Thermofield Dynamics

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1 Introduction

There are many formalisms for incorporating thermal effects in Quantum Field Theories[1]. Here, I present the basic ideas of one of them, the so called Thermofield Dynamics[2]. It basically consists of applying a general technique of purifying a system by enlarging the Hilbert Space of the theory to the framework of Quantum Field Theory, allowing one to calculate, with know techniques such as Feynman Rules and Diagrams, thermal averages of quantities by a simple pure state "vacuum" expectation value of a local operator.

2 Purification and a new "vacuum"

Let's start with an interesting mathematical factoid. We know that in Statistical Mechanics, we are usually interested in the thermal (ensemble) average of an operator:

$$\langle A \rangle_\beta = Z^{-1}(\beta) Tr\{A\rho\} = Z^{-1}(\beta) \sum_i e^{-\beta E_i} \langle i|A|i\rangle$$

with ρ and $Z(\beta)$ being the density operator and the partition function of the system, respectively.

We also know that in Quantum Field Theory, a quantity of great importance is the so called vacuum expectation value of an operator, $\langle 0|A|0\rangle$, related to transition amplitudes of various processes.

What if we could come up with a state $|0(\beta)\rangle$ for which a thermal average could be expressed as a simple "vacuum" expected value?

$$\langle A \rangle_\beta = \langle 0(\beta)|A|0(\beta)\rangle \tag{1}$$

[1] A great introductory reference for the different formalisms, their power, limitations and applications is the book by Ashok Das, *Finite Temperature Field Theory*.

[2] For a great comprehensive exploration of the formalism by some of its main developers, see *Thermofield Dynamics and Condensed States*, by H. Umezawa, H. Matsumoto and M. Tachiki.

This would be interesting as Quantum Field Theory arsenal of techniques could be applied for thermal systems. It turns out such a thing is possible by enlarging our system in a very beautiful way. Let's see how this goes.

Let $\mathcal{H}$ be the Hilbert space of our initial system, and let's suppose such a $|0(\beta)\rangle$ exists. If it lives in $\mathcal{H}$, we can expand it in a basis of $\mathcal{H}$. So let's investigate this:

If $\{|i\rangle\}$ is a basis of $\mathcal{H}$, take

$$|0(\beta)\rangle = \sum_i |i\rangle \langle i|0(\beta)\rangle = \sum_i g_i(\beta) |i\rangle \tag{2}$$

now, plugging this in equation (1), we get

$$Z^{-1}(\beta) \sum_i e^{-\beta E_i} \langle i|A|i\rangle = \langle 0(\beta)|A|0(\beta)\rangle = \sum_i \sum_j g_i^*(\beta) g_j(\beta) \langle i|A|j\rangle \tag{3}$$

which would require the functions $g_i(\beta)$ to satisfy

$$g_i^*(\beta) g_j(\beta) = Z^{-1}(\beta) e^{-\beta E_i} \delta_{ij} \tag{4}$$

which cannot be done, since the g's are just complex numbers. This could be a suggestion that such a state doesn't exist, however we can find a state satisfying (1) if we place it in other Hilbert space. For this, let $\tilde{\mathcal{H}}$ be a copy of $\mathcal{H}$ and take $|0(\beta)\rangle \in \mathcal{H} \otimes \tilde{\mathcal{H}}$. We call this a doubling of the Hilbert space. Then, we write

$$|0(\beta)\rangle = \sum_n g_n(\beta) |n, \tilde{n}\rangle \tag{5}$$

so that the "vacuum" expectation value of an operator (in $\mathcal{H}$) is given by

$$\langle 0(\beta)|A|0(\beta)\rangle = \sum_n \sum_m g_n^*(\beta) g_m(\beta) \langle n, \tilde{n}|A|m, \tilde{m}\rangle \tag{6}$$

now, since A is a local operator (acting only in $\mathcal{H}$), this ends up being, guess what:

$$\sum_n \sum_m g_n^*(\beta) g_m(\beta) \langle n, \tilde{n}|A|m, \tilde{m}\rangle = \sum_n \sum_m g_n^*(\beta) g_m(\beta) \langle n|A|m\rangle \delta_{nm} \tag{7}$$

