From tensor networks to quantum computing in lattice field theory

Karl Jansen

- **2+1-dimionsional U(1) gauge theory**
  - Hamiltonian formulation
  - truncation of the theory
  - electric and magnetic basis
- **3+1-dimionsional U(1) gauge theory**
- **Hamiltonian formulation of topological term opening path**
  - * classical calculations: tensor networks
  - * quantum calculations: quantum computer
- **Conclusion**

Towards quantum computations of a U(1) gauge theory in d=2 space dimensions

(Jan Haase, Luca Dellantonio, Alessio Celi, Danny Paulson, Angus Kan, K.J., Christine Muschik,
Quantum 5 (2021) 393)

- lattice Hamiltonian, lattice spacing a, periodic boundary conditions

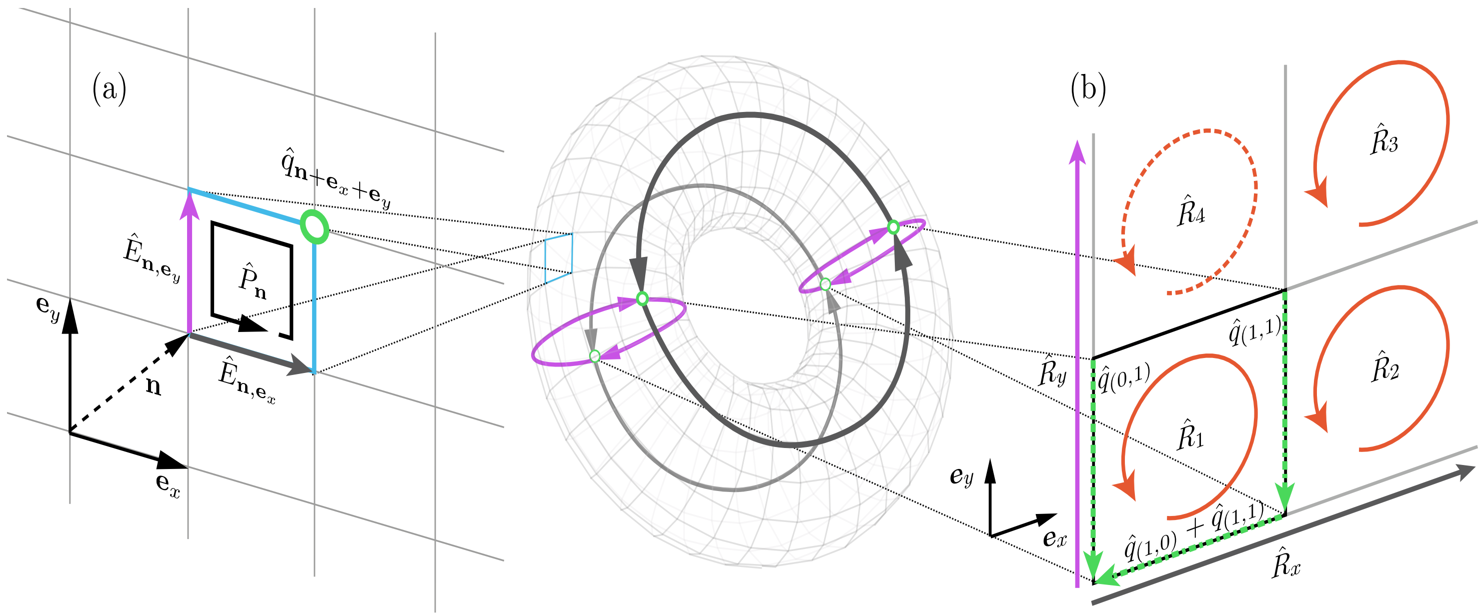
$$\hat{H}_{\text{gauge}} = \hat{H}_E + \hat{H}_B$$

$$\hat{H}_E = \frac{g^2}{2}\sum_{\boldsymbol{n}}\left(\hat{E}^2_{\boldsymbol{n},\boldsymbol{e}_x} + \hat{E}^2_{\boldsymbol{n},\boldsymbol{e}_y}\right) \;, \hat{H}_B = -\frac{1}{2g^2a^2}\sum_{\boldsymbol{n}}\left(\hat{P}_{\boldsymbol{n}} + \hat{P}^\dagger_{\boldsymbol{n}}\right)$$

- electric field operator: $\hat{E}_{\boldsymbol{n},\boldsymbol{e}_\mu}\left|E_{\boldsymbol{n},\boldsymbol{e}_\mu}\right\rangle = E_{\boldsymbol{n},\boldsymbol{e}_\mu}\left|E_{\boldsymbol{n},\boldsymbol{e}_\mu}\right\rangle , \quad E_{\boldsymbol{n},\boldsymbol{e}_\mu} \in \mathbb{Z}$
- plaquette operator: $\hat{P}_n = \hat{U}_{n,e_x}\hat{U}_{n+e_x,e_y}\hat{U}^\dagger_{n+e_y,e_x}\hat{U}^\dagger_{n,e_y}$
  $\rightarrow$ represented as lowering and raising operators, i.e. $\hat{P}_n|p_n\rangle = |p_n - 1\rangle$
- "naive" continuum limit: $\hat{H} \xrightarrow[a\to 0]{} \int \mathrm{d}\boldsymbol{x}[E(\boldsymbol{x})^2 + B(\boldsymbol{x})^2]$
- Gauss law

