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Thermodynamic properties of the free massless Bose field on a lattice

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Abstract A study is presented of the sensitivity of the energy density of the massless Bose field on a finite lattice, at finite temperature, when modes of different components are excluded from the partition function.

1. Introduction

The idea of describing Quantum Field Theories (QFT) on a lattice' has given many new insights into non-perturbative phenomena. From analogies drawn with statistical mechanics, it has become possible to borrow many well-known techniques. These include high temperature expansions (strong coupling), mean field theory, random walks and Monte Carlo simulations. The latter is used to evaluate path integrals numerically[2].

When QFT was studied on a lattice, questions about finite temperature calculations, in the continuum, were being investigated[3,4,5]. The next step was naturally the study of QFT at finite temperature on a finite lattice[6]. Either at finite or zero temperature, the finite lattice serves as a useful tool from which the continuum limit can be recovered.

A particular point of interest is to know the effect of finite lattice structure in finite temperature calculations. One attempt to answer this question came

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in a paper by Engels, Karsch and Satz[7], who discussed the simplest QFT: non interacting Bose and Fermi fields on a finite lattice. Considering the Bose field, particular attention was paid to the massless case, whose partition function was surprisingly found to be divergent. This divergence is due to the fact that periodic boundary conditions, p.b.c., were imposed in the space directions as well as in the temperature direction. In momentum space, this divergence turns out to be due to the zero mode contribution, $q_\mu = 0$ for all μ. Their way out of this problem was to drop this mode from the final partition function. Although finite, the solution seemed to be in contradiction with the third law of thermodynamics, as pointed out by Gorenstein, Lipskikh and Sorin[8]. In an attempt to correctly evaluate the partition function of the free massless scalar field, the latter authors eliminated not only the zero mode but also the 3-momentum zero modes from it. Their results then were in agreement with the third law of thermodynamics, but at the price of excluding from the partition function many degrees of freedom.

It is remarkable, however, that both cases have the same continuum limit for the energy density, given by the known Stefan-Boltzmann law, ϵ_{SB}. With better convergence or not, due to the lack of some modes contributing to the energy density, the role of individual components in the lattice model is not at all clear. We therefore present a study of the behaviour of the energy density when different modes are excluded from the partition function. We analyse the general contribution of isolated modes to the energy density ϵ and the convergence of the ratio ϵ/ϵ_{SB} in the continuum limit, showing the sensitivity of ϵ for practical Monte Carlo lattice sizes.

2. Basic formalism and previous results

Let us start by recalling the partition function of a system described by a Hamiltonian H

$$Z = \exp(-\beta H) \tag{2.1}$$

which can be written as the following functional integral, in Euclidean space[9]

$$Z = N \int [D\pi] \underbrace{\int}_{\text{periodic}} [D\phi] \exp\left\{ \int_0^\beta d\tau \int d^3x \left(i\pi\dot{\phi} - \mathcal{H}(\phi,\pi) \right) \right\} \tag{2.2}$$

Here $\mathcal{H}(\phi,\pi)$ is the Hamiltonian density, given in terms of the Wick rotated field $\phi(x)$ and its conjugate momentum $\pi(x)$; $\beta = (k_B T)^{-1}$ is the inverse of the physical temperature, k_B is the Boltzmann constant, set equal to 1 and N is a normalizing factor. (Note that $\dot{\phi} = d\phi/d\tau$). The periodic paths considered in the above functional integral are those for which $\phi(\vec{x},0) = \phi(\vec{x},\beta)$. As $\mathcal{H}$ usually has only quadratic dependence on r, the r-integration can be performed to give

$$Z = N'(\beta) \underbrace{\int}_{\text{periodic}} [d\phi] \exp(-S(\phi) \tag{2.3}$$

where $N'(\beta)$ is a temperature-dependent normalisation factor and $S(\phi)$ is the Euclidean action, given in terms of the Lagrangean density of the system

$$S(\phi) = -\int_0^\beta d\tau \int d^3x \mathcal{L}(\phi) \tag{2.4}$$

The above finite temperature field theory formalism is used for the case of the free massive scalar Bose field on a Euclidean lattice[7]. The aim is to evaluate the partition function and the thermodynamic properties derived from it. Consider the following Hamiltonian density

$$\mathcal{H}(\phi,\pi) = 1/2(\tilde{a}^2 + (\nabla\phi)^2 + m^2\phi^2) \tag{2.5}$$

