frac{i}{\exp(i\beta z) - 1} \approx \frac{T}{z} + \mathcal{O}(1) .$$
 (2.31)

Therefore, the residue at any pole is T. This means that we can replace the sum in Eq. (2.29) by a complex integral:

$$S = \oint \frac{\mathrm{d}p}{2\pi i} f(p) i n_{\mathrm{B}}(ip) \equiv \int_{-\infty - i0^{+}}^{+\infty - i0^{+}} \frac{\mathrm{d}p}{2\pi} f(p) n_{\mathrm{B}}(ip) + \int_{+\infty + i0^{+}}^{-\infty + i0^{+}} \frac{\mathrm{d}p}{2\pi} f(p) n_{\mathrm{B}}(ip) , \quad (2.32)$$

where, as indicated, the integration contour runs clockwise around the real axis of the complex p-plane.

In the latter term in Eq. (2.32), we can furthermore substitute integration variables as $p \to -p$, and note that

$$n_{\rm B}(-ip) = \frac{1}{\exp(-i\beta p) - 1} = \frac{\exp(i\beta p) - 1 + 1}{1 - \exp(i\beta p)} = -1 - n_{\rm B}(ip) .$$
(2.33)

We thereby get the final formula

$$S = \int_{-\infty-i0^{+}}^{+\infty-i0^{+}} \frac{\mathrm{d}p}{2\pi} \left\{ f(-p) + [f(p) + f(-p)]n_{\mathrm{B}}(ip) \right\}$$

=
$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{2\pi} f(p) + \int_{-\infty-i0^{+}}^{+\infty-i0^{+}} \frac{\mathrm{d}p}{2\pi} [f(p) + f(-p)]n_{\mathrm{B}}(ip) , \qquad (2.34)$$

where in the first term we were able to return to the real axis (because there are no singularities there), and substitute once again $p \to -p$. Thus we have managed to convert the sum in Eq. (2.29) to a complex integral.

The first term in Eq. (2.34) is temperature-independent: it gives the zero-temperature "vacuum" contribution. The latter term determines how thermal effects change the result.

As a technical point let us note, furthermore, that in the lower half plane,

$$|n_{\rm B}(ip)| \stackrel{p=x-iy}{=} \left| \frac{1}{e^{i\beta x} e^{\beta y} - 1} \right| \stackrel{y\gg T}{\approx} e^{-\beta y} \stackrel{y\gg x}{\approx} e^{-\beta|p|} .$$

$$(2.35)$$

Therefore, if the function f(p) grows slower than $e^{\beta|p|}$ at large |p| (in particular, polynomially), the integration contour can be closed in the lower half plane, and the result is determined by the pole locations and residues of the function f(p) + f(-p). Physically, we therefore say that the thermal contribution to S is related to "on-shell" particles.

Let us now apply the general formula in Eq. (2.34) to the particular example of Eq. (2.27). In fact, without any additional cost, we can consider a slight generalization,

$$i(E;c) \equiv T \sum_{\omega_n} \frac{1}{(\omega_n + c)^2 + E^2} , \quad c \in \mathbb{C} .$$
 (2.36)

In terms of Eq. (2.29), we then have

$$f(p) = \frac{1}{(p+c)^2 + E^2} = \frac{i}{2E} \left[\frac{1}{p+c+iE} - \frac{1}{p+c-iE} \right]$$
(2.37)

$$f(p) + f(-p) = \frac{i}{2E} \left[\frac{1}{p+c+iE} + \frac{1}{p-c+iE} - \frac{1}{p+c-iE} - \frac{1}{p-c-iE} \right]. \quad (2.38)$$

For Eq. (2.34), we need the poles in the lower half plane; for $|\operatorname{Im} c| < E$, these are at $p = \pm c - iE$. According to Eq. (2.38), the residue at each pole is i/2E. The vacuum term in Eq. (2.34) then produces

$$\frac{1}{2\pi}(-2\pi i)\frac{i}{2E} = \frac{1}{2E} , \qquad (2.39)$$

while the matter part yields

$$\frac{1}{2\pi}(-2\pi i)\frac{i}{2E}\left[\frac{1}{e^{\beta(E-ic)}-1} + \frac{1}{e^{\beta(E+ic)}-1}\right].$$
(2.40)

In total, then,

$$i(E;c) = \frac{1}{2E} \left[1 + n_{\rm B}(E - ic) + n_{\rm B}(E + ic) \right].$$
(2.41)

We note, first of all, that the result is periodic in $c \to c + 2\pi Tn$, $n \in \mathbb{Z}$, as it must be according to Eq. (2.36); and that the appearance of *ic* resembles that of a *chemical potential*. Indeed, as we will see in Exercise 2, setting $ic \to \mu$ corresponds to a situation where we have averaged over a particle (chemical potential μ) and an antiparticle (chemical potential $-\mu$.)