$$\left[\sum_{\mu=x,y}\left(\hat{E}_{n,e_\mu} - \hat{E}_{n-e_\mu,e_\mu}\right) - \hat{q}_n\right]|\Phi\rangle = 0 \forall n \quad \Longleftrightarrow |\Phi\rangle \in \{\text{ physical states }\}$$

pictorial representation



Electric field and plaquette **periodic torus** **rotators and strings**

Truncation of electric and magnetic degrees of freedom

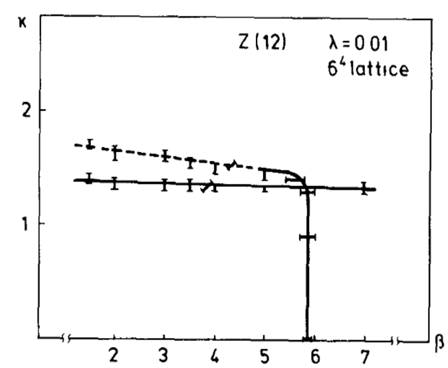
- Hamiltonian in *electric basis*

- Finite computational resources
  $\Rightarrow$ need to truncate theory: $\hat{E}_{\boldsymbol{n},\boldsymbol{e}_\mu} \left|E_{\boldsymbol{n},\boldsymbol{e}_\mu}\right\rangle = E_{\boldsymbol{n},\boldsymbol{e}_\mu} \left|E_{\boldsymbol{n},\boldsymbol{e}_\mu}\right\rangle , \quad E_{\boldsymbol{n},\boldsymbol{e}_\mu} \in [-L, L]$
  $\rightarrow$ suitable for strong coupling, $g^2 \gg 1 \rightarrow L \propto O(10)$

- problem: when $g^2 \rightarrow 0 \Rightarrow L \rightarrow \infty$
  $\Rightarrow$ cannot reach continuum limit

- strategy
  - use a double compact (U(1)) formulation for E and B fields
  - approximate $U(1)$ by $\mathbb{Z}_{2L+1}$

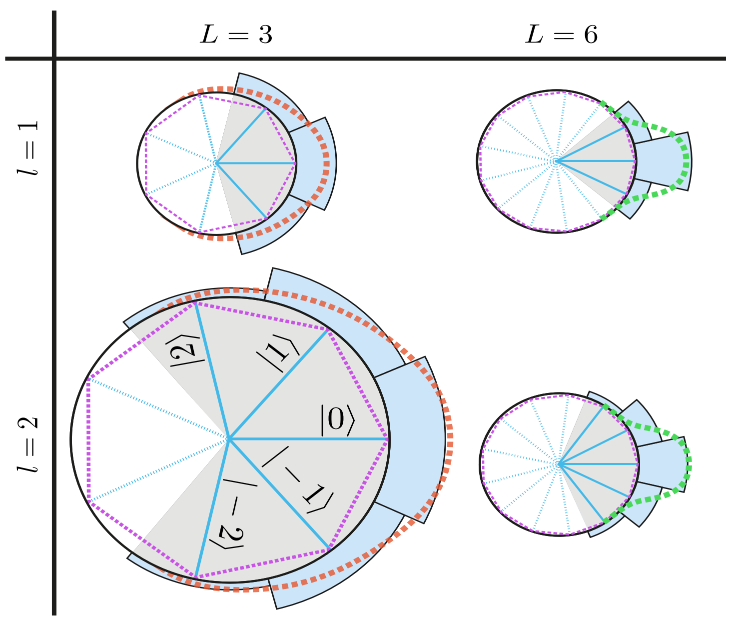
- new problem: L small:
  hit a freezing phase transition
  $\Rightarrow$ cannot reach continuum limit



from: J. Jersak, C.B. Lang, T. Neuhaus, G. Vones, K.J., NPB 265 (1986) 129

Steps towards quantum simulation of LGT
I: Mitigation the of truncation problem

- strategy: use only $2l + 1$ degrees of freedom centered at $|0\rangle$ state
  - when $g^2 \gg 1$, L can be small and $l = L$
  - when $g^2 \ll 1$, $L \gg 1$ but still $l \ll L$
  - L plays role of *resolution* l plays role of *truncation*



$g^2 \gg 1$: $L \sim l$ $g^2 \ll 1$: $L \gg 1$ but $l \ll L$

- when $g^2 \propto O(1)$: interplay between L and l
- doesn't work for Markov chain Monte Carlo $\rightarrow$ autocorrelation