and introduce it in eq.(2.2). The discretized partition function is given by

$$Z_E(N_\sigma, N_\beta, a_\sigma, a_\beta) = N' \int \Pi_\alpha d\phi(x_\alpha) \exp(-S(\phi)) \tag{2.6}$$

where the scalar field ϕ takes a value $\phi(x_\alpha)$ on each site x, of a lattice of N_σ^3 x N_β sites, with spacings a, and a_β in the space and temperature directions respectively. Here N' is the temperature dependent normalisation factor

$$N' = \left(\frac{a_\sigma^3}{2\pi a_\beta}\right)^{N_\sigma^3 N_\beta/2} \tag{2.7}$$

(fixed so that the partition function is dimensionless) and the action ***S(4)*** is

$$S(\phi) = 1/2a_\sigma^3 a_\beta \sum_\alpha \left\{ \sum_{\mu=1}^{3} \left(\frac{\phi(x_\alpha + \epsilon_\mu) - \phi(x_\alpha)}{a_\sigma}\right)^2 + \left(\frac{\phi(x_\alpha + \epsilon_0) - \phi(x_\alpha)}{a_\beta}\right)^2 + m^2\phi^2(x_\alpha)\right\} \tag{2.8}$$

where E, is a vector of length ***a,*** $(\mu = 1,2,3)$ or a_β $(\mu = 0)$ in the μ direction. The sum in α runs over all sites of the lattice. Also, periodic boundary conditions in all directions are imposed on the fields: $\phi(x_\alpha + N_\alpha\epsilon_\mu) = \phi(x_\alpha), \mu = 1,2,3; \phi(x_\alpha + N_\beta\epsilon_0) = \phi(x_\alpha)$. Notice that in the naive continuum limit ***a,, a,*** $\to \beta$ the action of the massive free field theory is recovered.

The diagonalization of ***S(4)*** by means of a Fourier transform gives the result

$$Z_E(N_\sigma, N_\beta, a_\sigma, \xi) = \xi^{N_\sigma^3 N_\beta}\Pi_q G^{1/2}(a_\sigma, \xi, q) \tag{2.9}$$

where ξ r a_σ/a_β and $G(a_\sigma, \xi, q)$ is the dimensionless lattice free field propagator given by

$$G^{-1}(a_\sigma, \xi, q) = (ma_\sigma)^2 + 4\sum_{\mu=1}^{3}\sin^2\left(\frac{1}{2}q_\mu a_\sigma\right) + 4\xi^2\sin^2\left(\frac{1}{2}q_0 a_\beta\right) \tag{2.10}$$

The four-momenta q take values in the first Brillouin zone of the reciprocal lattice

$$\begin{aligned} \mu &= 0 \\ q_0 &= \frac{2\pi j_0}{N_\beta a_\beta} \\ j_0 &= \begin{cases} 0, \pm1, ..., \pm(N_\beta/2 - 1), N_\beta/2; (N_\beta \text{ even}) \\ o, \pm1, ..., \pm(N_\beta - 1)/2; (N, \text{ odd}) \end{cases} \end{aligned} \tag{2.11}$$

$$\mu = 1,2,3$$
$$q_\mu = \frac{2\pi j_\mu}{N_\sigma a_\sigma}$$
$$j_\mu = \begin{cases} 0, \ \pm1, ..., \pm(N_\sigma/2 - 1), N_\sigma/2; (\text{Nu even}) \\ 0, \ \pm1, ..., \pm(N_\sigma - 1)/2; (N_\sigma \text{ odd}) \end{cases}$$

The important feature of expression (2.9) is that for the free massless case the zero mode $q_\mu = 0$ for all μ, gives an infinite contribution, as can be seen from eq.(2.10) with m = 0. Tracing this contribution in the functional integral, we find that whenever $\phi(x_\alpha)$ is the same constant for all sites $x_\alpha, \phi(x_\alpha) = \phi(x'_\alpha)$, the integrand in eq.(2.6) is also a constant and therefore the contribution of constant configurations to the integral is infinite. It is then clear that the divergence arises because periodic boundary conditions were imposed not only in the temperature direction but in the space direction as well. If we take $\phi = 0$ boundary conditions, this divergence disappears. The integration along the line of constant field configuration for all sites then gives one contribution, which is zero. By performing this calculation with zero boundary conditions we get a finite answer, but we have an extra constraint, $\phi(x_\alpha + N_{\alpha,\beta}\epsilon_\mu) = \phi(x_\alpha) = 0$, therefore restricting the number of degrees of freedom.