Now, choosing $g_i(\beta) = Z^{-1/2}(\beta) e^{-\beta E_i/2}$, we get

$$\begin{aligned} \langle 0(\beta)|A|0(\beta)\rangle &= \sum_n \sum_m g_n^*(\beta) g_m(\beta) \langle n|A|m\rangle \delta_{nm} \\ &= Z^{-1}(\beta) \sum_n e^{-\beta E_i} \langle n|A|n\rangle \\ &= \langle A\rangle_\beta \end{aligned} \tag{8}$$

In conclusion, we see that, by enlarging the Hilbert space we work in, we were able to define a new (thermal) "vacuum" for which the expected value of operators equals the thermal ensemble averages we deal with in usual descriptions of thermal systems. Our new thermal "vacuum" state is given by

$$|0(\beta)\rangle = \frac{1}{\sqrt{Z(\beta)}} \sum_n e^{-\beta E_n/2} |n, \tilde{n}\rangle \tag{9}$$

3 An Illustration

We may gain a little of intuition about this formalism by considering it in a fairly simple system, a bosonic oscillator.

We begin with a single oscillator Hamiltonian

$$H = \omega a^\dagger a$$

and impose bosonic commutation relations:

$$[a, a^\dagger] = 1$$

We now make a copy of our Hamiltonian

$$\tilde{H} = \omega \tilde{a}^\dagger \tilde{a}$$

also imposing the same commutation relations

$$[\tilde{a}, \tilde{a}^\dagger] = 1$$

with all other commutators being 0. Now we construct our thermal vacuum:

$$|0(\beta)\rangle = \sum_n g_n(\beta) |n, \tilde{n}\rangle \tag{10}$$

which from eq. (9) is given by

$$|0(\beta)\rangle = \sqrt{1 - e^{-\beta\omega}} \sum_n e^{-\beta\omega n/2} |n, \tilde{n}\rangle \tag{11}$$

we may write this as

$$\begin{aligned} |0(\beta)\rangle &= \sqrt{1 - e^{-\beta\omega}} \sum_n \frac{(e^{-\beta\omega/2})^n}{n!} (a^\dagger \tilde{a}^\dagger)^n |0, \tilde{0}\rangle \\ &= \sqrt{1 - e^{-\beta\omega/2}} \exp\left(e^{-\beta\omega} a^\dagger \tilde{a}^\dagger\right) |0, \tilde{0}\rangle \end{aligned} \tag{12}$$

Which makes more transparent the connection between the two vacua of our theories. I confess it's not clear why one would be interested in such a thing, but I hope it will become clearer as we move on. For now, take it as a different way of writing things. But let's probe deeper. With not much work we see that, with the definitions

$$\cosh\theta(\beta) = \frac{1}{\sqrt{1-e^{\beta\omega}}}$$

and

$$\sinh\theta(\beta) = \frac{e^{-\beta\omega/2}}{\sqrt{1-e^{\beta\omega}}},$$

we may write

$$|0(\beta)\rangle = U(\theta(\beta))\,|0,\tilde{0}\rangle\,, \tag{13}$$

with

$$U(\theta) = exp\{-iG(\theta)\} = exp\{-\theta(\beta)(\tilde{a}a - a^{\dagger}\tilde{a}^{\dagger})\},$$

where I have suppressed the β dependence just for notation sake.

Now, this is pretty neat. We found that we induce a "thermal vacuum" from a beautiful (formally) unitary transformation on the (doubled) initial vacuum. The transformation given by $U(\theta)$ is called *two-mode squeezing*. Written like this, we see that it is generated by $G(\theta)$, which is called a *Bogoliubov* transformation.