To conclude this section, let us integrate the result of Eq. (2.41) with respect to E, in order to obtain a generalization of the function in Eq. (2.28),

$$j(E;c) \equiv T \sum_{\omega_n} \frac{1}{2} \ln[(\omega_n + c)^2 + E^2] .$$
 (2.42)

The relation given in Eq. (2.27) continues to hold in the presence of c. Noting that

$$\frac{1}{e^x - 1} = \frac{e^{-x}}{1 - e^{-x}} = \frac{\mathrm{d}}{\mathrm{d}x} \left(1 - e^{-x} \right) \,, \tag{2.43}$$

we immediately get

$$j(E;c) = \text{const.} + \frac{E}{2} + \frac{T}{2} \left\{ \ln \left[1 - e^{-\beta(E-ic)} \right] + \left[1 - e^{-\beta(E+ic)} \right] \right\},$$
(2.44)

where the constant can depend on T and c.

Setting now c = 0, and comparing with Eqs. (2.24), (2.26), we notice that we have been lucky: the extra terms in Eq. (2.24) are such that they precisely cancel against the integration constant in Eq. (2.44). So, the full physical result containing j(E;0) can be deduced directly from i(E;0). That the same is true even for $\mu \equiv ic \neq 0$, if we interpret j(E;c) as a free energy density averaged over a particle and an antiparticle (in a harmonic oscillator potential, i.e. a free field), is shown in Exercise 2.

2.4. Exercise 2

Compute the partition function of the harmonic oscillator in the presence of a chemical potential,

$$e^{-\beta F(T,\mu)} \equiv \mathcal{Z}(T,\mu) \equiv \operatorname{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right],$$
(2.45)

and show that the expression

$$\frac{1}{2}\left[F(T,ic) + F(T,-ic)\right] \tag{2.46}$$

agrees with the E-dependent part of Eq. (2.44).

Solution to Exercise 2

Trivially,

$$\langle n|(\hat{H}-\mu\hat{N})|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right) - \mu n = (\hbar\omega-\mu)n + \frac{\hbar\omega}{2}.$$
(2.47)

Evaluating the partition function in the energy basis yields

$$\mathcal{Z}^{\rm HO} = \sum_{n=0}^{\infty} \exp\left(-\frac{\hbar\omega}{2T} - \frac{\hbar\omega - \mu}{T}n\right) = \frac{\exp\left(-\frac{\hbar\omega}{2T}\right)}{1 - \exp\left(-\frac{\hbar\omega - \mu}{T}\right)} \,. \tag{2.48}$$

Putting $\hbar \to 1, \, \omega \to E, \, \mu \to ic$, we can rewrite the result as

$$\mathcal{Z}^{\text{HO}} = \exp\left\{-\frac{1}{T}\left[\frac{E}{2} + T\ln\left(1 - e^{-\frac{E-ic}{T}}\right)\right]\right\}.$$
(2.49)

Reading from here $F(T, \mu)$ according to Eq. (2.45), and computing $\frac{1}{2} \left[F(T, ic) + F(T, -ic) \right]$, yields directly the *E*-dependent part of Eq. (2.44).

2.5. Low-temperature expansion

Our next goal is to carry out the momentum integration in Eqs. (2.24), (2.26). We denote

$$J(m,T) \equiv \int \frac{\mathrm{d}^{d}\mathbf{k}}{(2\pi)^{d}} \left[\frac{E_{\mathbf{k}}}{2} + T \ln\left(1 - e^{-\beta E_{\mathbf{k}}}\right) \right]$$
(2.50)

$$= T \sum_{\omega_n} \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \left[\frac{1}{2} \ln(\omega_n^2 + E_\mathbf{k}^2) - \text{const.} \right], \qquad (2.51)$$

$$I(m,T) \equiv \frac{1}{m} \frac{\mathrm{d}}{\mathrm{d}m} J(m,T)$$
(2.52)