In ref.7, which we refer to as (EKS), the interest was in the massless case and this problem was circumvented by dropping the zero mode term from eq.(2.9). All the subsequent calculations were therefore performed using the partition function as

$$Z_E(N_\sigma, N_\beta, a_\sigma, \xi) = \xi^{N_\sigma^3 N_\beta} \Pi'_q G^{1/2}(a_\sigma, \xi, q) \tag{2.12}$$

where the dash stands for the absence of the q = 0 mode, $q = (q_0, \vec{q})$.

The value of the energy density, normalized to zero at T = 0, (see appendix), was then given by

$$\epsilon_{EKS} = -\frac{\xi^3}{N_\sigma^3 N_\beta a_\sigma^4} \sum_j{}' \frac{\sin^2(\pi j_0/N_\beta)}{b^2(\vec{j}) + \xi^2 \sin^2(\pi j_0/N_\beta)}$$
$$+ \frac{\xi^3}{N_\sigma^3 a_\sigma^4} \sum_j \left[b(\xi^2 + b^2)^{1/2} + \xi^2 + b^2\right]^{-1} \tag{2.13}$$

We can sum the j_0 component[8] to get

$$\epsilon_{EKS} = \frac{\xi}{N_\sigma^3 a_\sigma^4} \sum_j{}' \frac{b}{(b^2 + \xi^2)^{1/2}} \left\{\mathrm{cth}\left[N_\beta sinh^{-1}(b/\xi)\right] - 1\right) + \frac{\xi}{N_\sigma^3 N_\beta a_\sigma^4} \tag{2.14}$$

with

$$b^2(\vec{j}) = \sum_{\mu=1}^{3} \sin^2(\pi j_\mu/N_\sigma) \tag{2.15}$$

(again the dash means that the zero mode is absent).

The effect of the finite lattice approximation was seen by comparing the above expression for the energy density with the well-known continuum form for the energy density of a photon *gas.* This is given by the Stefan-Boltzmann law[10]

$$\epsilon_{SB} = \frac{\pi^2}{30}\beta^{-4} \tag{2.16}$$

This problem was next examined by Gorenstein, Lipskikh and Sorin[8], hereafter referred to as (GLS), when considering the quantization of the free massless Bose field in a finite volume V. Starting from the Hamiltonian

$$H = \int_v d^3x \mathcal{H}(\Pi, \phi) = 1/2 \int d^3x\left(\Pi^2 + (\vec{\nabla}\phi)^2\right) \tag{2.17}$$

they considered the quantized system in which the above Hamiltonian is written in terms of creation and annihilation operators and the vacuum energy is zero

$$H = \sum_{\vec{k}}{}' \omega_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} \tag{2.18}$$

where the dash rneans absence of the $\vec{k}=0$ mode.

Repeting the same analysis as before, their partition function for the massless free field, with the above Hamiltonian is given in terms of δ function

$$Z = \underbrace{\int}_{\text{periodic}} [D\phi]\Pi_\tau \left\{\delta\Big(\int_v d^3x\, \phi(\vec{x},\tau)\Big)\cdot\delta\Big(\int_v d^3x\, \Pi(\vec{x},\tau)\Big)\cdot(2\pi)^4\right\}$$
$$\cdot \exp\left\{\int_0^{\beta} d\tau \int d^3x\big(i\pi\dot{\phi} - \mathcal{H}(\Pi,\phi)\big)\right\} \tag{2.19}$$

And the final partition function on the Iattice is

$$Z_{GLS}(N_\sigma, N_\beta, a_\sigma, \xi) = N\xi^{(N_\sigma^3 - 1)N_\beta} \frac{\Pi'_q G^{1/2}(a_\sigma,\xi,q)}{\Pi'_{q_0} G^{1/2}(a_\sigma,\xi,q_0)} \tag{2.20}$$

where $G^{-1}(a_\sigma,\xi,q)$ is given by eq.(2.10) for m = 0 and N is a ξ-independent normalisation factor.