4 Operators

Still in our example, in this new space, with this new thermal vacuum (to be honest, up to now, there is no apparent reason why this state should be called vacuum at all, but hold on), the a's operators no longer act how we expect, that is

$$a\,|0(\beta)\rangle \neq 0 \neq \tilde{a}\,|0(\beta)\rangle$$

But look at eq. (13). We are effectively changing our basis! Therefore, we shouldn't simply look at the action of our old operators, but of new operators induced by the $U(\theta)$ transformation, that is

$$\begin{aligned} a(\beta) &= U(\theta)aU^{\dagger}(\theta) \\ a^{\dagger}(\beta) &= U(\theta)a^{\dagger}U^{\dagger}(\theta) \\ \tilde{a}(\beta) &= U(\theta)\tilde{a}U^{\dagger}(\theta) \\ \tilde{a}^{\dagger}(\beta) &= U(\theta)\tilde{a}^{\dagger}U^{\dagger}(\theta). \end{aligned}$$

Now check this out

$$a(\beta)\,|0(\beta)\rangle = U(\theta)aU^{\dagger}(\theta)U(\theta)\,|0,\tilde{0}\rangle = U(\theta)a\,|0,\tilde{0}\rangle = 0$$

Aha! $|0(\beta)\rangle$ is indeed a vacuum state, we just had to look at the right operators!

Since $U(\beta)$ is a unitary operator, it follows that the algebra of the initial operators a and $\tilde{a}$ is preserved, that is, we have

$$[a(\beta), a^\dagger(\beta)] = [\tilde{a}(\beta), \tilde{a}^\dagger(\beta)] = 1 \tag{14}$$

with the other commutators being zero.

Now, what about the Hamiltonian? What happens if we apply it to the our new vacuum state?

$$H\,|0(\beta)\rangle = \omega a^\dagger a \sum_n e^{-\beta\omega n/2}\,|n, \tilde{n}\rangle = \omega \sum_n n e^{-\beta\omega n/2}\,|n, \tilde{n}\rangle \neq 0$$

That is, our thermal vacuum is not even an eigenstate of the original Hamiltonian H, the same holds for $\tilde{H}$. We should expect that the dynamical operator we ought to look at would involve both H and $\tilde{H}$, since our vacuum lives in both spaces. Now, lets look at a different operator $\hat{H} = H - \tilde{H}$. We have that

$$\begin{aligned}
\hat{H}\,|0(\beta)\rangle &= 0 \\
\hat{H}a^\dagger(\beta)\,|0(\beta)\rangle &= \omega a^\dagger(\beta)\,|0(\beta)\rangle \\
\hat{H}\tilde{a}^\dagger(\beta)\,|0(\beta)\rangle &= -\omega\tilde{a}^\dagger(\beta)\,|0(\beta)\rangle \\
\hat{H}a^\dagger(\beta)\tilde{a}^\dagger(\beta)\,|0(\beta)\rangle &= 0.
\end{aligned}$$

We see then that our thermal vacuum is an eigenstate of this new operator $\hat{H}$. The message is that in dealing with thermal systems, look for $|0(\beta)\rangle$, $U(\theta(\beta))$ and $\hat{H}$[3].

5 Fields (Finally!)

Let's finally delve into fields territory. In field theory we usually start with the Lagrangian for a given theory, and based on the discussion above about the fact that the dynamical operator we should look at is $\hat{H}$, I believe it's not hard to convince oneself that in field theory, what we should start with is not simply $\mathcal{L}$, regarding the degrees of freedom in $\mathcal{H}$ only, but $\hat{\mathcal{L}} = \mathcal{L} - \tilde{\mathcal{L}}$, with both $\mathcal{H}$ and $\tilde{\mathcal{H}}$ at play. It is instructive to construct the formalism already within an example. The model we consider is the free scalar field:

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi - \frac{1}{2}m^2\phi^2 \tag{15}$$

We already know how to proceed, define our tilde fields $\tilde{\phi}$ and write our doubled Lagrangian:

$$\hat{\mathcal{L}} = \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{1}{2}\partial_\mu\tilde{\phi}\,\partial^\mu\tilde{\phi} + \frac{1}{2}m^2\tilde{\phi}^2 \tag{16}$$

[3] Here I should thank our class friend Leonardo Lessa for a great insight into what is going on. Basically, the operation $|\psi\rangle\langle\phi| \to |\psi\rangle\,|\phi\rangle$, which is how we constructed the thermal vacuum, is antilinear in the dual variables (the tilde variables, in our case), which results in a complex conjugation for the tilde variables when constructing the time evolution operator.

