

A numerical approach to modular Hamiltonians in quantum field theory

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Modular Hamiltonians for (massive) quantum fields

- Numerical approximation scheme for a scalar field on regions of $(1+1)$ and $(1+3)$ -dimensional Minkowski spacetime.
[\[Bostelmann–Cadamuro–M. 2023\]](#)
arXiv:2209.04681
- Analytic results for fermions of small mass in $(1+1)$ -dimensional Minkowski spacetime.
[\[Cadamuro–Fröb–M. 2024\]](#)
arXiv:2312.04629
- Numerical approximation scheme for fermions on regions of $(1+1)$ Minkowski and cylinder spacetimes.
[\[Bostelmann–Cadamuro–M.\]](#)
(paper in preparation)
- The numerical scheme applied to a scalar field on regions of the half-space $\mathbb{R} \times \mathbb{R}_+$ with a Robin boundary condition at the spatial boundary.
[\[M.–Tonni\]](#)
(paper in preparation)
- Modular Hamiltonians for a scalar field on regions of flat spacetime in arbitrary dimension with a point defect (including massless bosons in even spatial dimensions where Huygens' principle is violated).
[\[Mintchev–M.–Tonni\]](#)
(work in progress)

(Reviews of) modular theory for physicists

- “Notes on some entanglement properties of quantum field theory” [[Witten 2018](#)] includes comments on the classification of von Neumann algebras
- “An intuitive construction of modular flow” [[Sorce 2023](#)] starts with thermal states in physics and
- “Modular theory, non-commutative geometry and quantum gravity” [[Bertozzini-Conti-Lewkeeratiyutkul 2010](#)] reasons to consider modular theory without reference to classical theory, but classical spacetime as an “emergent” structure from non-commutative geometry

What can we learn from modular theory

- Entanglement is part of the algebras in QFT, not just the states.
- The modular operator can be used to compute relative (entanglement) entropies.
- It plays a role in the classification of von Neumann algebras [[Connes 1973](#)].
- Since it is related to the spacetime symmetries, it captures geometric properties of underlying spacetime regions.

A canonical (Gibbs) ensemble

Hamiltonian H_{can} and an inverse temperature $\beta = (k_B T)^{-1}$ determine a **density matrix**

$$\rho = \frac{1}{Z} e^{-\beta H_{\text{can}}}, \quad Z := \text{tr}\left(e^{-\beta H_{\text{can}}}\right),$$

as long as $Z < \infty$, as on a lattice, for example.

A state with density matrix

For any invertible density matrix ρ ,

$$H = -\log \rho$$

- is the **modular Hamiltonian** of ρ
- is the Hamiltonian of a system in a thermal state (in units where $\beta = 1$).

State properties in quantum field theory

For a spacetime region \mathcal{O} (typically a double cone), we have an algebra \mathcal{A} of operators supported in that region. We consider a von Neumann algebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ that acts on some Hilbert space \mathcal{H} .

A normalised vector $\Omega \in \mathcal{H}$ is

- **cyclic:** $\mathcal{A}\Omega$ is dense in \mathcal{H}
all states can be approximated arbitrarily well,
- **separating:** $\forall a \in \mathcal{A} : a\Omega = 0 \Rightarrow a = 0$
it distinguishes operators.

Vacuum states in QFT are cyclic and separating [Reeh–Schlieder 1961].

How does a state in QFT define a modular Hamiltonian?

The modular operator

The *Tomita operator* T_Ω is the closure of the map

$$\forall a \in \mathcal{A} : \quad a\Omega \mapsto a^*\Omega$$

It is an unbounded involution, with unique polar decomposition $T_\Omega = J\Delta^{1/2}$ into

- the modular conjugation J (anti-unitary), and
- the **modular operator** $\Delta = T_\Omega^* T_\Omega$ (self-adjoint, positive definite).

[Tomita 1969; Takesaki 1972]

The *modular Hamiltonian* is now

$$H := -\log \Delta$$

Example (bi-partite finite dimensional system)

A bi-partite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with algebras \mathcal{A}_A and \mathcal{A}_B acting only on their components.

$$\Psi = \sum_k c_k |k\rangle_A \otimes |k\rangle_B$$

$$T_{\Psi,A} : (a \otimes \mathbb{1})\Psi \mapsto (a^* \otimes \mathbb{1})\Psi$$

$$\rho_A = \sum_k |c_k|^2 |k\rangle_A \langle k|_A$$

$$\rho_B = \sum_k |c_k|^2 |k\rangle_B \langle k|_B$$

$$\Delta_{\Psi,A} = \rho_A \otimes \rho_B^{-1}$$

The Hilbert spaces \mathcal{H}_A and \mathcal{H}_B can be understood as dual to each other.

Linear quantum field theory

Consider the CCR/CAR algebras for a single particle.

Examples in $(1 + 1)$ -dimensional Minkowski space:

scalar: $\partial_t^2 \psi = (-\partial_x^2 + m^2) \psi,$
 $\hat{D} := p^2 + m^2.$

fermion: $\partial_t \psi_{\pm} = (-\partial_x \pm m) \psi_{\mp},$
 $\hat{D}^{\pm \frac{1}{2}} := \frac{m \pm i p}{\sqrt{p^2 + m^2}}.$

We want to compute the modular Hamiltonian $H = -\log \Delta$ corresponding to the vacuum state Ω over some subspace.

