Thermal field theories and shifted boundary conditions

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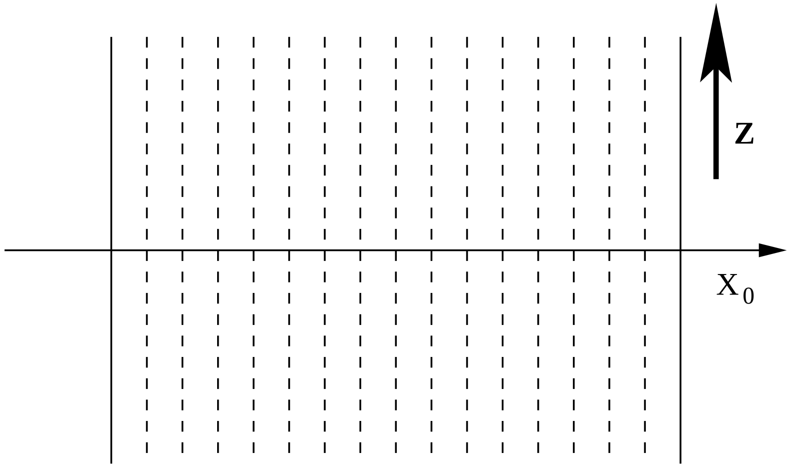
Related presentations: L. G., M. Pepe Poster Session B; H. B. Meyer, D. Robaina talk session 1C.

Outline

- Free-energy density with "shifted" boundary conditions

$$f\left(\sqrt{L_0^2 + \boldsymbol{z}^2}\right) = - \lim_{V\to\infty} \frac{1}{L_0 V} \ln Z(L_0, \boldsymbol{z})$$

$$\phi(L_0, \boldsymbol{x}) = \phi(0, \mathbf{x} - \boldsymbol{z})$$



- Ward Identities in infinite and finite volume

- Applications on the lattice

- Conclusions and outlook

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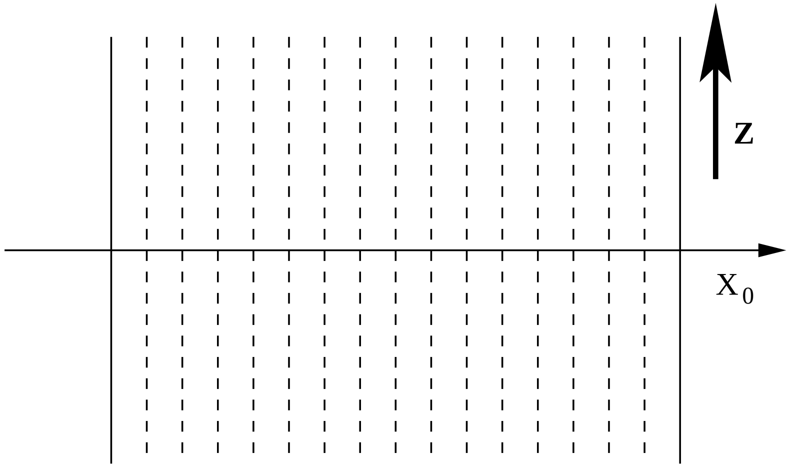

- Ward Identities in infinite and finite volume
- Applications on the lattice
- Conclusions and outlook

Path integrals with shifted boundary conditions: infinite-volume limit (I)

- We are interested in the partition function

$$\phi(x) = \phi(x + V_{\rm sbc} m) \quad m \in \mathbb{Z}^4$$

$$Z(L_0, \boldsymbol{\xi}) = \mathrm{Tr}\left\{ e^{-L_0(\widehat{H} - i\boldsymbol{\xi}\cdot\widehat{\boldsymbol{P}})} \right\}$$

$$V_{\rm sbc} = \begin{pmatrix} L_0 & 0 & 0 & 0 \\ L_0\xi_1 & L_1 & 0 & 0 \\ L_0\xi_2 & 0 & L_2 & 0 \\ L_0\xi_3 & 0 & 0 & L_3 \end{pmatrix}$$

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- By making an Euclidean ”boost” rotation

$$\gamma_1 = \frac{1}{\sqrt{1+\xi_1^2}}$$

$$\Lambda = \begin{pmatrix} \gamma_1 & \gamma_1\xi_1 & 0 & 0 \\ -\gamma_1\xi_1 & \gamma_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