$$= \int \frac{\mathrm{d}^{d}\mathbf{k}}{(2\pi)^{d}} \frac{1}{2E_{\mathbf{k}}} \Big[1 + 2n_{\mathrm{B}}(E_{\mathbf{k}}) \Big]$$
(2.53)

$$= T \sum_{\omega_n} \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} , \qquad (2.54)$$

where d is the space dimension, $E_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}$, and we made use of the fact that $m^{-1}d/dm = E_{\mathbf{k}}^{-1}d/dE_{\mathbf{k}}$. In order to simplify the notation in the following, we will denote

$$\oint_{\tilde{K}} \equiv T \sum_{\omega_n} \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} , \quad \oint_{\tilde{K}}' \equiv T \sum_{\omega'_n} \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} , \quad \int_{\mathbf{k}} \equiv \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} , \quad (2.55)$$

where $\tilde{K} \equiv (\omega_n, \mathbf{k})$, and a prime denotes that the zero-mode is omitted. The tilde in \tilde{K} is a reminder for Euclidean metric.

At low temperatures, $T \ll m$, we expect that the results resemble those of the zero-temperture theory. Therefore we can write

$$J(m,T) = J_0(m) + J_T(m) , I(m,T) = I_0(m) + I_T(m) , \qquad (2.56)$$

where J_0 is the temperature-independent vacuum energy density,

$$J_0(m) \equiv \int_{\mathbf{k}} \frac{E_{\mathbf{k}}}{2} , \qquad (2.57)$$

and J_T is the thermal part of the free energy density,

$$J_T(m) \equiv \int_{\mathbf{k}} T \ln \left(1 - e^{-\beta E_{\mathbf{k}}} \right) \,. \tag{2.58}$$

The sum-integral I(m,T) can be divided in a similar way. It is clear that $J_0(m)$ is ultraviolet divergent, and can only be evaluated in the presence of a regularization; as indicated by Eq. (2.55), we will mostly be employing dimensional regularization here. In contrast, the integrand in J_T is exponentially small for $|\mathbf{k}| \gg T$, and therefore the integral is well convergent.

Let us start by evaluating $J_0(m)$. Writing the mass dependence explicitly, the task is to evaluate

$$J_0(m) = \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \frac{1}{2} \left(\mathbf{k}^2 + m^2\right)^{\frac{1}{2}} , \qquad (2.59)$$

and subsequently insert $d = 3 - 2\epsilon$. For generality and future reference, we will in fact first compute

$$F(m,d,A) \equiv \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \frac{1}{(\mathbf{k}^2 + m^2)^A} , \qquad (2.60)$$

and obtain then J_0 as $J_0(m) = \frac{1}{2} F(m, d, -\frac{1}{2})$.

Since the integrand only depends on $|\mathbf{k}|$, angular integrations can be carried out, and the integration measure obtains the known form²

$$d^{d}\mathbf{k} = \frac{\pi^{d/2}}{\Gamma(d/2)} (\mathbf{k}^{2})^{\frac{d-2}{2}} d(\mathbf{k}^{2}) , \qquad (2.61)$$

where $\Gamma(s)$ is the Euler gamma function (we reiterate some of its basic properties in Sec. 2.7). Substituting $\mathbf{k}^2 \to z \to m^2 t$ in Eq. (2.60), we get

$$F(m, d, A) = \frac{\pi^{d/2}}{\Gamma(d/2)} \frac{1}{(2\pi)^d} \int_0^\infty dz \, z^{\frac{d-2}{2}} (z+m^2)^{-A} = \frac{m^{d-2A}}{(4\pi)^{d/2} \Gamma(d/2)} \int_0^\infty dt \, t^{d/2-1} (1+t)^{-A} \,.$$
(2.62)

A further substitution $t \to 1/s - 1$, $dt \to -ds/s^2$ yields

$$F(m,d,A) = \frac{m^{d-2A}}{(4\pi)^{d/2}\Gamma(d/2)} \int_0^1 \mathrm{d}s \, s^{A-d/2-1} (1-s)^{d/2-1} \,. \tag{2.63}$$

We now recognize a standard integral that can be expressed in terms of the gamma function:

$$F(m,d,A) = \int \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \frac{1}{(\mathbf{k}^2 + m^2)^A} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(A - d/2)}{\Gamma(A)} \frac{1}{(m^2)^{A - d/2}} \,. \tag{2.64}$$