The comparison between eq.(2.20) and eq.(2.12) shows that the total 3-momentum zero mode contribution has been extracted from the propagator via the term

$$\Pi'_q G^{1/2}(a_\sigma, \xi, q = (q_0, \vec{0}))$$

The contribution of this term to the energy density is such that

$$\epsilon_{GLS} = \frac{\xi}{N_\sigma^3 a_\sigma^4} \sum_j{}' \frac{b}{(b^2+\xi^2)^{1/2}} \left\{\mathrm{cth}\left[N_\beta \sinh^{-1}(b/\xi)\right] - 1\right\}$$
$$= \epsilon_{EKS} - \frac{\xi}{N_\sigma^3 N_\beta a_\sigma^4} \tag{2.21}$$

It is clear then that the role of the 6 function in eq.(2.19) was to subtract the term $\xi/(N_\sigma^3 N_\beta a_\sigma^4)$. The main feature of this subtraction is that this term contributes with an N_β-independent term to the specific heat C,, which does not vanish in the zero temperature ($N_\beta \to \infty$) limit, preventing the validity of the third law of thermodynamics. We should remind the reader that the third law of thermodynamics concerns the fact that in the zero temperature limit the entropy vanishes and, as a consequence, so does the specific heat.

We see that the exclusion of modes in the (GLS) case has changed the thermodynamic properties of the lattice model, so that the third law of thermodynamics now holds. However, even though we have some advantages brought up with the exclusion of these modes, the way this is carried out in both approaches ís still arbitrary. On the one hand, (EKS) treated the zero mode in a way such that the supression of the integration over constant field configurations resulted in dropping the zero mode from the partition function. On the other hand, when considering the Hamiltonian as the one that has zero vacuum energy, the (GLS) case, the actual claim was that the constant field configurations were excluded from the functional integral via 6 functions. But this turned out to suppress not only the zero mode but modes of the form $q = (q_0, 0)$ as well, for any q_0, that is, the 3-momentum zero mode for the whole temperature range. As a result, the third law now holds; the thermodynamics of the discretized system has really changed.

Therefore, facing this apparent contradiction in dealing with different modes of the partition function, it remains inconclusive how other modes actually contribute to the energy density, without altering the continuum limit or thermodynamic quantities like the specific heat. To study the sensitivity of the energy density we take (EKS)'s partition function as a standard result, because it has all modes of the 4 components - except the $q = 0$ mode. We then consider various cases in which different modes are suppressed each time from Z_{EKS} and evaluate the energy density c. Then we analyse the ration ϵ/ϵ_{SB} for different size lattices, which show how the initial results were affected. We therefore shall be dealing with partition functions that are written as

$$Z_i = \frac{Z_{EKS}}{I_i(a_\sigma, \xi)} \tag{2.22}$$

where I_i(a,, ξ) denotes the contribution of isolated modes taken away from the massless propagator $G(a_\sigma, \xi, q)$, given by eq.(2.10) for $m = 0$, that is

$$I_i(a_\sigma, \xi) \propto \underbrace{\Pi'_q}_{\text{individual modes}} G^{1/2}(a_\sigma, \xi, q) \tag{2.23}$$

Thus the energy density will be of the form (see appendix),

$$\epsilon_i = \epsilon_{\text{EKS}} + \delta\epsilon_i \tag{2.24}$$

where

$$\delta\epsilon_i = -\frac{\xi^2}{N_\sigma^3 a_\sigma^4} \frac{\partial}{\partial\xi} \left(\frac{\ln I_i}{N_\beta} - \lim_{N_\beta \to \infty} \frac{\ln I_i}{N_\beta} \right)_{a_\sigma, N_\sigma, N_\beta} \tag{2.25}$$

3. Results

We have considered 5 different cases at random, for which we present joint graphs for comparison with the (EKS) and (GLS) cases.

Case 1 - Consider I_i (a,, ξ) such that it removes from the propagator the zero modes: $q_\mu = 0$ for $\mu = 0, 2, 3$ or equivalently $j_\mu = 0$, $\mu = 0, 2, 3$

$$I_1(a_\sigma, \xi) = \Pi'_{j_1} G^{1/2}(a_\sigma, \xi, j = 0, j_1, 0, 0)) \tag{3.1}$$

We can immediately see from eq.(2.10) that I_i is ξ-independent, which means that $\delta\epsilon_1$ given by eq.(2.25) is zero, that is, $\epsilon_1 = \epsilon_{\text{EKS}}$. In other words, modes that do not contribute with a ξ-dependence can be removed from the partition function without altering the (EKS) result.