Steps towards quantum simulation of LGT
II: Eliminating degrees of freedom

- consider single periodic plaquette

- charge conservation $\sum_n \hat{q}_n = 0$ in Gauss law provides constraints

$$\hat{E}_{(0,0),\boldsymbol{e}_x} + \hat{E}_{(0,0),\boldsymbol{e}_y} - \hat{E}_{(1,0),\boldsymbol{e}_x} - \hat{E}_{(0,1),\boldsymbol{e}_y} = \hat{q}_{(0,0)}$$

$$\hat{E}_{(0,1),\boldsymbol{e}_x} + \hat{E}_{(0,1),\boldsymbol{e}_y} - \hat{E}_{(1,1),\boldsymbol{e}_x} - \hat{E}_{(0,0),\boldsymbol{e}_y} = \hat{q}_{(0,1)}$$

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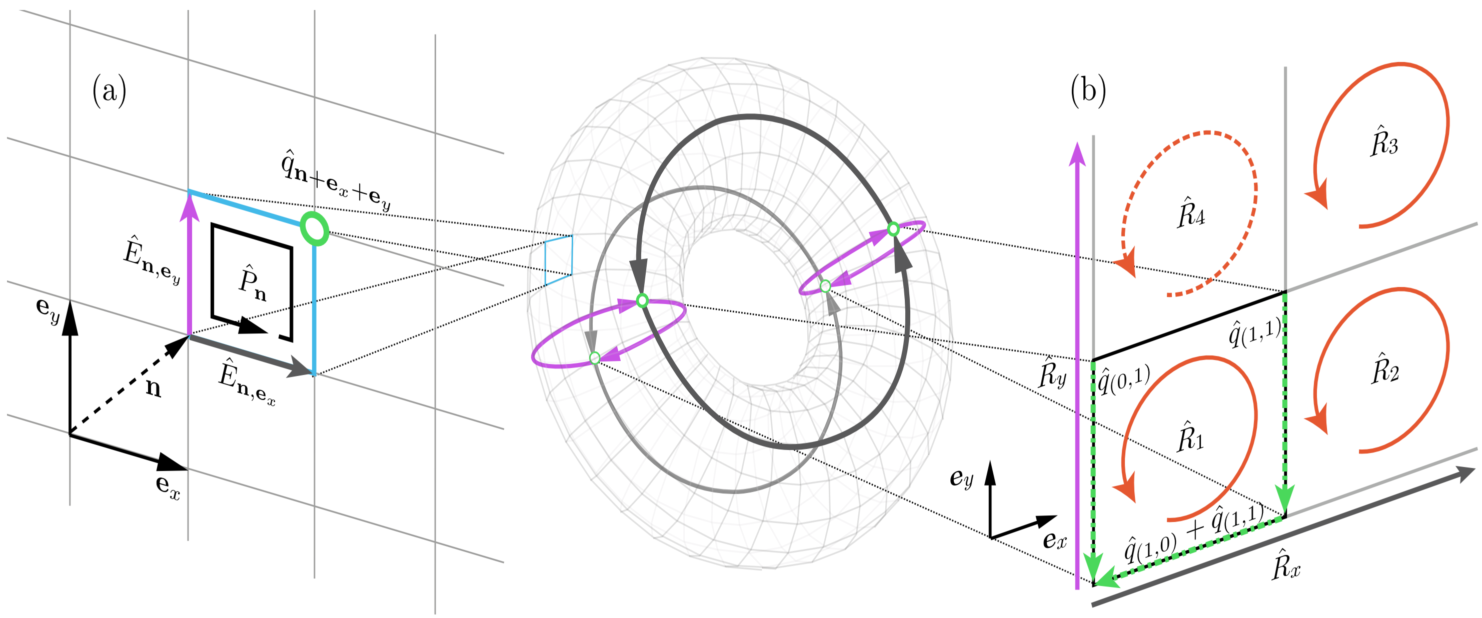
$$\hat{E}_{(1,0),\boldsymbol{e}_x} + \hat{E}_{(1,0),\boldsymbol{e}_y} - \hat{E}_{(0,0),\boldsymbol{e}_x} - \hat{E}_{(1,1),\boldsymbol{e}_y} = \hat{q}_{(1,0)}$$

- solving these equations
  - allows to eliminate some degrees of freedom
  - leads to complicated, non-local interactions

Using rotators and strings

- reformulate Hamiltonian
  - rotators
  - strings e.g. $\hat{E}_{(0,0),\boldsymbol{e}_y} + \hat{E}_{(0,1),\boldsymbol{e}_y} = \hat{R}_y$



Electric field and plaquette **periodic torus** **rotators and strings**

Relation between electric field operator and rotators and strings

- relation between electric fields and rotators and strings

$$\hat{E}_{(0,0),\boldsymbol{e}_x} = \hat{R}_1 + \hat{R}_x - \left(\hat{q}_{(1,0)} + \hat{q}_{(1,1)}\right), \quad \hat{E}_{(1,0),\boldsymbol{e}_x} = \hat{R}_2 - \hat{R}_3 + \hat{R}_x$$

$$\hat{E}_{(1,0),\boldsymbol{e}_y} = \hat{R}_1 - \hat{R}_2 - \hat{q}_{(1,1)}, \quad \hat{E}_{(1,1),\boldsymbol{e}_y} = -\hat{R}_3$$