One-particle structure for linear fields

- a real, separable Hilbert space \mathcal{H}_r
- a closed subspace $\mathcal{H}_{r,A} \subset \mathcal{H}_r$
- and a positive operator D on \mathcal{H}_r with dense range such that

$$D^s \mathcal{H}_{r,A}^s \cap D^{-s} \mathcal{H}_{r,A}^{-s} = \{0\}$$

and similar for the orthogonal complement $\mathcal{H}_{r,A}^{\perp}.$

The gray super-scripts $\pm s$ on the Hilbert spaces $\mathcal{H}_{r,A}$ in this expression denote certain domain closures that are required in the bosonic case, where D is an unbounded operator, see

[Bostelmann–Cadamuro–M. 2023].

One-particle structure for linear fields

Real, separable Hilbert space $\mathcal{H}_r := L^2_{\mathbb{R}}(\mathbb{R}^{d-1})$ and subspace $\mathcal{H}_{r,A} := L^2_{\mathbb{R}}(A)$ for two pieces of initial data. Together they form a complex Hilbert space $\mathcal{H} = \mathcal{H}_r^{1/4} \oplus \mathcal{H}_r^{-1/4}$ with **complex structure**

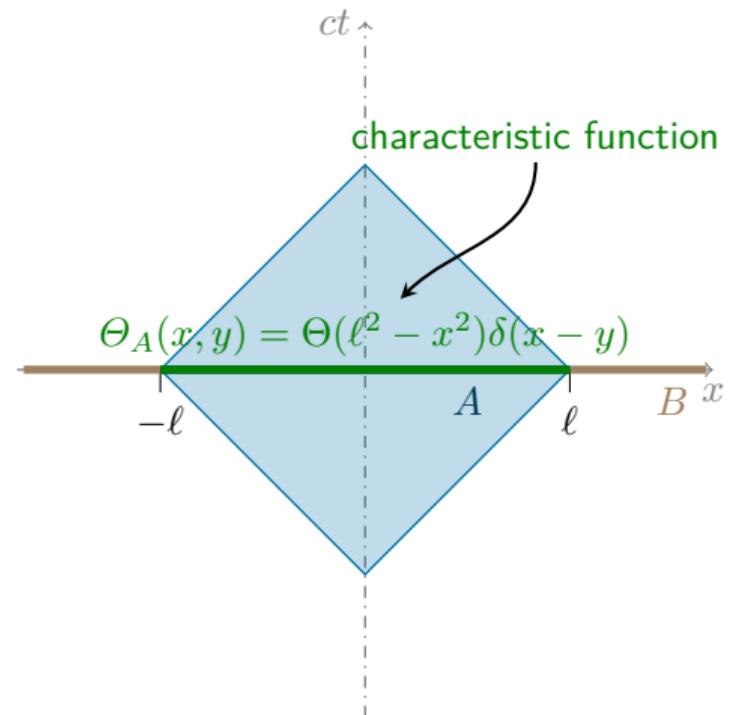
$$I = \begin{pmatrix} 0 & D^{-\frac{1}{2}} \\ -D^{+\frac{1}{2}} & 0 \end{pmatrix},$$

and a *standard* subspace $\mathcal{H}_A \subset \mathcal{H}$ (meaning $\mathcal{H}_A \cap I\mathcal{H}_A = \{0\}$, $\overline{\mathcal{H}_A + I\mathcal{H}_A} = \mathcal{H}$).

There are **subspace projectors**

$$P = \Theta_{\frac{1}{4}, A} \oplus \Theta_{-\frac{1}{4}, A} \quad (\text{scalar fields})$$

$$E = \Theta_A \oplus \Theta_A \quad (\text{fermions}).$$



Staying at the one-particle level

For all self-adjoint operators $F = F^*$,
 $G = G^* \in \mathcal{A}(\mathcal{O})$

$$\hat{T} : (F + iG)\Omega \mapsto (F - iG)\Omega$$

which corresponds to the complex conjugation at the one-particle level ($f, g \in \mathcal{H}_A$)

$$f + Ig \mapsto f - Ig,$$

with the Tomita operator $T = J\Delta^{1/2}$ as the closure.

On Fock space, the modular operator is the second quantization $\hat{\Delta} = \Gamma(\Delta)$ for bosons [Eckmann–Osterwalder 1973] and for fermions [Foit 1983]; see also [Longo 2019].

From the projectors to the modular operator

The one-particle Tomita operator $T = J\Delta^{1/2}$, the cutting projection P and orthogonal projector E are related [Figliolini–Guido 1994, Longo 2022],

$$\begin{aligned} -I \log \Delta &= 2I \operatorname{arcoth}(P - IPI - 1), \\ -I \log \Delta &= 2I \operatorname{tanh}(E - IEI - 1). \end{aligned}$$

$$-I \log \Delta = \begin{pmatrix} 0 & M_- \\ -M_+ & 0 \end{pmatrix},$$

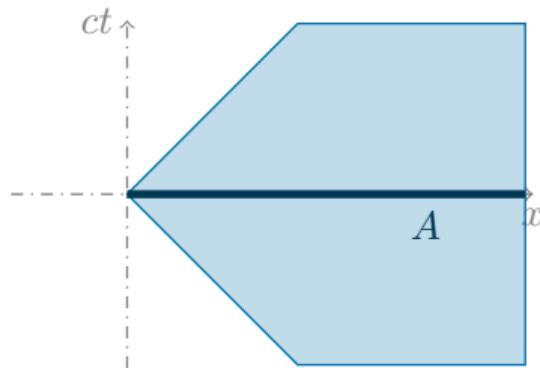
$$M_{\pm} = 2D^{\pm\frac{1}{4}} \frac{\operatorname{arcoth}(Z)D^{\pm\frac{1}{4}}}{\operatorname{tanh}} \quad \begin{array}{l} \rightarrow \text{bosonic} \\ \rightarrow \text{fermionic} \end{array}$$

$$Z = D^{+\frac{1}{4}} \Theta_{+\frac{1}{4}, A} D^{-\frac{1}{4}} + D^{-\frac{1}{4}} \Theta_{-\frac{1}{4}, A} D^{+\frac{1}{4}} - 1.$$