Case 2 - In this case, we choose I_2 *(a,,* ξ) in order to remove from the propagator a fixed non-zero 3-momentum vector $\vec{q}$, or equivalently, a non-zero 3-vector $\vec{j}$ as in eq.(2.11), i.e.,

$$I_2(a_\sigma, \xi) = \Pi'_{j_0} G^{1/2}(a_\sigma, \xi, j = (j_0, \vec{j})), \text{for fixed } \vec{j}, \vec{j} \neq 0 \tag{3.2}$$

This is a very special case which can be directly compared with (GLS), for which $\vec{j} = 0$ (cf. eq. 2.20).

The energy density here is given by

$$\epsilon_2 = \epsilon_{\mathrm{EKS}} - \frac{\xi}{N_\sigma^3 a_\sigma^4} \frac{b}{(b^2 + \xi^2)^{1/2}} \{\mathrm{cth}\left[N_\beta \sinh^{-1}(b/\xi)\right] - 1\} \tag{3.3}$$

or

$$\epsilon_2 = \epsilon_{\mathrm{EKS}} + \delta\epsilon_2$$

where b is given by eq.(2.15). We have considered particular values of $\vec{j}$:

1) $\vec{j} = (0,0,1)$ 2) $\vec{j} = (0,1,1)$

3) $\vec{j} = (1,1,1)$ 4) $\vec{j} = (N_\sigma/2, N_\sigma/2, N_\sigma/2)$

Comparing $\epsilon_2/\epsilon_{\mathrm{SB}}$ with $\epsilon_{\mathrm{EKS}}/\epsilon_{\mathrm{SB}}$ we found that the only significant difference comes from $\vec{\mathbf{j}} = (0,0,1)$, which we show in *figs.* 1, 2, **3.** *For all* the other values of $\vec{j}$, the difference is negligible, especially for increasing values of N_σ, N_β, where we have ę =,,é ,.

We should point out that the (GLS) case can be recovered by taking the $\vec{q} \to 0$ $(b \to 0)$ limit in $\delta\epsilon_2$. The behaviour of ϵ_2/ϵ_{SB} is therefore crucially different from the one where $\vec{q} \neq 0$, and so are other thermodynamic properties as for instance, the specific heat. Here, unlike the $\vec{q} = 0$ case, the specific heat (derived in the appendix) does not vanish in the limit $N_\beta \to \infty$ (T $\to$ 0).

Case 3 - Let us remove from the partition function the two zero components of the 3-momentum, through $I_3(a,, \xi)$ given by

$$I_3(a_\sigma, \xi) = \Pi'_{j_0,j_1} G^{1/2}(a_\sigma, \xi, j = (j_0, j_1, 0, 0)) \tag{3.4}$$

which can be rewritten as the products

$$I_3 = \Pi'_{j_0} G^{1/2}(a_\sigma, \xi, j = (j_0, 0, 0, 0)) \cdot \Pi_{\substack{j_0,j_1 \\ j_0 \neq 0}} G^{1/2}(a_\sigma, \xi, j) = (j_0, j_1, 0, 0)) \tag{3.5}$$

This shows directly that we have included the (GLS) case. Hence the energy density is

$$\epsilon_3 = \epsilon_{GLS} - \frac{\xi}{N_\sigma^3 a_\sigma^4} \sum_{j_1} \frac{b}{(b^2 + \xi^2)^{1/2}} \{\mathrm{cth}[N_\beta \sinh^{-1}(b\xi)] - 1\} \tag{3.6}$$

where in this case

$$b^2(\vec{j}) = \sin^2(\pi j_1 / N_\sigma) \tag{3.7}$$

Once the (GLS) case has been included, we expect the ratio ϵ_3/ϵ_{SB} to be smaller than $\epsilon_{GLS}/\epsilon_{SB}$. In fact we should note that this case is actually a combination of a Case **2** and (GLS) case, which stresses even more the difference from $\epsilon_{EKS}/\epsilon_{SB}$, especially for small values of N_σ and N_β, (see fig. 1). An increase in N_β at fixed N_σ (low temperature limit) makes ϵ_3/ϵ_{SB} approach zero rapidly again, as opposed to the divergent behaviour of $\epsilon_{EKS}/\epsilon_{SB}$. Larger values of N_σ and N_β (with $N_\sigma >> N_\beta$) make this ratio converge to 1, but in a slower way than in (GLS), see figs. 2 and **3**.