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Lorentz [SO(4)] invariance implies

$$Z(L_0, \boldsymbol{\xi}) = \mathrm{Tr}\left\{ \exp -L_1\gamma_1(\widetilde{H} + i\xi_1 \widetilde{P}_0) \right\}, \qquad V'_{\rm sbc} = \Lambda\, V_{\rm sbc} = \begin{pmatrix} L_0/\gamma_1 & L_1\gamma_1\xi_1 & 0 & 0 \\ 0 & L_1\gamma_1 & 0 & 0 \\ 0 & 0 & L_2 & 0 \\ 0 & 0 & 0 & L_3 \end{pmatrix}$$

Path integrals with shifted boundary conditions: infinite-volume limit (II)

- Assuming that $\widetilde{H}$ has a translationally-invariant vacuum and a mass gap [$\boldsymbol{\xi} = \{\xi_1, 0, 0\}$]

$$Z(L_0, \boldsymbol{\xi}) = \mathrm{Tr}\left\{ \exp -L_1\gamma_1(\widetilde{H} + i\xi_1 \widetilde{P}_0)\right\}, \qquad V'_{\rm sbc} = \Lambda\, V_{\rm sbc} = \begin{pmatrix} L_0/\gamma_1 & L_1\gamma_1\xi_1 & 0 & 0 \\ 0 & L_1\gamma_1 & 0 & 0 \\ 0 & 0 & L_2 & 0 \\ 0 & 0 & 0 & L_3 \end{pmatrix}$$

the right hand side becomes insensitive to the phase in the limit $L_1 \to \infty$ at fixed ξ_1

$$f\left(L_0\sqrt{1+\xi_1^2}\right) = -\lim_{V\to\infty} \frac{1}{L_0 V} \ln Z(L_0, \boldsymbol{\xi}) \qquad V''_{\rm sbc} = \begin{pmatrix} L_0/\gamma_1 & 0 & 0 & 0 \\ 0 & L_1\gamma_1 & 0 & 0 \\ 0 & 0 & L_2 & 0 \\ 0 & 0 & 0 & L_3 \end{pmatrix}$$

- Thanks to cubic symmetry (infinite volume)

$$f\left(L_0\sqrt{1+\boldsymbol{\xi}^2}\right) = -\lim_{V\to\infty} \frac{1}{L_0 V} \ln Z(L_0, \boldsymbol{\xi}), \qquad \phi(L_0, \boldsymbol{x}) = \phi(0, \boldsymbol{x} - L_0\boldsymbol{\xi})$$

for a generic shift $\boldsymbol{\xi}$

Thermal field theory in a moving frame

- If $\widehat{H}$ and $\widehat{\boldsymbol{P}}$ are the Hamiltonian and the total momentum operator expressed in a moving frame, the standard partition function is

$$\mathcal{Z}(L_0, \boldsymbol{v}) \equiv \mathrm{Tr}\left\{e^{-L_0\,(\widehat{H} - \boldsymbol{v}\cdot\widehat{\boldsymbol{P}})}\right\}$$

- If we continue $\mathcal{Z}$ to imaginary velocities $\boldsymbol{v} = i\boldsymbol{\xi}$

$$Z(L_0, \boldsymbol{\xi}) = \mathrm{Tr}\,\{e^{-L_0(\widehat{H} - i\boldsymbol{\xi}\cdot\widehat{\boldsymbol{P}})}\}$$

- The functional dependence $f(L_0\sqrt{1+\boldsymbol{\xi}^2})$ is consistent with modern thermodynamic arguments on the Lorentz transformation of the temperature and the free-energy

  [Ott 63; Arzelies 65; see Przanowski 11 for a recent discussion]

- In the zero-temperature limit the invariance of the theory (and of its vacuum) under the Poincaré group forces its free energy to be independent of the shift $\boldsymbol{\xi}$

- At non-zero temperature the finite length L_0 breaks SO(4) softly, and the free energy depends on the shift (velocity) explicitly but only through the combination $\beta = L_0\sqrt{1+\boldsymbol{\xi}^2}$

Ward identities for correlators of $\overline{T}_{\mu\nu}$ at zero shift

- In the path integral formalism

$$L_0 \, \langle \overline{T}_{01} \, T_{01} \rangle_c = \langle T_{00} \rangle - \langle T_{11} \rangle$$

$$L_0^3 \, \langle \overline{T}_{01} \, \overline{T}_{01} \, \overline{T}_{01} \, T_{01} \rangle_c = 9 \, \langle T_{11} \rangle - 9 \, \langle T_{00} \rangle + 3 \, L_0 \, \langle \overline{T}_{00} T_{00} \rangle_c \ ,$$

$$\ldots$$

where $\overline{T}_{\mu\nu}(x_0) = \int d^3x \, T_{\mu\nu}(x)$.