Analytic expressions for local subspaces in $(1 + 1)$ -dimensional Minkowski space

Right wedge region

[Bisognano–Wichmann 1975]

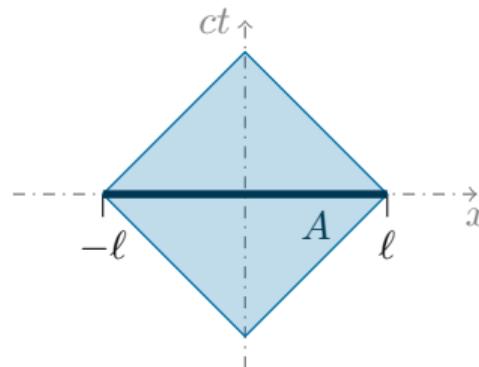
 $\Delta^{-it} =$ boosts (symmetries of the wedge subspace)

For massive Majorana fermions:

$$M_{\pm}(x, y) = 2\pi x \left(m\delta(x - y) \mp \delta'(x - y) \right)$$

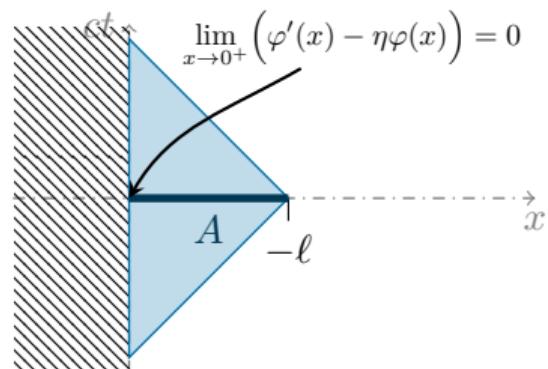
Double cone region

[Hislop–Longo 1982]

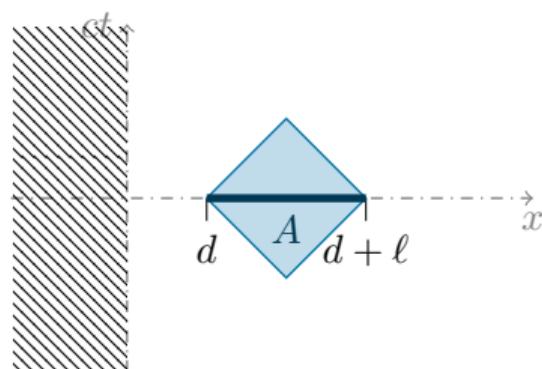
 $\Delta^{-it} =$ conformal transformations (symmetries of the double cone) – massless!What can we find out about **massive** particles?

Analytic expressions for local subspaces in flat spacetime with spatial boundary

Region over an adjacent interval [Cardy–Tonni 2016]



Region over a separated interval



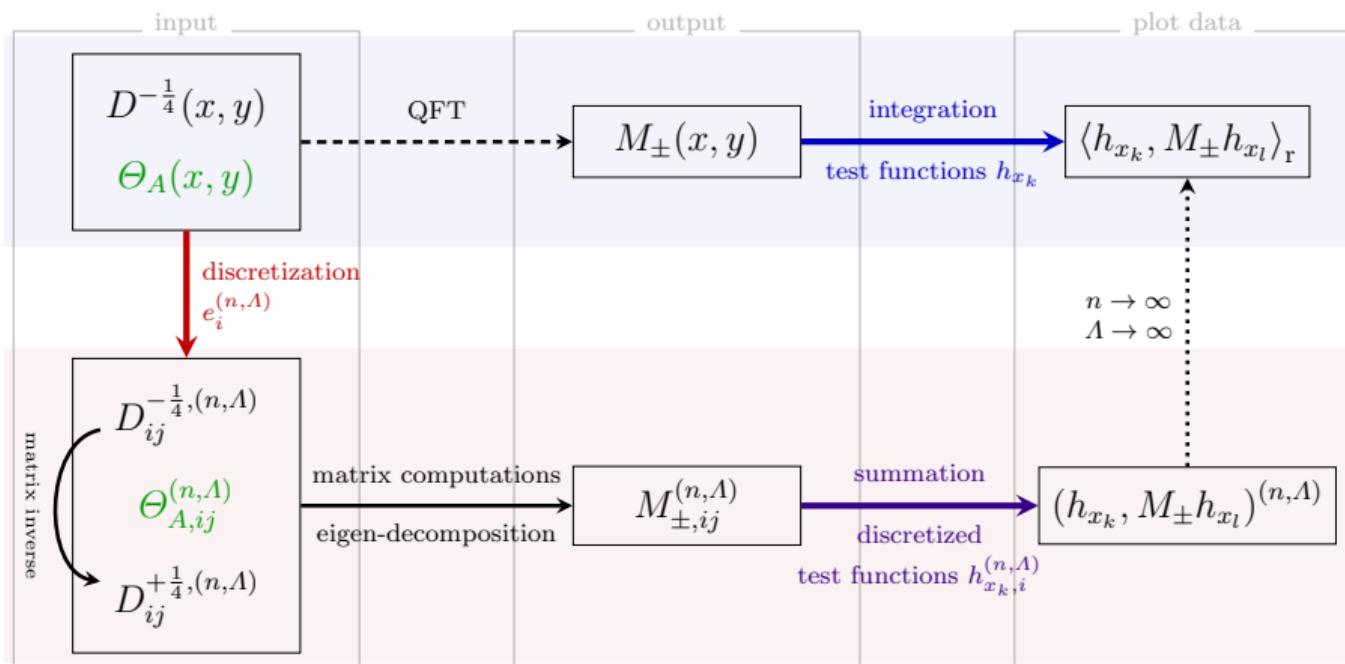
Boundary conformal field theory (massless boson)
for a Neumann or Dirichlet boundary condition:

$$M_-(x, y) = 2\pi \frac{\ell^2 - x^2}{2\ell} \delta(x - y),$$

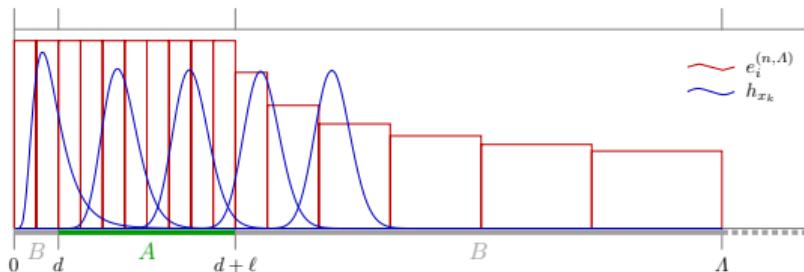
(shown with a magenta line in later plots).

In the bosonic case, there is no known solution for this region in the massless and massive regimes yet.

Scheme of the numerical approach



Functions for discretization and smearing

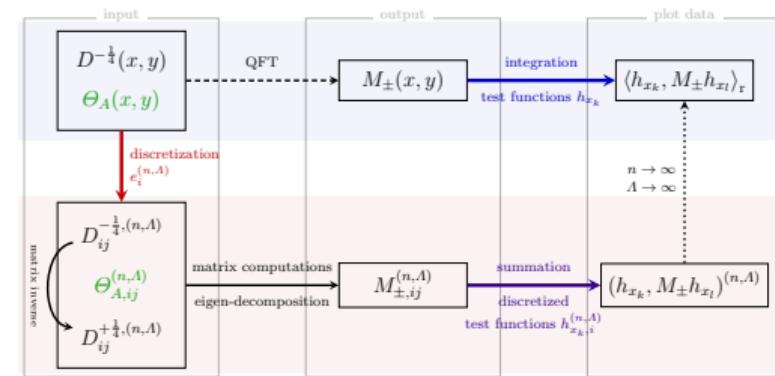


$$e_i^{(n,A)}(x) := \frac{\Theta(x - a_i)\Theta(b_i - x)}{\sqrt{b_i - a_i}},$$

$$O_{ij}^{(n,A)} := \left\langle e_i^{(n,A)}, O e_j^{(n,A)} \right\rangle_r,$$

$h_{x_k}(x)$:= L²-normalized log-Gaussian ,

$$h_{x_k,i}^{(n,A)} := \left\langle e_i^{(n,A)}, h_{x_k} \right\rangle_r,$$

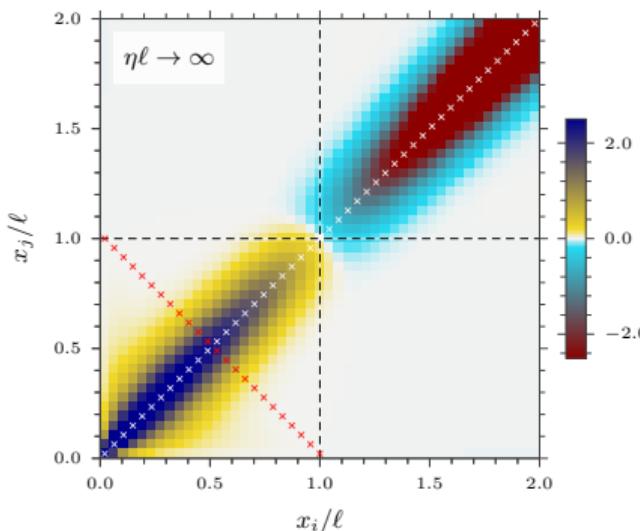


$$\langle h_{x_k}, M_{\pm} h_{x_l} \rangle_r ,$$

$$\sum_{i,j=0}^{n-1} h_{x_k,i}^{(n,A)} M_{\pm,ij}^{(n,A)} h_{x_l,j}^{(n,A)} =: (h_{x_k}, M_{\pm} h_{x_l})^{(n,A)} .$$