Case 4 - This is the simplest case considered, in which only one mode is suppressed from the original partition function

$$I_4(a_\sigma, \xi) = G^{1/2}(a_\sigma, \xi, j), \text{ for fixed } j = (j_0, \vec{j}), \quad j \neq 0 \tag{3.8}$$

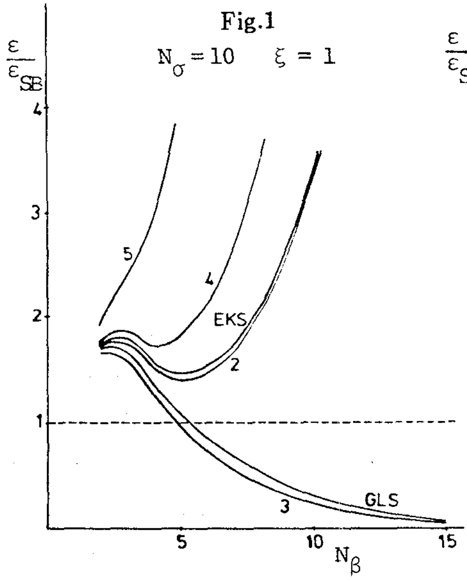
In contrast with the previous case, its contribution to the energy density has increased ϵ_{EKS} by a positive number

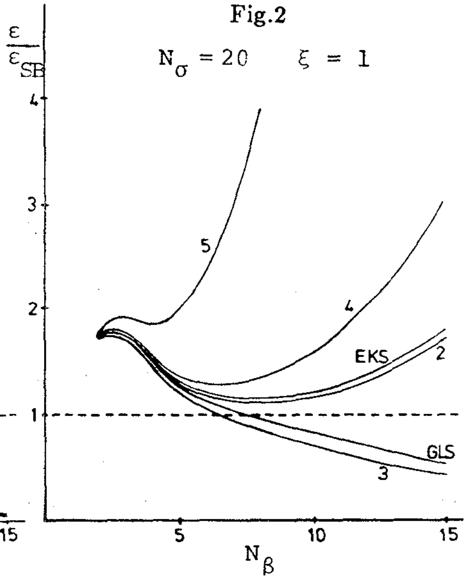
$$\delta\epsilon_4 = \frac{\xi^3}{N_\sigma^3 N_\beta a_\sigma^4} \frac{\sin^2(\pi j_0/N_\beta)}{b^2 + \xi^2 \ \sin^2(\pi j_0/N_\sigma)} \tag{3.9}$$

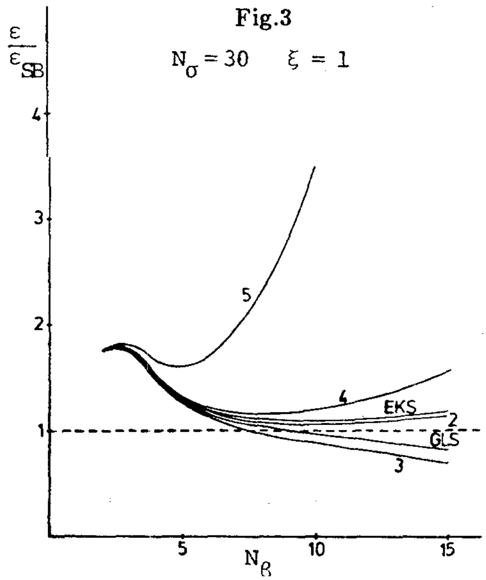
The reason why we now have $\delta\epsilon > 0$ is due to the fact that the vacuum contribution of this isolated mode is zero (see eq.2.25). To see by how much ϵ_{EKS} is increased, we have considered special values of $j; j = (j_0, j_1, j_2, j_3)$

a) $j = (1,0,0,0)$ b) $j = (N_\beta/2,0,0,0)$ c) $j = (1,1,0,0)$

d) $j = (N_\beta/2,1,0,0)$ e) $j = (1, N_\sigma/2, N_\sigma/2, N_\sigma/2)$







The ratios of energy densities: $\epsilon_{EKS}/\epsilon_{SB}$, $\epsilon_{EKS}/\epsilon_{SB}$ and ϵ_i/ϵ_{SB} $(\mathbf{i} = 2,3,4,5)$ as functions of N_β at fixed N_σ and with $\xi = 1$. **Fig.1** - $N_\sigma = 10$. Fig.2 - N_σ **= 20. Fig.3** - N_σ **= 30.**