- Note that:
  - $*$ All operators at non-zero distance
  - $*$ Number of EMT on the two sides different
  - $*$ On the lattice they can be imposed to fix the renormalization of $T_{\mu\nu}$

- These WIs implies that the total energy and momentum distributions are related

Ward identities at non-zero shift

- When $\boldsymbol{\xi} \neq 0$ odd derivatives in the ξ_k do not vanish anymore, and new interesting WIs hold. The first non-trivial one is

$$\langle T_{0k} \rangle_{\boldsymbol{\xi}} = \frac{\xi_k}{1-\xi_k^2} \left\{ \langle T_{00} \rangle_{\boldsymbol{\xi}} - \langle T_{kk} \rangle_{\boldsymbol{\xi}} \right\} \; .$$

which implies

$$s = -\frac{L_0 \, (1+\boldsymbol{\xi}^2)^{3/2}}{\xi_k} \langle T_{0k} \rangle_{\boldsymbol{\xi}}$$

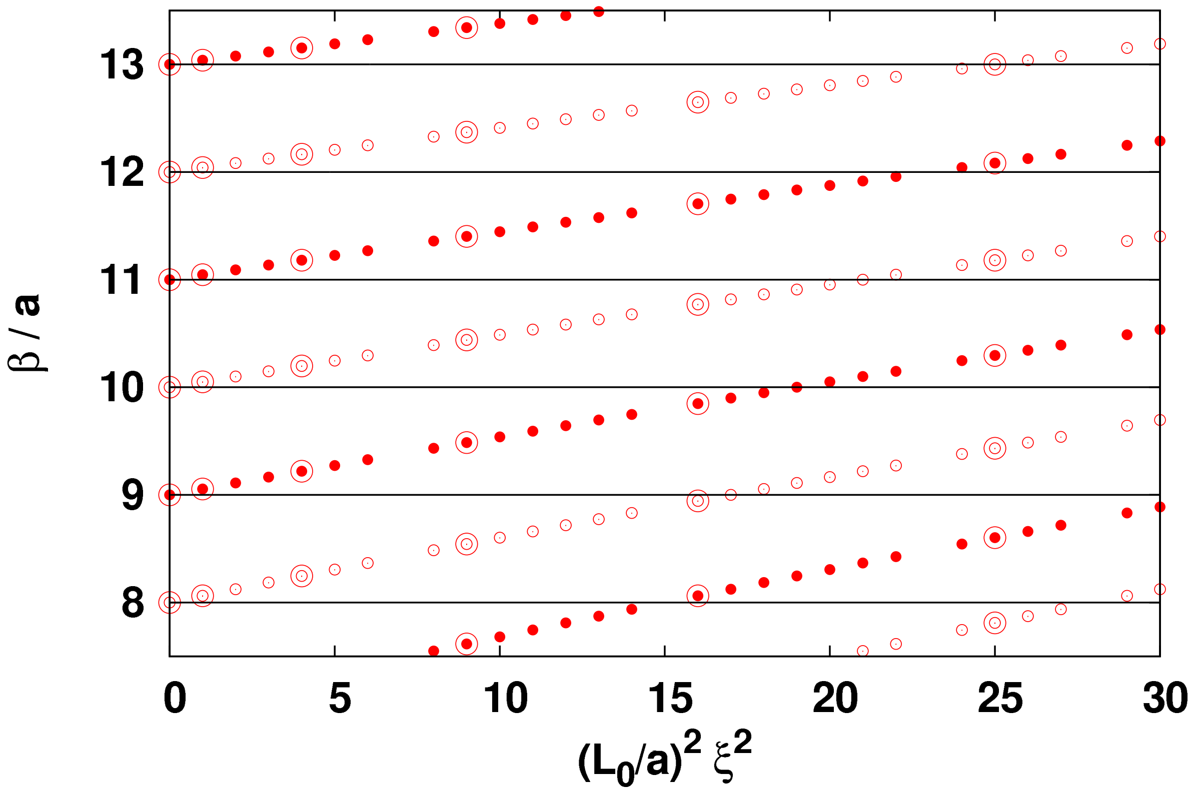
- By deriving twice with respect to the ξ_k

$$\langle T_{0k} \rangle_{\boldsymbol{\xi}} = \frac{L_0 \xi_k}{2} \sum_{ij} \left\langle \overline{T}_{0i} \, T_{0j} \right\rangle_{\boldsymbol{\xi},\, c} \left[\delta_{ij} - \frac{\xi_i \, \xi_j}{\boldsymbol{\xi}^2} \right] \; .$$