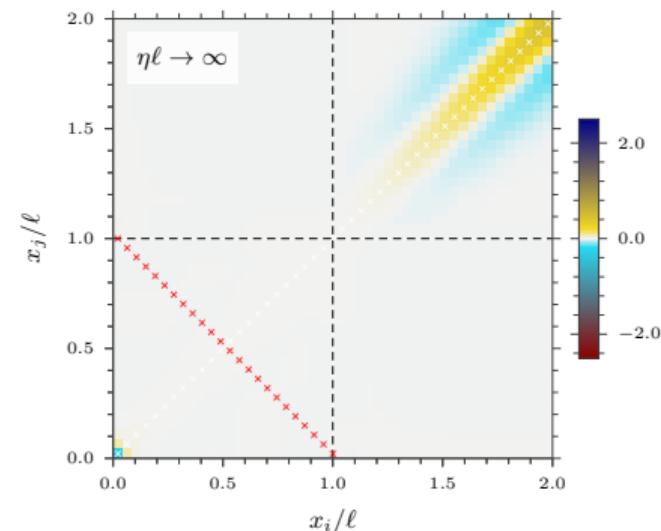
Massless regime

A scalar boson on the adjacent interval, massless regime



Smeared numeric results

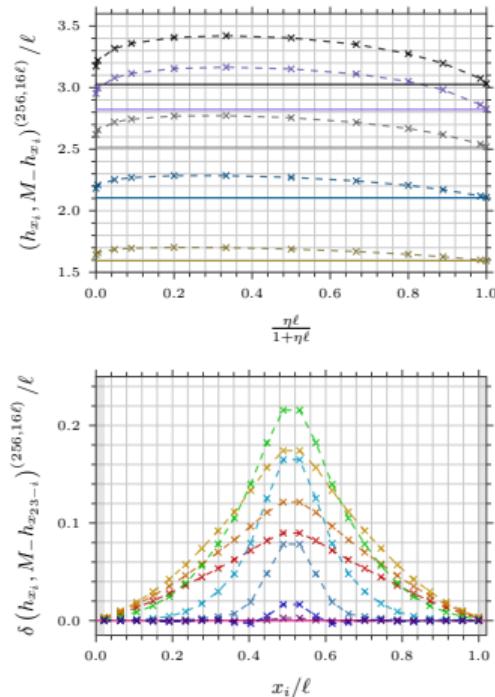
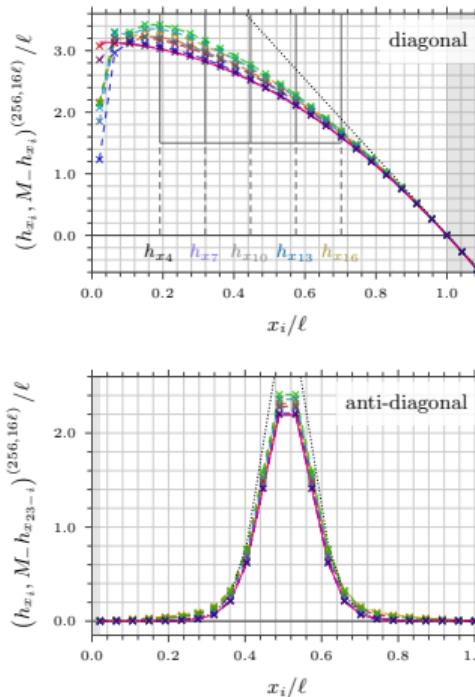
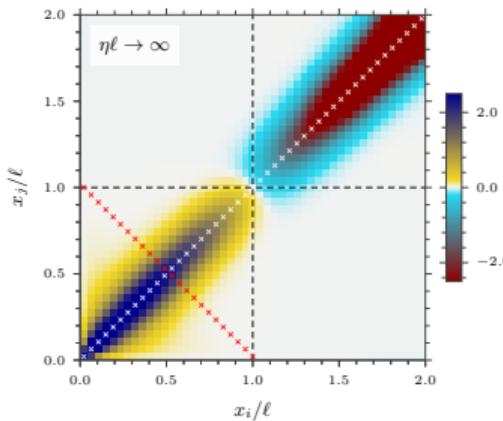
$$(h_{x_k}, M_- h_{x_l})^{(n, \Lambda)} := \sum_{i,j} h_{x_k, i}^{(n, \Lambda)} M_{\pm, ij}^{(n, \Lambda)} h_{x_l, j}^{(n, \Lambda)}$$



Smeared difference between the numeric results and the analytic BCFT reference

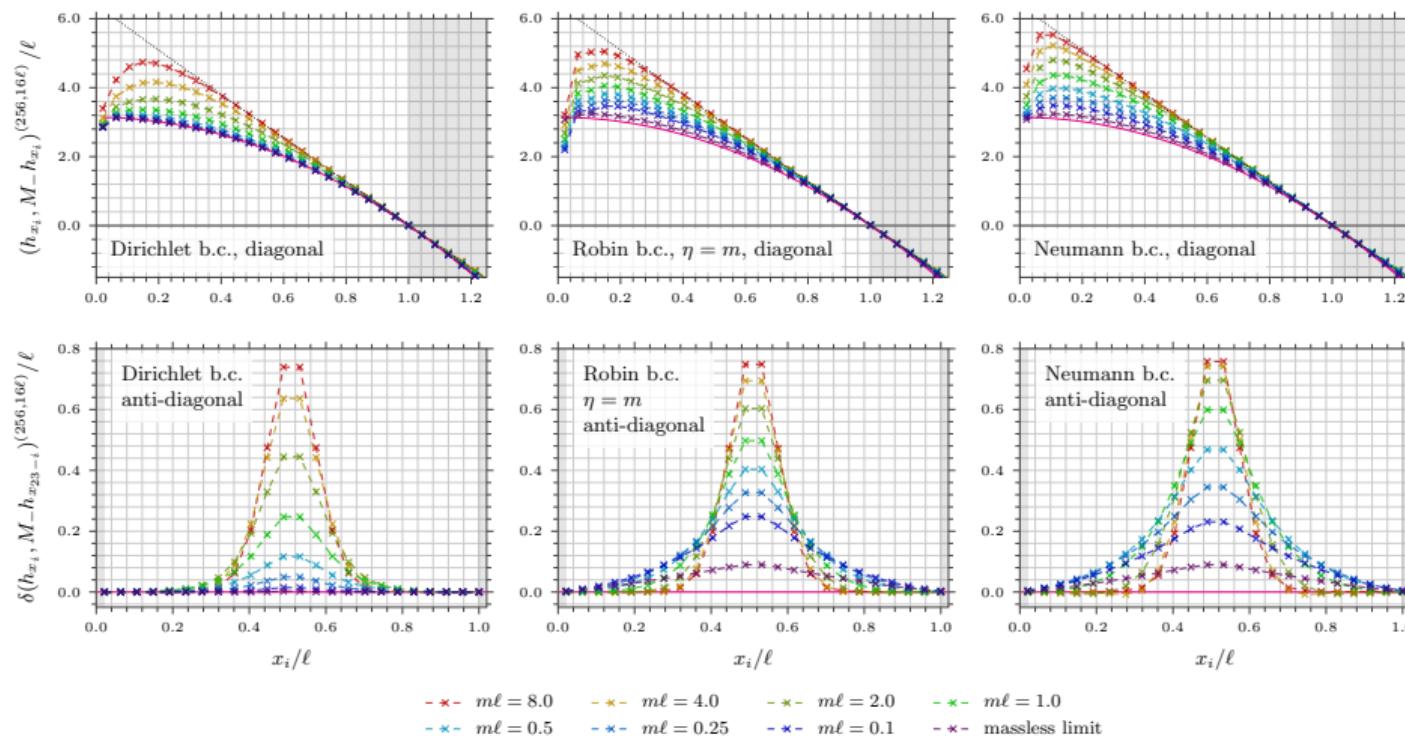
$$\delta (h_{x_k}, M_- h_{x_l})^{(n, \Lambda)} := (h_{x_k}, M_- h_{x_l})^{(n, \Lambda)} - \langle h_{x_k}, M_-^{\text{BCFT}} h_{x_l} \rangle_r$$