$$\hat{E}_{(0,1),\boldsymbol{e}_x} = -\hat{R}_1, \quad \hat{E}_{(1,1),\boldsymbol{e}_x} = \hat{R}_3 - \hat{R}_2$$

$$\hat{E}_{(0,0),\boldsymbol{e}_y} = \hat{R}_2 - \hat{R}_1 + \hat{R}_y - \hat{q}_{(0,1)}, \quad \hat{E}_{(0,1),\boldsymbol{e}_y} = \hat{R}_3 + \hat{R}_y$$

inverted version:

$$\hat{R}_1 = -\hat{E}_{(0,1),\boldsymbol{e}_x}$$

$$\hat{R}_2 = -\hat{E}_{(0,1),\boldsymbol{e}_x} - \hat{E}_{(1,0),\boldsymbol{e}_y} - \hat{q}_{(1,1)}$$

$$\hat{R}_3 = -\hat{E}_{(1,1),\boldsymbol{e}_y}$$

$$\hat{R}_x = -\hat{E}_{(0,0),\boldsymbol{e}_x} + \hat{E}_{(0,1),\boldsymbol{e}_x} + \hat{q}_{(1,0)} + \hat{q}_{(1,1)}$$

$$\hat{R}_y = \hat{E}_{(0,1),\boldsymbol{e}_y} + \hat{E}_{(1,1),\boldsymbol{e}_y}$$

Hamiltonian in terms of rotators and strings

- setting all charges to zero $\left[\hat{H}_{\text{gauge}}, \hat{R}_x\right] = 0 \Rightarrow$ string operator irrelvant
- Hamiltonian becomes rather simple
  $\rightarrow$ eliminate (arbitrarily) $\hat{P}_4$

$$\hat{H}_E^{(\mathrm{e})} = 2g^2 \left[\hat{R}_1^2 + \hat{R}_2^2 + \hat{R}_3^2 - \hat{R}_2 \left(\hat{R}_1 + \hat{R}_3\right)\right]$$

$$\hat{H}_B^{(\mathrm{e})} = -\frac{1}{2g^2 a^2} \left[\hat{P}_1 + \hat{P}_2 + \hat{P}_3 + \hat{P}_1 \hat{P}_2 \hat{P}_3 + \mathrm{H.c.}\right]$$

Steps towards quantum simulation of LGT
III: Switching to the magnetic basis

- discrete Fourier transformation

$$\hat{\mathcal{F}}^{\dagger}_{2L+1} = \frac{1}{\sqrt{2L+1}} \sum_{\mu,\nu=-L}^{L} \mathrm{e}^{-i\frac{2\pi}{2L+1}\mu\nu} |\mu\rangle\langle\nu$$

diagonalizes lowering plaquette operator (γ integer)

$$\hat{\mathcal{F}}_{2L+1}\hat{P}^{\gamma}\hat{\mathcal{F}}^{\dagger}_{2L+1} = \sum_{r=-L}^{L} \exp^{-i\frac{2\pi}{2L+1}\gamma r} |r\rangle\langle r|$$

- rotators can be treated by Fourier expansion (up to a constant)

$$\hat{R} \mapsto \sum_{\nu=1}^{2L} f^{s}_{\nu} \sin\left(\frac{2\pi\nu}{2L+1}\hat{R}\right) \;, \hat{R}^2 \mapsto \sum_{\nu=1}^{2L} f^{c}_{\nu} \cos\left(\frac{2\pi\nu}{2L+1}\hat{R}^2\right)$$

Hamiltonian in magnetic basis

- electric part

$$\hat{H}_E^{(\mathrm{b})} = g^2 \sum_{\nu=1}^{2L} \left\{ f_\nu^c \sum_{j=1}^{3} \hat{R}_j^\nu + \frac{f_\nu^s}{2} \left[\hat{R}_2^\nu - \left(\hat{R}_2^\dagger \right)^\nu \right] \right.$$

$$\left. \times \sum_{\mu=1}^{2L} f_\mu^s \left[\hat{R}_1^\mu + \hat{R}_3^\mu \right] \right\} + \mathrm{H.c.}$$

  – f_μ^s, f_μ^c known coefficients

- (diagonal) magnetic part $|\boldsymbol{r}\rangle = |r_1 r_2 r_3\rangle$

$$\hat{H}_B^{(\mathrm{b})} = -\frac{1}{g^2 a^2} \sum_{r=-L}^{L} \left[\cos\left(\frac{2\pi r_1}{2L+1} \right) \right.$$

$$+ \cos\left(\frac{2\pi r_2}{2L+1} \right) + \cos\left(\frac{2\pi r_3}{2L+1} \right)$$

$$\left. + \cos\left(\frac{2\pi (r_1 + r_2 + r_3)}{2L+1} \right) \right] |\boldsymbol{r}\rangle \langle \boldsymbol{r}|$$