We now return to $J_0(m)$ in Eq. (2.59), i.e. set $A = -\frac{1}{2}$, $d = 3 - 2\epsilon$, $A - \frac{d}{2} = -2 + \epsilon$ in Eq. (2.64), and multiply by $\frac{1}{2}$. The basic property $\Gamma(s) = s^{-1}\Gamma(s+1)$ allows to transport the argument of the gamma function to the vicinity of 1/2 or 1, where a Taylor expansion is easily carried out (basic formulae can be found in Sec. 2.7):

$$\Gamma(-2+\epsilon) = \frac{1}{(-2+\epsilon)(-1+\epsilon)\epsilon} \Gamma(1+\epsilon)$$
(2.65)

$$= \frac{1}{2\epsilon} \left(1 + \frac{\epsilon}{2} \right) \left(1 + \epsilon \right) (1 - \gamma_E \epsilon) + \mathcal{O}(\epsilon) , \qquad (2.66)$$

$$\Gamma(-\frac{1}{2}) = -2\Gamma(\frac{1}{2}) = -2\sqrt{\pi}.$$
 (2.67)

The other parts of Eq. (2.64) are written as

$$(4\pi)^{-\frac{3}{2}+\epsilon} = \frac{2\sqrt{\pi}}{(4\pi)^2} \Big[1 + \epsilon \ln(4\pi) \Big] + \mathcal{O}(\epsilon^2) , \qquad (2.68)$$

$$(m^2)^{2-\epsilon} = m^4 \mu^{-2\epsilon} \left(\frac{\mu^2}{m^2}\right)^{\epsilon} = m^4 \mu^{-2\epsilon} \left(1 + \epsilon \ln \frac{\mu^2}{m^2}\right) + \mathcal{O}(\epsilon^2) , \qquad (2.69)$$

where μ is an arbitrary scale parameter, introduced as $1 = \mu^{-2\epsilon} \mu^{2\epsilon}$.

Collecting now everything together, we get

$$J_0(m) = -\frac{m^4}{64\pi^2} \mu^{-2\epsilon} \left[\frac{1}{\epsilon} + \ln \frac{\mu^2}{m^2} + \ln(4\pi) - \gamma_E + \frac{3}{2} + \mathcal{O}(\epsilon) \right].$$
(2.70)

It is convenient at this point to introduce the $\overline{\text{MS}}$ scheme scale parameter $\bar{\mu}$, through

$$\ln \bar{\mu}^2 \equiv \ln \mu^2 + \ln(4\pi) - \gamma_E .$$
 (2.71)

²On one hand, $\int d^d k \exp(-tk^2) = [\int_{-\infty}^{\infty} dk_1 \exp(-tk_1^2)]^d = (\pi/t)^{d/2}$. On the other, $\int d^d k \exp(-tk^2) = c(d) \int_0^{\infty} dk \, k^{d-1} \exp(-tk^2) = c(d)t^{-d/2} \int_0^{\infty} dx \, x^{d-1}e^{-x^2} = c(d)\Gamma(d/2)/2t^{d/2}$. Thereby $c(d) = 2\pi^{d/2}/\Gamma(d/2)$.

Thereby

$$J_0(m) = -\frac{m^4 \mu^{-2\epsilon}}{64\pi^2} \left[\frac{1}{\epsilon} + \ln \frac{\bar{\mu}^2}{m^2} + \frac{3}{2} + \mathcal{O}(\epsilon) \right].$$
(2.72)

For $I_0(m)$, we obtain from Eqs. (2.52), (2.72) the expression

$$I_0(m) = \int_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} = -\frac{m^2 \mu^{-2\epsilon}}{16\pi^2} \left[\frac{1}{\epsilon} + \ln \frac{\bar{\mu}^2}{m^2} + 1 + \mathcal{O}(\epsilon) \right].$$
(2.73)

Incidentally, note that $\int_{-\infty}^{\infty} dk_0/(2\pi) \times 1/(k_0^2 + E_k^2) = 1/(2E_k)$, so that $I_0(m)$ can also be written as

$$I_0(m) = \int \frac{\mathrm{d}^{d+1}\mathbf{k}}{(2\pi)^{d+1}} \frac{1}{\mathbf{k}^2 + m^2} \,. \tag{2.74}$$