We can quantize our fields in the standard manner, canonically. First we get the canonical conjugate momenta:

$$\pi_\phi = \frac{\partial \hat{\mathcal{L}}}{\partial(\partial_t \phi)}, \tag{17}$$

$$\tilde{\pi}_{\tilde{\phi}} = \frac{\partial \hat{\mathcal{L}}}{\partial(\partial_t \tilde{\phi})}. \tag{18}$$

We now impose the (equal time) commutation relations:

$$[\phi(x), \pi_\phi(y)] = i\delta(x-y), \tag{19}$$

$$[\tilde{\phi}(x), \tilde{\pi}_{\tilde{\phi}}(y)] = i\delta(x-y), \tag{20}$$

with the other commutators being zero. Expanding now our fields operators in momentum modes,

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} (a_k e^{-ikx} + a_k^\dagger e^{ikx}), \tag{21}$$

$$\tilde{\phi}(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} (\tilde{a}_k e^{ikx} + \tilde{a}_k^\dagger e^{-ikx}), \tag{22}$$

we induce commutation relations between the a's operators. Our knowledge about the bosonic now comes in handy, since the algebra induced by our field operators is exactly the same, that is,

$$[a_p, a_q^\dagger] = [\tilde{a_p}, \tilde{a}_q^\dagger] = (2\pi)^3 \delta_{pq}. \tag{23}$$

We now know how to induce a thermal vacuum and thermal fields with the thermal bosonic operators:

$$|0(\beta)\rangle = U(\theta)\,|0,\tilde{0}\rangle\,, \tag{24}$$

$$\phi_\beta(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_k} (a_k(\beta) e^{-ikx} + a_k^\dagger(\beta) e^{ikx}). \tag{25}$$

Let's stop to understand what is going on. Being more explicit, the initial vacuum is given, in Fock states language, by

$$|0,\tilde{0}\rangle = \otimes_k\,|0_k, \tilde{0}_k\rangle\,,$$

and the thermal transformation is similarly a product of the transformations in each mode,

$$U(\theta) = \prod_k U(\theta_k), \text{ with } U(\theta_k) = exp\{-\theta_k(\beta)(a_k\tilde{a}_k - a_k^\dagger \tilde{a}_k^\dagger)\},$$

where the $\theta_k(\beta)$ are defined exactly how we did for a single bosonic mode, but now we have one $\theta_k(\beta)$ for each energy ω_k.

6 The (thermal) Propagator

With this, we are pretty much ready for action. Let's derive the form of the thermal propagator of our fields. Let me remind the reader that for zero temperature the propagator is defined[4] as

$$iS(x-y) = \langle 0|\phi(x)\phi(y)|0\rangle \tag{26}$$

and has it's Fourier transform given by

$$i\tilde{S}(k) = \frac{1}{k^2 - m^2 + i\epsilon}. \tag{27}$$

Here, and only here, the tilde has nothing to do with the doubled space structure, it denotes the Fourier Transform of S. Now, the thermal propagator for our theory (recall the motivation for defining the thermal vacuum the way we did) will be given by

$$iS_\beta(x-y) = \langle 0(\beta)|\phi(x)\phi(y)|0(\beta)\rangle \tag{28}$$

where the fields are not thermal ones (See eq. (1))! With this, we have the tools we need to roll up our sleeves and do the calculation, which would go something like

$$\begin{aligned} iS_\beta(x-y) &= \langle 0(\beta)|\phi(x)\phi(y)|0(\beta)\rangle \\ &= \int \frac{d^3k d^3p}{(2\pi)^6}\frac{1}{4\omega_k\omega_p}\left\langle 0(\beta)\right|(a_k e^{-ikx} + a_k^\dagger e^{ikx})(a_p e^{-ipy} + a_p^\dagger e^{ipy})\left|0(\beta)\right\rangle, \end{aligned}$$

and here one would have to take care of each term of the product, such as

$$\langle 0(\beta)|e^{-i(kx+py)}a_k a_p|0(\beta)\rangle$$

(integrated over p and k momenta). This is not trivial, for the fields are not thermal, but the vacuum is. One can handle such expressions by working out the inverse Squeezing transformations of the non-thermal fields into thermal ones and then act with them on the thermal vacuum, it is not so complicated[5]. However, there is a pretty nice way to explore the structure of the thermal transformations in the creation operators, check out the appendix for the explanation of such matrix structure for the single oscillator case.