Efficient formulation for quantum and tensor network simulations

- electric part

$$\hat{H}_{\mathrm{E}}^{(b)} = g^2 \sum_{\nu=1}^{2L} \left\{ f_\nu^c \sum_{j=1}^{3} \left(\hat{V}_j^-\right)^\nu + \frac{f_\nu^s}{2} \left[\left(\hat{V}_2^-\right)^\nu - \left(\hat{V}_2^+\right)^\nu \right] \right.$$

$$\left. \times \sum_{\mu=1}^{2L} f_\mu^s \left[\left(\hat{V}_1^-\right)^\mu + \left(\hat{V}_3^-\right)^\mu \right] \right\} + \mathrm{H.c.}$$

- (diagonal) magnetic part

$$\hat{H}_{\mathrm{B}}^{(b)} = -\frac{1}{g^2} \left[\sum_{i=1}^{3} \cos\left(\frac{2\pi \hat{S}_i^z}{2L+1} \right) + \cos\left(\frac{2\pi \left(\hat{S}_1^z + \hat{S}_2^z + \hat{S}_3^z \right)}{2L+1} \right) \right]$$

- $\hat{S}^z$, z-component of spin operator, $\hat{V}^-$ ladder operator
  $\rightarrow$ expressible in Pauli operators

$$\hat{V}^- \equiv \begin{bmatrix} 0 & \dots & \dots & 0 \\ 1 & \dots & \dots & 0 \\ 0 & \ddots & \vdots & 0 \\ 0 & \dots & 1 & 0 \end{bmatrix}$$

Steps towards quantum simulation of LGT
IV: The observable

- having a single plaquette, the observable is

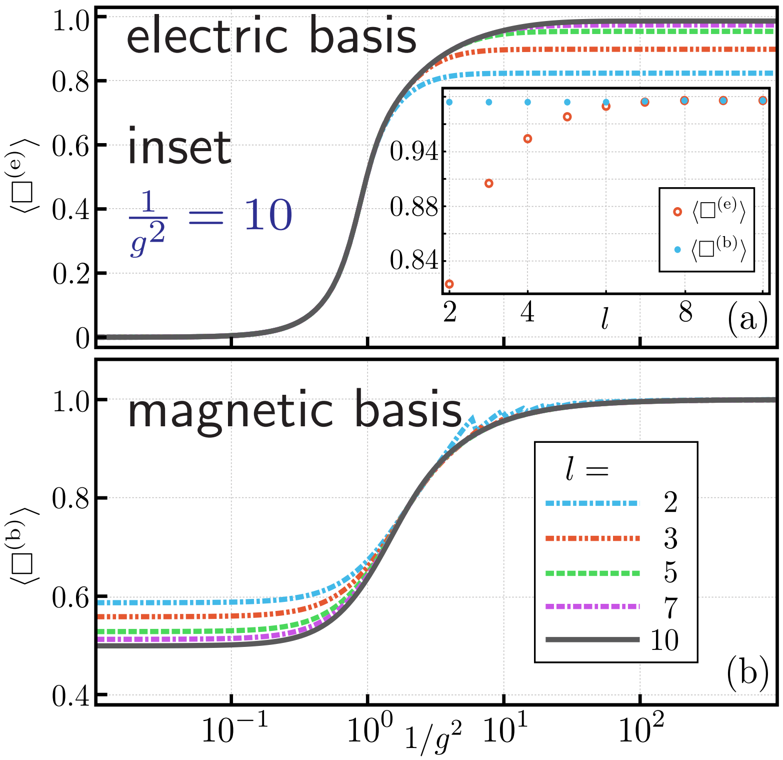
$$\langle \Box \rangle = -\frac{1}{V} \left\langle \Psi_0 \left| \hat{H}_B \right| \Psi_0 \right\rangle$$

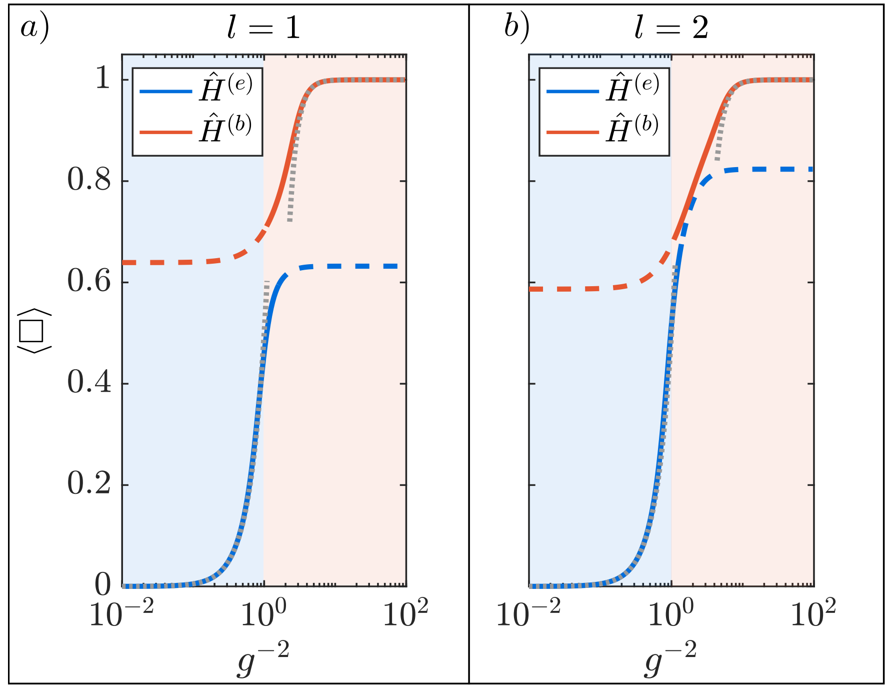
  i.e. the plaquette expectation value in the ground state