Boundary dependence in the massless regime

Dependence on the boundary parameter η in the massless regime

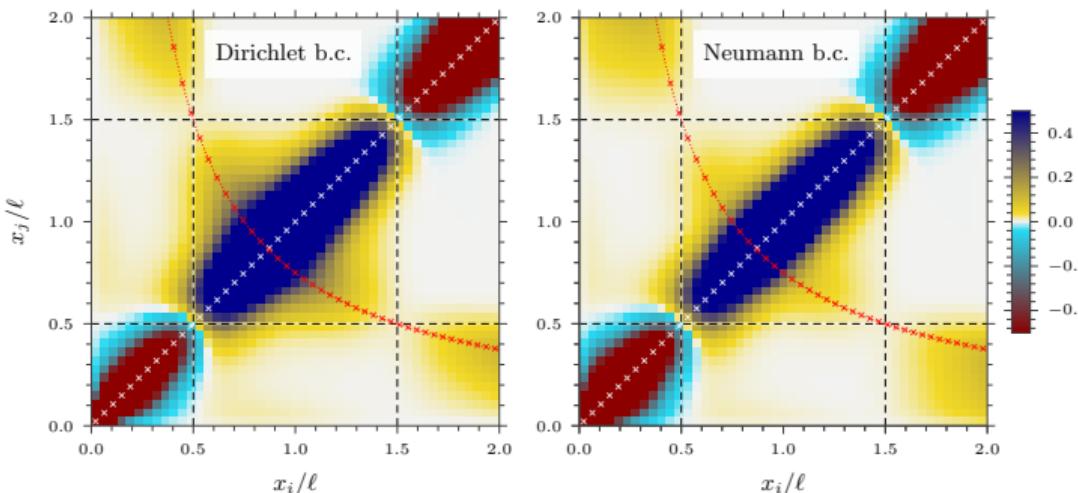
- - - Neumann b.c.	- - - $\eta\ell = 0.005$	- * - $\eta\ell = 0.05$	- * - $\eta\ell = 0.5$
- - - $\eta\ell = 2.0$	- - - $\eta\ell = 8.0$	- - - $\eta\ell = 64.0$	- - - Dirichlet b.c.

Massive regime

Dependence on the mass parameter m 

Plotting curves and analytic reference

Plotting curves



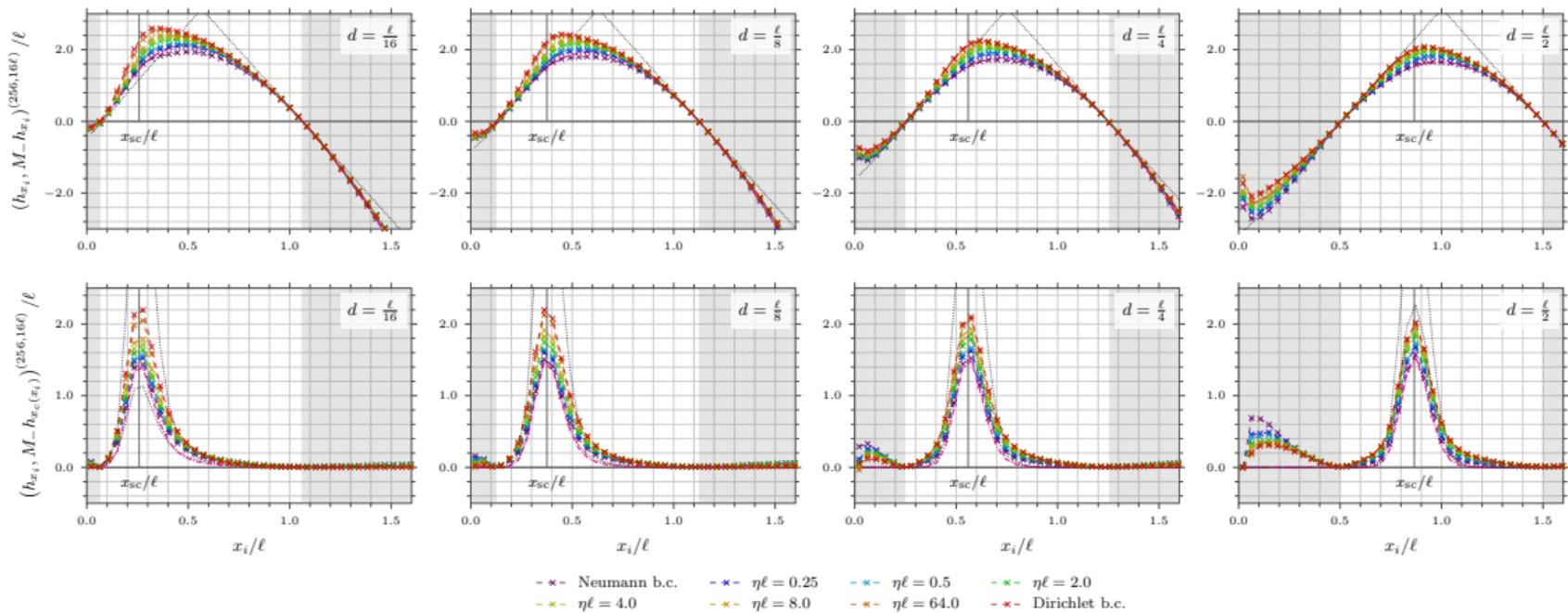
Main diagonal (white crosses) and conjugate curve (red crosses),