Here, we define a doublet for the fields (suppressing spacetime dependence)

[4] Yes, I know, there should be a Time Ordering operator there, but since I'm only concerned about the structure of the thing, I'm not going to be bothered to put it there. But for a strictly formal description, it should be there.

[5] And a good place to see this calculation done is in section 8.1 of the book *Thermal Quantum Field Theory - Algebraic Aspects and Applications*, by Khanna, Malbouisson, Malbouisson (yep, two of them) and Santana.

$$\Phi = \begin{pmatrix} \phi \\ \tilde{\phi}^\dagger \end{pmatrix},$$

such that we can express the thermal doublet in a simpler way (again, see the appendix for clarification)

$$\Phi_\beta = \begin{pmatrix} \phi_\beta \\ \tilde{\phi}^\dagger_\beta \end{pmatrix} = \bar{U}(\theta) \begin{pmatrix} \phi \\ \tilde{\phi}^\dagger \end{pmatrix},$$

with $\bar{U}(\theta)$ being a "simple" matrix. Actually, this matrix isn't by any means simple, after all the Squeezing transformation for the fields is an infinite product (had we quantized our theory in a box, it would be a finite one, but still), which makes $\bar{U}$ a tensor product of an infinite (or just insanely huge) number of two by two matrices, but since in the end we are going to talk about the propagator in momentum space, only one mode will be important, we will really only need to worry about two by two matrices. We will see how that goes.

With this structure, we define the propagator matrix in terms of the doublet,

$$iS^{ab}_\beta(x-y) = \langle 0(\beta)|\Phi^a(x)\Phi^b(y)|0(\beta)\rangle \tag{29}$$

with the superscripts labeling the components. Let's work the calculations in this matrix framework:

$$\begin{aligned} iS^{ab}_\beta(x-y) &= \langle 0(\beta)|\Phi^a(x)\Phi^b(y)|0(\beta)\rangle \\ &= \langle 0,\tilde{0}|U^\dagger(\theta)\Phi^a(x)U(\theta)U^\dagger(\theta)\Phi^b(y)U(\theta)|0,\tilde{0}\rangle \\ &= \langle 0,\tilde{0}|U(-\theta)\Phi^a(x)U^\dagger(-\theta)U(-\theta)\Phi^b(y)U^\dagger(-\theta)|0,\tilde{0}\rangle \end{aligned}$$

And here comes the point of the matrix notation, since $U(-\theta)\Phi U^\dagger(-\theta)$ ("componentwise") can be written as $\bar{U}(\theta)\Phi$ ("matrixwise"), we can write

$$\begin{aligned} iS^{ab}_\beta(x-y) &= \langle 0,\tilde{0}|U(-\theta)\Phi^a(x)U^\dagger(-\theta)U(-\theta)\Phi^b(y)U^\dagger(-\theta)|0,\tilde{0}\rangle \\ &= (\bar{U}(-\theta))^{ac}\,\langle 0,\tilde{0}|\Phi^c(x)\Phi^d(y)|0,\tilde{0}\rangle\,(\bar{U}^\intercal(-\theta))^{dc}. \end{aligned}$$

Now look at the last line, the object between the $\bar{U}$'s is a zero temperature propagator (in this doubled space)! So we ended up with a pretty neat expression. In momentum space, the thermal propagator is then written as (in proper matrix notation)

$$\begin{aligned} i\tilde{S}_\beta(k) = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \frac{1}{k^2-m^2+i\epsilon} & 0 \\ 0 & \frac{-1}{k^2-m^2-i\epsilon} \end{pmatrix} \times \\ \times \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix}. \end{aligned} \tag{30}$$