When we take **j** as in a) or b), because their 3-momentum $\vec{j} = 0$, the energy density is trivially reduced to

$$\epsilon_4 = \epsilon_{EKS} + \frac{\xi}{N_\sigma^3 N_\beta a_\sigma^4}$$

that is, $\delta\epsilon_4$ gives exactly the same absolute value at $\delta\epsilon_{GLS}$ (cf. eq. 2.21). Thus the deviation from ϵ_{EKS} is very large. For the other values of j we note that when j_0 is large and $\vec{j}$ has small j_1, j_2 and j_3 components, ϵ_4/ϵ_{SB} is very large, compared to $\epsilon_{EKS}/\epsilon_{SB}$ as shown in figs. 1, 2, 3 for different values of N_β and N_σ, with $\epsilon = 1$. If $\vec{j}$ has higher values of j_1, j_2, j_3, the result is that $\epsilon \cong \epsilon_{EKS}$.

Case 5 - Suppose that we remove from the partition function modes with j_0, j_2 and j_3 fixed. This is accomplished with I_5(a,, ξ) given by

$$I_5(a_\sigma, \xi) = \Pi_{j_1} G^{1/2}(a_\sigma, \xi, j), \quad j = (j_0, j_1, j_2, j_3) \tag{3.10}$$

for fixed j_0, j_2 and $j_3, j_0 \neq 0$. The energy density, as in case 4, will be given by $\epsilon_5 = \epsilon_{EKS} + \delta\epsilon_5, \delta\epsilon_5 > 0$, and with

$$\delta\epsilon_5 = \frac{\xi^4}{N_\sigma^2 N_\beta a_\sigma^4} \frac{\sin^2(\pi j_0/N_\beta)}{\left(b^2 + \xi^2 \sin^2(\pi j_0/N_\beta)\right)^{1/2}} \frac{\mathrm{cth}\left[N_\sigma \sinh^{-1}\left(b^2 + \xi^2 \sin(\pi j_0/N_\beta)\right)^{1/2}\right]}{\left(1 + b^2 + \xi^2 \sin(\pi j_0/N_\beta)\right)^{1/2}} \tag{3.11}$$

where

$$b^2(j) = \sin^2(\pi j_2/N_\sigma) + \sin^2(\pi j_3/N_\sigma)$$

We have analysed the following special cases of (j_0, j_2, j_3) :

a) $(1,0,0)$; b) $(1, N_\sigma/2, 0)$; c) $(N_\beta/2, 0, 0)$; d) $(N_\beta/2, N_\sigma/2, 0)$

Although the amount $\delta\epsilon_5$ of the contributes to ϵ_{EKS} is much greater than $\delta\epsilon_4$ in Case 4, the conclusions for this case remain almost the same: an increase in j_2 and j_3 with small j_0 makes $\delta\epsilon_5$ small. Nevertheless, going through intermediate values of j_2, j_3 and j_0 we see great changes in the energy density, especially for the case $j_0 = N_\beta/2$ and $j + 2 = j_3 = 0$, which is shown in figs. 1, 2 and 3. It is interesting to note that no change takes place in the energy density ϵ_{EKS} for $j_0 = j_2 = j_3 = 0$; it is when Case 1 is recovered (cf. eq. 3.1 and 3.10). The difference between this case and GLS is remarkable, since in both there is the lack of one full component of momenta, (see figs.).

4. Discussion and Conclusions

We have investigated the behaviour of the energy density of a free massless Bose field on a finite Euclidean lsttice, at finite temperatures, when different modes plus the zero mode contributiori are suppressed from the partition function.

From two already existing models to correctly evaluate the partition function of this field theory, we took the first, the (EKS) case, as standard and studied the change caused by the exclusion of other modes to physical quantities such as the energy density. We should point out that we were not interested in establishing a new model system for this field theory, but in analysing the general contribution of isolated modes to the energy density. We have done so in view of the arbitrariness of those approaches, especially the (GLS) case, which has implemented great changes in the thermodynamic quantities such as the specific heat. Notice that this case also excludes the 4-momentum zero mode in their treatment and this is why we took the (EKS) case as standard.