$$x_c(x) := \frac{d(d + \ell)}{x} .$$

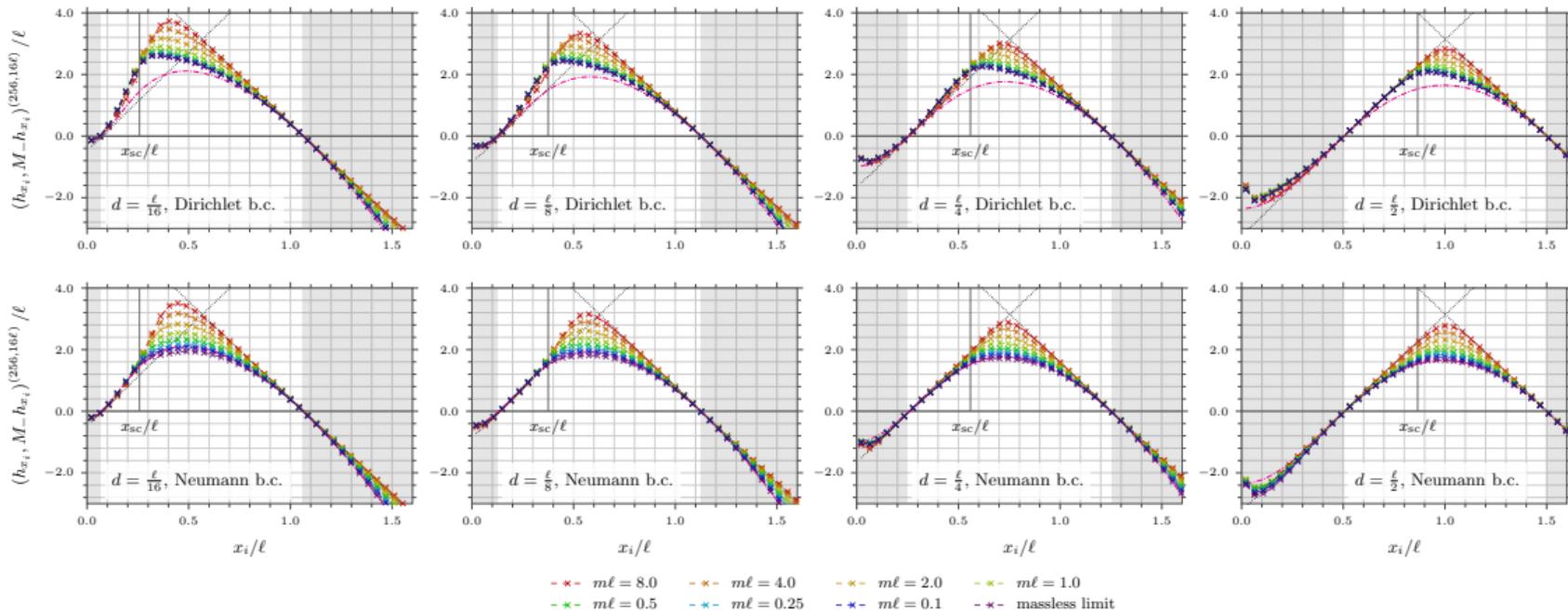
There is no known reference for the bosonic theory, so we consider the local part of the solution in the corresponding fermionic BCFT [Mintchev–Tonni 2021] as analytic reference (dash dot magenta line below)

$$M_-^{\text{loc}}(x, y) = \frac{\pi}{\ell} \frac{[x^2 - d^2][(d + \ell)^2 - x^2]}{d(d + \ell) + x^2} \delta(x - y) .$$

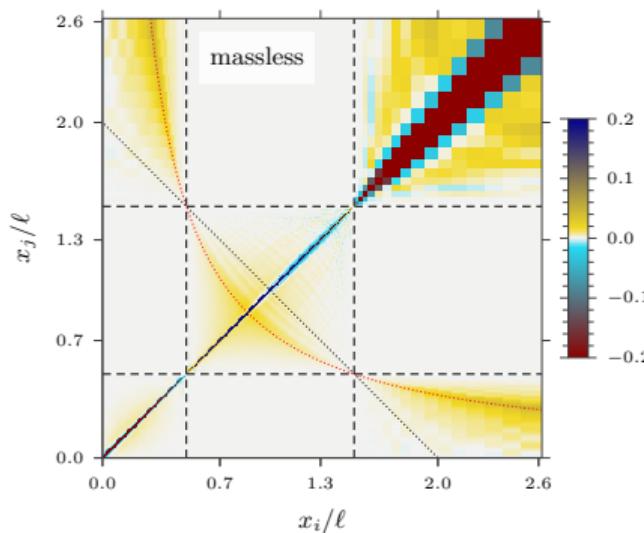
Boundary dependence in the massless regime