We then move to the finite-temperature parts, $J_T(m)$ and $I_T(m)$. As already mentioned, the corresponding integrals are finite. Therefore, we can normally set d = 3 to begin with.³ Substituting $|\mathbf{k}| \to Tx$ in Eq. (2.58), and taking the derivative in Eq. (2.52), we find

$$J_T(m) = \frac{T^4}{2\pi^2} \int_0^\infty dx \, x^2 \, \ln\left(1 - e^{-\sqrt{x^2 + y^2}}\right)_{y \equiv m/T}, \qquad (2.75)$$

$$I_T(m) = \frac{T^2}{2\pi^2} \int_0^\infty \frac{\mathrm{d}x \, x^2}{\sqrt{x^2 + y^2}} \left. \frac{1}{e^{\sqrt{x^2 + y^2}} - 1} \right|_{y \equiv m/T} \,. \tag{2.76}$$

Unfortunately, these integrals cannot be expressed in terms of elementary functions. In retrospective, though, this may even be "understandable": as we will see, they contain so much important physics that it would be unrealistic to find it in any simple well-behaved analytic function! At the same time, Eqs. (2.75), (2.76) can of course be numerically evaluated without problems.

Even though Eq. (2.75) cannot be evaluated exactly, we can still find approximate expression valid in various limit. In this section we are interested in low temperatures, i.e. $y = m/T \gg 1$. Let us thus evaluate the leading term of Eq. (2.75) in an expansion in $\exp(-y)$ and 1/y. We can write

$$\int_{0}^{\infty} \mathrm{d}x \, x^{2} \ln\left(1 - e^{-\sqrt{x^{2} + y^{2}}}\right) = -\int_{0}^{\infty} \mathrm{d}x \, x^{2} \, e^{-\sqrt{x^{2} + y^{2}}} + \mathcal{O}(e^{-2y})$$

$${}^{w \equiv \sqrt{x^{2} + y^{2}}} - \int_{y}^{\infty} \mathrm{d}w \, w \sqrt{w^{2} - y^{2}} e^{-w} + \mathcal{O}(e^{-2y})$$

$${}^{v \equiv w^{-y}} - e^{-y} \int_{0}^{\infty} \mathrm{d}v (v + y) \sqrt{2vy + v^{2}} e^{-v} + \mathcal{O}(e^{-2y})$$

$$= -\sqrt{2}y^{\frac{3}{2}} e^{-y} \int_{0}^{\infty} \mathrm{d}v \, v^{\frac{1}{2}} \left(1 + \frac{v}{y}\right) \left(1 + \frac{v}{2y}\right)^{\frac{1}{2}} e^{-v} + \mathcal{O}(e^{-2y})$$

$$= -\sqrt{2}\Gamma\left(\frac{3}{2}\right)y^{\frac{3}{2}} e^{-y} \left[1 + \mathcal{O}\left(\frac{1}{y}\right) + \mathcal{O}\left(e^{-y}\right)\right], \quad (2.77)$$

where $\Gamma(3/2) = \sqrt{\pi}/2$.

Inserting into Eq. (2.58), we thus obtain

$$J_T(m) = -T^4 \left(\frac{m}{2\pi T}\right)^{\frac{3}{2}} e^{-\frac{m}{T}} \left[1 + \mathcal{O}\left(\frac{T}{m}\right) + \mathcal{O}\left(e^{-m/T}\right)\right].$$
(2.78)

The derivative in Eq. (2.52) subsequently yields

$$I_T(m) = \frac{T^3}{m} \left(\frac{m}{2\pi T}\right)^{\frac{3}{2}} e^{-\frac{m}{T}} \left[1 + \mathcal{O}\left(\frac{T}{m}\right) + \mathcal{O}\left(e^{-m/T}\right)\right].$$
(2.79)

³In multiloop computations, $J_T(m)$ or $I_T(m)$ could get multiplied by a divergent term, $1/\epsilon$, in which case contributions of $\mathcal{O}(\epsilon)$ would be needed as well. They could then be obtained by noting from Eq. (2.61) that $\mu^{2\epsilon} d^d \mathbf{k}/(2\pi)^d = \{1 + \epsilon [\ln(\bar{\mu}^2/4\mathbf{k}^2) + 2] + \mathcal{O}(\epsilon^2)\} d^3 \mathbf{k}/(2\pi)^3$, for $d = 3 - 2\epsilon$ and an integrand only depending on \mathbf{k}^2 .