Working out the multiplication and writing explicitly the θ_k dependence in terms of β and ω_k, we get

$$i\tilde{S}_\beta(k) = \begin{pmatrix} \frac{1}{k^2-m^2+i\epsilon} & 0 \\ 0 & \frac{-1}{k^2-m^2-i\epsilon} \end{pmatrix} + \\ - 2i\pi\bar{n}(\omega_k)\delta(k^2-m^2)\begin{pmatrix} 1 & e^{\beta\omega_k/2} \\ e^{\beta\omega_k/2} & 1 \end{pmatrix}, \quad (31)$$

where $\bar{n}(\omega_k) = (e^{\beta\omega_k}-1)^{-1}$ is the average occupation number for bosons.

There are a number of things we can comment on this result. Fist, we notice that there is a nice split between the zero temperature and the finite temperature contributions to the propagator. This does not happen in all formalisms for finite temperature quantum field theory and is a nice feature of the Thermofield Dynamics formalism[6]. Also, we note that the δ function is selecting on-shell modes, forbidding us from having ultraviolet problems. This is a very general result[7], if our zero temperature theory is free of ultraviolet divergences, the thermal theory is also free of such problems, that is, the zero temperature counterterms are enough to renormalize the thermal theory (unfortunately, this does not help us with infrared problems). The last thing I find worth mentioning is the appearance of off-diagonal terms in the thermal contribution. The appearance of such terms makes sense in light of what we expect thermality to do to our system, as we trace out the extra degrees of freedom to recover our original system, we lose information, which makes sense!

[6] Ashok Das - *Finite Temperature Field Theory*
[7] *Ibid.*, 3.5

A Appendix: Matrix Structure

There is a very nice property that is very useful when doing calculations, and is based on a very simple observation. Let's look again at the single bosonic mode. We saw in section 4 that the thermal operators were generated by the $U(\theta)$ transformation, working out the expressions, with the help of know identities such as "Baker–Campbell–Hausdorff"-like formulas, we get the following:

$$\begin{aligned} a(\beta) &= U(\beta)aU^{\dagger}(\beta) = \cosh{(\theta)}a - \sinh{(\theta)}\tilde{a}^{\dagger} \\ a^{\dagger}(\beta) &= U(\beta)a^{\dagger}U^{\dagger}(\beta) = \cosh{(\theta)}a^{\dagger} - \sinh{(\theta)}\tilde{a} \\ \tilde{a}(\beta) &= U(\beta)\tilde{a}U^{\dagger}(\beta) = \cosh{(\theta)}\tilde{a} - \sinh{(\theta)}a^{\dagger} \\ \tilde{a}^{\dagger}(\beta) &= U(\beta)\tilde{a}^{\dagger}U^{\dagger}(\beta) = \cosh{(\theta)}\tilde{a}^{\dagger} - \sinh{(\theta)}a. \end{aligned}$$

Looking carefully, we see that there is a nice separation between these transformations. In the sense that, if we define a vector-like quantity

$$A = \begin{pmatrix} a \\ \tilde{a}^{\dagger} \end{pmatrix}, \tag{32}$$

we can encode the transformation properties of both objects in A in a matrix form,

$$A(\beta) = \begin{pmatrix} a(\beta) \\ \tilde{a}^{\dagger}(\beta) \end{pmatrix} = \begin{pmatrix} \cosh\theta(\beta) & -\sinh\theta(\beta) \\ -\sinh\theta(\beta) & \cosh\theta(\beta) \end{pmatrix} \begin{pmatrix} a \\ \tilde{a}^{\dagger} \end{pmatrix} = \bar{U}(\theta)A \tag{33}$$

where the $\bar{U}(\theta)$ is defined by this expression and given by

$$\bar{U}(\theta) = \begin{pmatrix} \cosh\theta(\beta) & -\sinh\theta(\beta) \\ -\sinh\theta(\beta) & \cosh\theta(\beta) \end{pmatrix}. \tag{34}$$

In terms of components, we have

$$A^{a}(\beta) = \bar{U}(\theta)^{ab}A^{b} \tag{35}$$

For the two remaining operators, I believe you can convince yourself that we can define another vector-like object with them and the same structure would hold.