Dependence on the boundary parameter η and the separation distance d 

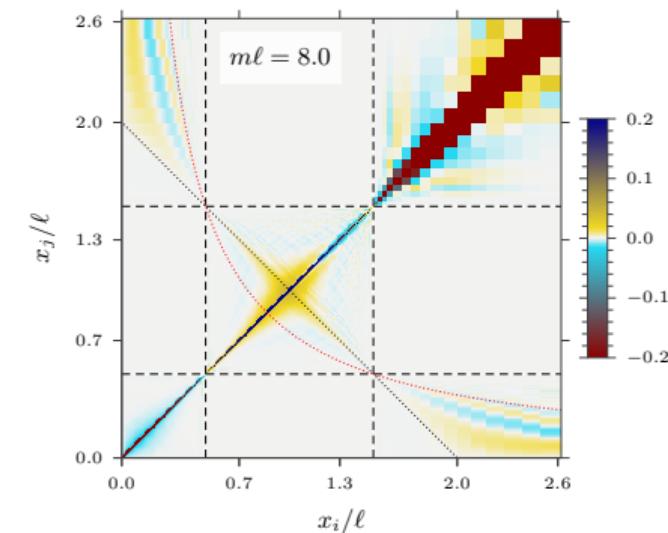
The diagonal in the massive regime

Dependence on the mass parameter m and the separation distance d 

Non-local contributions in the massive regime

Dependence on the mass parameter m with a Dirichlet boundary

$$x_c(x) := \frac{d(d + \ell)}{x} \quad (\text{dotted red})$$

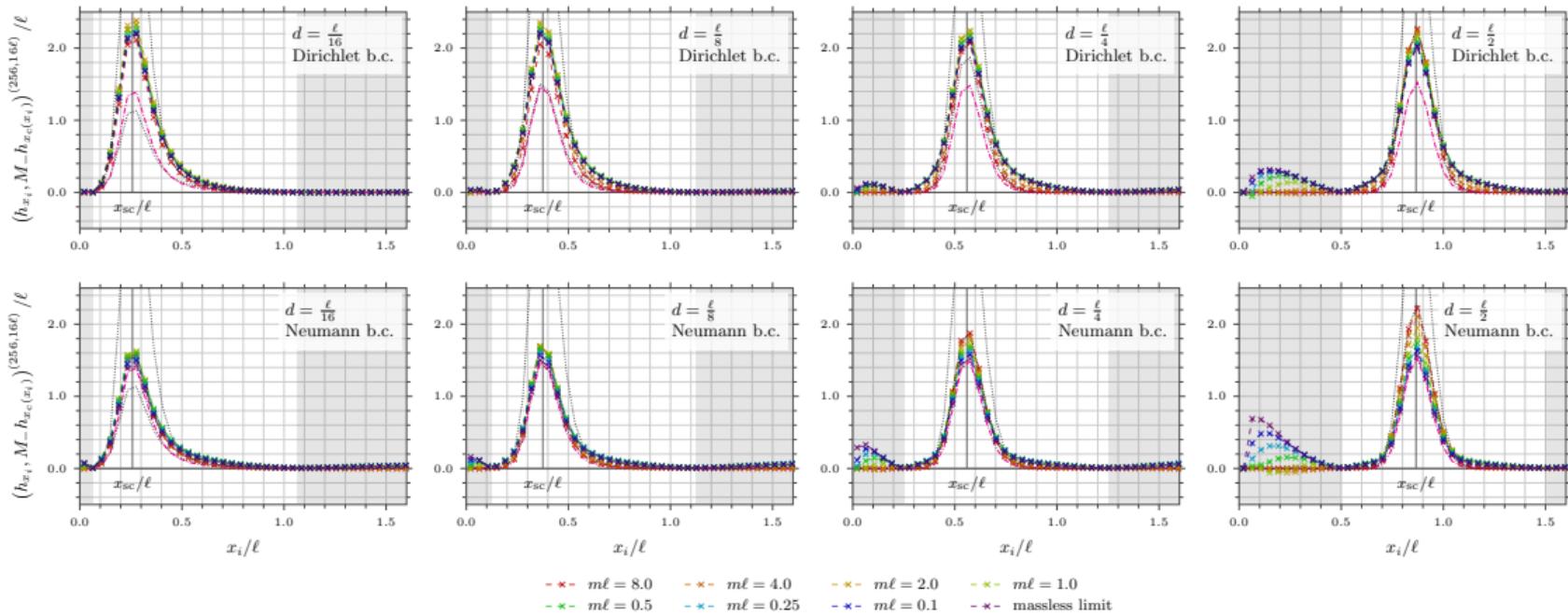


$$y(x) := \ell + 2d - x \quad (\text{dotted black})$$

Discretized numeric results $M_-^{(n,A)}$ (without smearing).

Non-diagonal contributions are mostly concentrated along and between these two curves.

The conjugate curve in the massive regime

Dependence on the mass parameter m for different separations d from the boundary

Summary

- The modular Hamiltonian $-\log \Delta$ can be used to compute relative entropies in QFT, for example, between the Fock vacuum ω and a coherent excitation described by the Weyl operator $W(f)$ for any vector f in the bosonic Hilbert space \mathcal{H} ,

$$\omega_f(\hat{a}) := \omega(W(f)^* \hat{a} W(f)) ,$$

$$S(\omega_f \| \omega) = \left\langle f, (\Theta_{-\frac{1}{4}, A} M_+ \oplus \Theta_{\frac{1}{4}, A} M_-) f \right\rangle_{\frac{1}{4} \oplus -\frac{1}{4}} .$$

- The modular operator Δ is defined through the Tomita operator $T_\Omega : a\Omega \mapsto a^*\Omega$.
- We can approximate it numerically in certain setups, even when we lack analytic solutions.

Challenges

- Is it possible to generalize the approach to curved spacetime?
- Could we study regions near horizons (in cosmology or black holes)?

Thank you for your interest.