Looking separately at each case we have treated, we note that apart from case 3, cases 2, 4 and 5 present the same general pattern: the ratio of energy densities ϵ/ϵ_{SB} shows that they all have a best N_β (sufficiently large), so that after that the curve diverges. This actually occurs in the EKS case. Increasing N_β and N_σ with $N_\sigma \geq N_\beta$, the curves flatten , and approach the value 1. The finite size effects for cases 4 and 5, where the.3-momentum modes were excluded at fixed temperature, are larger than for the ones where the temperature modes were excluded, as in cases **2** and 3. For the latter, case 3, the ratio of energy densities shows the same behaviour as (GLS), and we can see that what really made a change was the absence of the full 3-momentum zero mode for all temperature values. Here, this ratio is mainly a decreasing function of N_β, for fixed N_σ, ξ, tending to zero for large N_β, (zero temperature limit). If N_σ is also large as $N_\beta \rightarrow \infty$, it can then converge to **1,** if $N_\sigma > N_\beta$. The finite size effects are smaller when compared to (EKS), but larger if compared to (GLS). The difference that only one mode can make to the finite lattice size effects is surprising. Case 4, for instance, shows that the isolated influence of one mode is enormous when compared to the case where many modes have been dropped, such as case **2.**

Concerning other thermodynamic quantities, like for instance the specific heat, there are changes: whenever the zero 3-momentum mode is excluded, this change is such that C_v vanishes in the $T \rightarrow 0$ limit. This however only happens in (GLS) and case 3. Otherwise C_v is a constant in the zero temperature limit, contradicting results such as the third law of thermodynamics.

We conclude that the influence of finite lattice size is not negligibe in quantities like the energy density; isolated modes can drastically change finite size effects. Therefore, if one studies the free theory in order to use the knowledge learnt from it to apply to more complicated (interactive) systems, one has to be very careful before neglecting unwanted infinities. It may turn out that one would be dropping modes that give significant contributions to the energy density.

Appendix

Having evaluated the partition function Z_E, we can calculate thermodynamic quantities like the free energy, the energy density and so on. In the following we recall the definition of these quantities and their related discrete forms. On the lattice, since $V = N_\sigma^3 a_\sigma^3$ and $\beta = N_\beta a_\beta$, the discrete derivatives, given at fixed N_σ and N_β are (for $\xi = a_\sigma / a_\beta$) :

$$\left(\frac{\partial}{\partial \beta}\right)_v = -\frac{\xi^2}{N_\beta a_\sigma}\left(\frac{\partial}{\partial \xi}\right)_{a_\sigma, N_\sigma, N_\beta}$$

$$\left(\frac{\partial}{\partial V}\right)_\beta = \frac{1}{3N_\sigma^3 a_\sigma^2}\left(\frac{\partial}{\partial a_\sigma}\right)_{a_\beta, N_\sigma, N_\beta} = \frac{1}{3N_\sigma^3 a_\sigma^2}\left\{\left(\frac{\partial}{\partial a_\sigma}\right)_\xi + \frac{\xi}{a_\sigma}\left(\frac{\partial}{\partial \xi}\right)_{a_\sigma}\right\}$$

Thus, the energy density, defined by

$$\epsilon = \frac{\partial}{\partial \beta}(\beta f)_v$$

is written on a lattice as

$$\epsilon = -\frac{\xi^2}{N_\beta a_\sigma}\left\{\frac{\partial}{\partial \xi}\left(\frac{N_\beta a_\sigma}{\xi} f\right)\right\}_{a_\sigma, N_\sigma, N_\beta}$$

where f is the Helmholtz free energy density,

$$f = -\frac{1}{\beta V}\ln Z$$

Its discrete form, normalized to zero at zero temperatute $(N_\beta \to \infty)$ is

$$f = f_E - \lim_{N_\beta \to \infty} f_E$$

with

$$\begin{aligned} f_E &= -\frac{1}{N_\sigma^3 a_\sigma^3}\frac{\xi}{N_\beta a_\sigma}\ln Z_E \\ &= \frac{\xi}{a_\sigma^4}\ln \xi + \frac{\xi}{2N_\sigma^3 a_\sigma^4 N_\beta}\sum \ln G^{-1}(a_\sigma, \xi, q) \end{aligned}$$

Finally, the specific heat is defined by

$$C_v = \left(\frac{\partial \epsilon}{\partial T}\right)_v$$

and takes the following discrete form

$$C_v = N_\beta a_\sigma \left(\frac{\partial \epsilon}{\partial \xi}\right)_{a_\sigma}$$

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Resumo

Apresentamos um estudo da sensitividade da densidade de energia de um campo de Bose livre e não massivo numa rede finita e à temperatura finita, quando modos de componentes diferentes do momento são excluidos da função de partição.