  – can detect phase transitions
  – was also used in pioneering work by M. Creutz, Phys. Rev. D 21, 2308 (1980)
  – encodes the running coupling $\alpha_{\text{ren}} = g^2/\langle \Box \rangle^{1/4}$
  (Booth et.al., Phys.Lett.B 519 (2001) 229, hep-lat/0103023)
  $\leftarrow$ perturbative expansion of $\langle \Box \rangle$
  $\rightarrow$ provides non-perturbative Λ parameter
  i.e. scale, where non-perturbative physics sets in

Coupling dependence of plaquette

- plaquette dependence on g^2 and different truncations





truncation effect

from D. Paulson et.al., PRX Quantum 2 (2021) 030334

Truncation effects

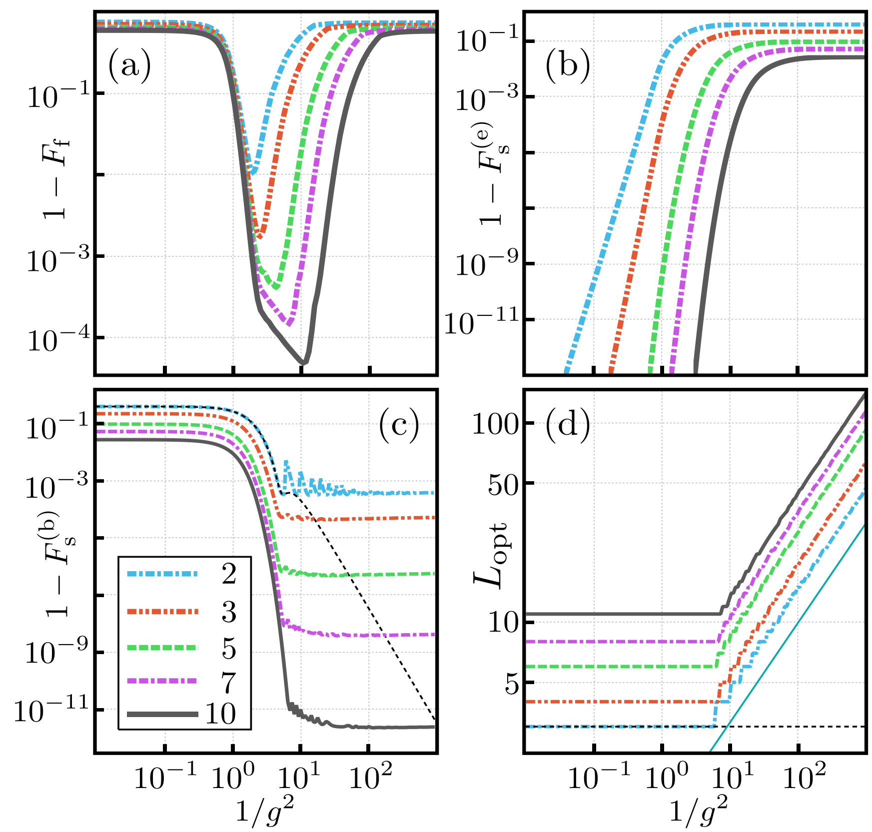
- measures for quantifying truncations effects
  - sequence fidelity

    $$F_{\mathrm{s}}^{(\mu)}(l,L) = \sum_{r=-l+1}^{l-1} \left\langle \psi^{(\mu)}(l-1,L) \mid \boldsymbol{r} \right\rangle \left\langle \boldsymbol{r} \mid \psi^{(\mu)}(l,L) \right\rangle$$

    → overlap of successive truncations $l-1$ and l
  - Fourier fidelity

    $$F_{\mathrm{f}}(l) = \max_{L>l} \left| \left\langle \psi^{(\mathrm{b})}(L,l) | \hat{\mathcal{F}}(L,l) | \psi^{(\mathrm{e})}(l) \right\rangle \right|^2$$

    → overlap of ground state in electric and magnetic representation

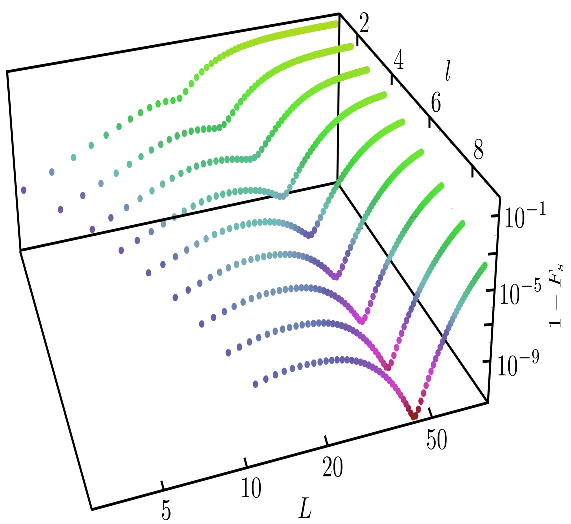


Steps towards quantum simulation of LGT
V: which L and l?