which implies for instance

$$s^{-1} = -\frac{1}{2(1+\boldsymbol{\xi}^2)^{3/2}} \sum_{ij} \frac{\left\langle \overline{T}_{0i} \, T_{0j} \right\rangle_{\boldsymbol{\xi},\, c}}{\langle T_{0i} \rangle_{\boldsymbol{\xi}} \langle T_{0j} \rangle_{\boldsymbol{\xi}}} \, \xi_i \xi_j \left[\delta_{ij} - \frac{\xi_i \xi_j}{\boldsymbol{\xi}^2} \right]$$

A finer scan in the temperature on the lattice



- A finer scan in the temperature values become possible at fixed lattice spacing

$$\frac{1}{aT} = \frac{\beta}{a} = \sqrt{\left(\frac{L_0}{a}\right)^2 + \left(\frac{L_0\xi_1}{a}\right)^2 + \left(\frac{L_0\xi_2}{a}\right)^2 + \left(\frac{L_0\xi_3}{a}\right)^2}$$

Non-perturbative renormalization of $T_{\mu\nu}$ (traceless components)

- On the lattice translational invariance is broken down to a discrete group and standard discretizations of $T_{\mu\nu}$ acquire finite ultraviolet renormalizations

- We focus here on the SU(3) Yang–Mills, but the analysis applies to other theories as well [Caracciolo et al. 88, 90]

$$T^{\mathrm{R}}_{01} = Z_T\, T_{01}$$

$$T^{\mathrm{R}}_{00} - T^{\mathrm{R}}_{11} = Z_T\, z_T\, (T_{00} - T_{11})$$

$$V_T = \begin{pmatrix} L_0 & 0 & 0 & 0 \\ \frac{L_0}{2} & \frac{5}{2}L_0 & 0 & 0 \\ 0 & 0 & L & 0 \\ 0 & 0 & 0 & L \end{pmatrix}$$

- There is a great freedom in choosing the renormalization conditions. A possibility is

$$z_T = \frac{3}{2}\frac{\langle T_{01}\rangle_{V_T}}{\langle T_{00}\rangle_{V_T} - \langle T_{11}\rangle_{V_T}}\,,$$

while Z_T can be determined in finite volume from (see also Robaina's talk)

$$Z_T = \frac{1}{L_0\langle T_{0k}\rangle_{V_T}}\frac{\partial}{\partial \xi_k}\ln Z(V_T)$$

- Once Z_T has been computed in a small volume (for instance), the entropy density can be computed as ($\xi_k \neq 0$)

$$s = -\frac{Z_T L_0 (1+\boldsymbol{\xi}^2)^{3/2}}{\xi_k} \langle T_{0k} \rangle_{V_{\rm sbc}}$$

thanks to the misalignment of the lattice axes with respect to the periodic directions

- Analogously the specific heat is given by (ξ_k and L_k chosen to be equal)

$$\frac{c_v}{s} = \frac{3}{\boldsymbol{\xi}^2} \frac{\left\langle \overline{T}_{01}\, T_{02} \right\rangle_{V_{\rm sbc},c} + \boldsymbol{\xi}^2 \left\langle \overline{T}_{01}\, T_{01} \right\rangle_{V_{\rm sbc},c}}{\left\langle \overline{T}_{01}\, T_{02} \right\rangle_{V_{\rm sbc},c} - \left\langle \overline{T}_{01}\, T_{01} \right\rangle_{V_{\rm sbc},c}}$$

- Note that:

  $*$ No ultraviolet-divergent power subtraction needed

  $*$ Renormalization constant fixed non-perturbatively by WIs

Entropy density from the response to the shift

- As we have seen in the continuum

$$s = -\lim_{V\to\infty} \frac{1}{V} \frac{\partial^2}{\partial \xi_k^2} \ln Z(L_0, \boldsymbol{\xi})\Big|_{\boldsymbol{\xi}=0}$$

- On the lattice the only difference is the discrete derivative

$$s = -\frac{1}{T^2} \lim_{V\to\infty} \lim_{a\to 0} \frac{2}{n_z^2 a^2 V} \ln\left[\frac{\mathcal{Z}(L_0, \{0,0,n_z a/L_0\})}{\mathcal{Z}(L_0, \{0,0,0\})}\right]$$

with n_z being kept fixed when $a \to 0$

- Note that:

  $*$ No ultraviolet renormalization

  $*$ Finite volume effects exponentially small

  $*$ Discretization effects $\mathcal{O}(a^2)$ once action improved

Conclusions and outlook (I)

- Lorentz invariance implies a great degree of redundancy in defining a relativistic thermal theory in the Euclidean path-integral formalism

- In the thermodynamic limit, the orientation of the compact periodic direction with respect to the spatial axes can be chosen at will and only its length is physically relevant

$$f\left(L_0\sqrt{1+\boldsymbol{\xi}^2}\right) = -\lim_{V\to\infty} \frac{1}{L_0 V} \ln Z(L_0,\boldsymbol{\xi})$$

- The redundancy in the description implies that the total energy and momentum distributions in the canonical ensemble are related

- For a finite-size system, the lengths of the box dimensions break this invariance. Being a soft breaking, however, interesting exact Ward Identities survive

- If the lightest screening mass $M \neq 0$, leading finite-size corrections exponentially small in (ML) as in the standard case

Conclusions and outlook (II)

- When the theory is regularized on a lattice, the overall orientation of the periodic directions with respect to the lattice coordinate system affects renormalized observables at the level of lattice artifacts

- As the cutoff is removed, the artifacts are suppressed by a power of the lattice spacing. They turn out to be rather small: at the level of per-mille in the step-scaling function of the entropy density [L. G., M. Pepe Poster Session B; see also H. B. Meyer, D. Robaina talk session 1C.]

- The flexibility in the lattice formulation added by the introduction of a triplet $\boldsymbol{\xi}$ of (renormalized) parameters has interesting consequences:

  * A finer scan of the temperature value
  * WIs to renormalize non-perturbatively $T_{\mu\nu}$
  * Simpler ways to compute thermodynamic potentials

$$s = -\frac{Z_T L_0 (1+\boldsymbol{\xi}^2)^{3/2}}{\xi_k} \langle T_{0k} \rangle_{V_{\rm sbc}}$$

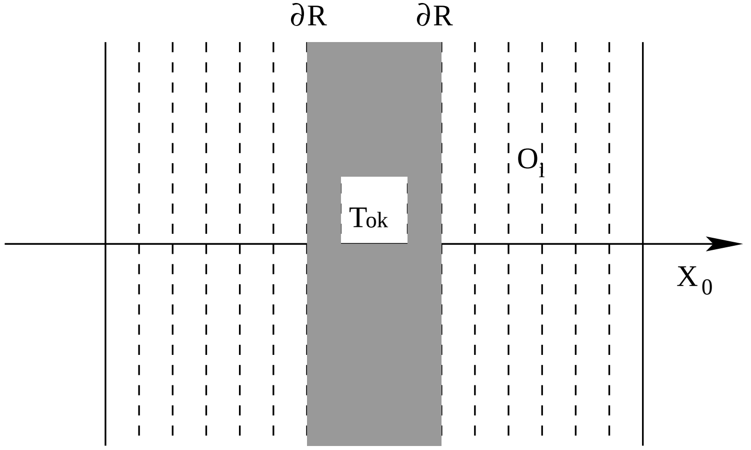
- It is also intriguing the fact that thermodynamic potentials can be directly inferred from the response of the partition function to the shift in the boundary conditions

Ward identities in a finite spatial box (III)

- The commutator of boost with momentum

$$[\hat{K}_k, \hat{p}_k] = i\hat{H}$$

is expressed in the Euclidean by the WIs



$$\int_{\partial R} d\sigma_\mu(x)\, \langle K_{\mu;0k}(x)\, \overline{T}_{0k}(y_0)\, O_1 \ldots O_n \rangle_c = \langle \overline{T}_{00}(y_0)\, O_1 \ldots O_n \rangle_c$$

when the O_i are localized external fields.

- In a 4D box boost transformations are incompatible with (periodic) boundary conditions. WIs associated with $SO(4)$ rotations must be modified by finite-size contributions

- The finite-volume theory is translational invariant, and it has a conserved $T_{\mu\nu}$. Modified WIs associated to boosts constructed from those associated to translational invariance

$$L_0\, \langle \overline{T}_{0k}(x_0)\, T_{0k}(y) \rangle_{V_{\rm sbc},c} - L_k\, \langle \widetilde{T}_{0k}(w_k)\, T_{0k}(z) \rangle_{V_{\rm sbc},c} = \langle T_{00} \rangle - \langle T_{kk} \rangle_{V_{\rm sbc},c}$$