- sequence fidelity

$$F_{\mathrm{s}}^{(\mu)}(l,L)=\sum_{r=-l+1}^{l-1}\left\langle\psi^{(\mu)}(l-1,L)\mid\boldsymbol{r}\right\rangle\left\langle\boldsymbol{r}\mid\psi^{(\mu)}(l,L)\right\rangle$$

$\rightarrow$ overlap of successive truncations $l-1$ and l



$1/g^2$	Standard truncation (electric basis)	Unscaled $\mathbb{Z}_N$ truncation (electric and magnetic basis)	Scaled $\mathbb{Z}_N$ truncation (electric and magnetic basis)
0.1	27	27	27
10	2197	1331	125
100	>9261	27	27

$g^2=1/100$
– optimal value L_{opt}
– suffiently large value of l

number of states drastically reduced
$\rightarrow$ computational cost reduced
$\Rightarrow$ **enormous gain**

Adding matter

- using staggered discretization
  - mass term

$$\hat{H}_M = m \sum_{n} (-1)^{n_x+n_y} \hat{\Psi}^\dagger_n \hat{\Psi}_n$$

  - kinetic term

$$\hat{H}_K = \kappa \sum_{\boldsymbol{n}} \sum_{\mu=x,y} \left[\hat{\Psi}^\dagger_{\boldsymbol{n}} \left(\hat{U}^\dagger_{\boldsymbol{n},\boldsymbol{e}_\mu} \right) \hat{\Psi}_{\boldsymbol{n}+\boldsymbol{e}_\mu} + \mathrm{H.c.} \right]$$

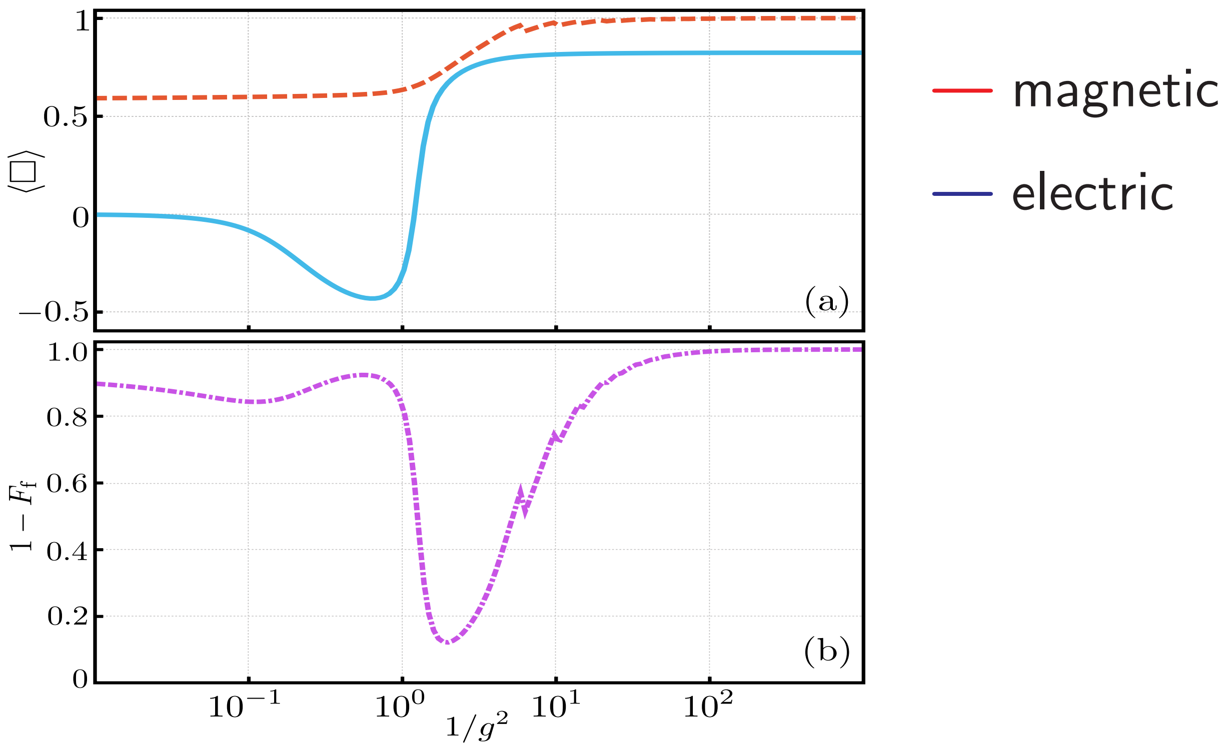
  - charge operator

$$\hat{q}_{\mathbf{n}} = q \left(\hat{\Psi}^\dagger_{\mathbf{n}} \hat{\Psi}_{\mathbf{n}} - \frac{\mathbb{1}}{2} \left[1 - (-1)^{n_x+n_y} \right] \right)$$

- performing the same transformations to magnetic basis
  $\rightarrow$ obtain Hamiltonian in magnetic basis

Identifying a phase transition

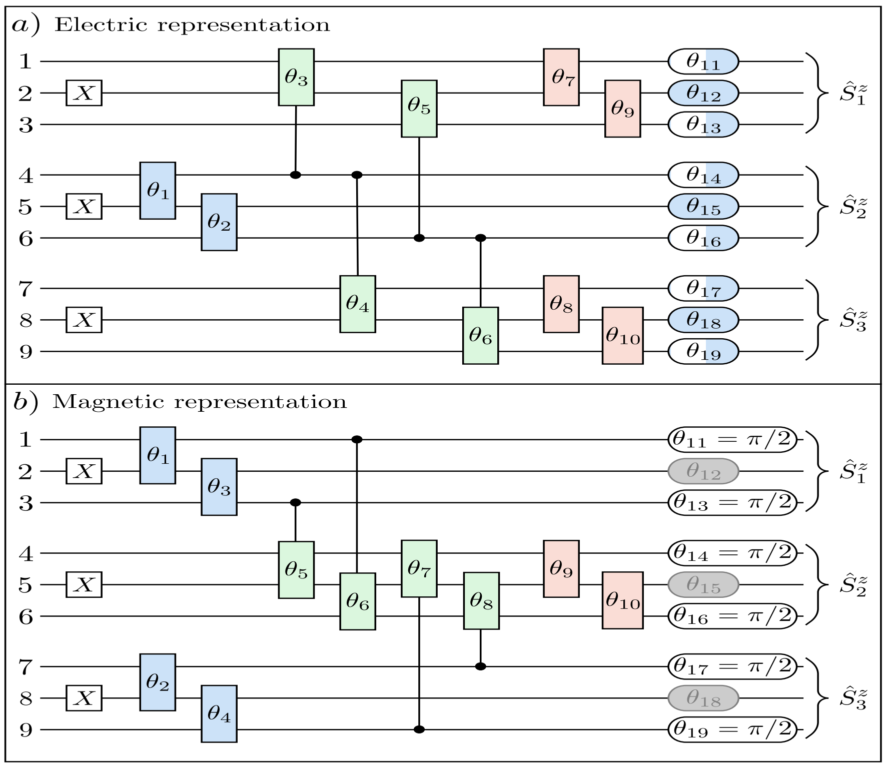
- using an open plaquette with dynamical matter
- coupling dependence of plaquette at negative fermion mass
  $\rightarrow$ competing effects of kinetic and magnetic terms
- a phase transition at negative fermion mass (?)
  $\rightarrow$ fidelity largish



Steps towards quantum simulation of LGT
VII: construct quantum circuit and measurement protocol

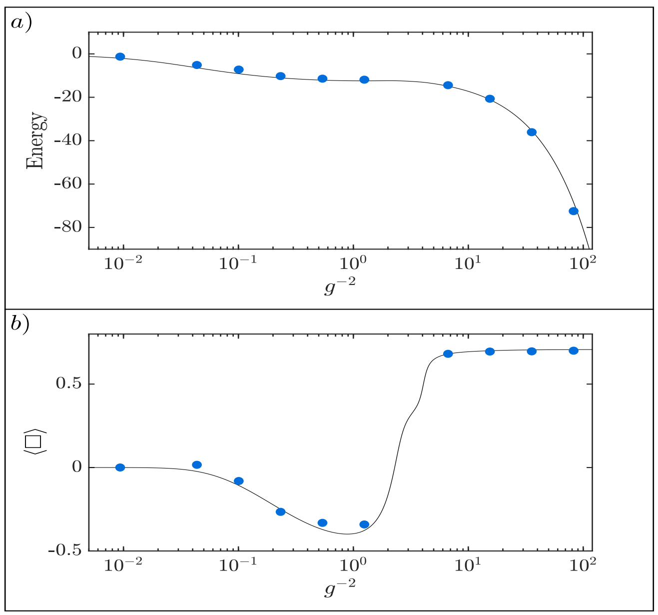
(D. Paulson, L. Dellantonio, J. Haase, A. Celi, A. Kan, A. Jena, C. Kokail, R. van Bijnen, K.J., P. Zoller, C. Muschik, PRX Quantum 2 (2021) 030334)

- designing the quantum circuit



Steps towards quantum simulation of LGT
VIII: demonstration of feasibility on NISQ devices

- perform classical variational quantum simulation
  - obtain measurement points
  - demonstrate effect:
    $\rightarrow$ indications of phase transition at negative fermion mass



Topological terms for 3+1 dimensional gauge theories

(Angus Kan, Lena Funcke, Stefan Kühn, Luca Dellantonio,
Jinglei Zhang, Jan Haase, Christine Muschik, K.J., Phys.Rev.D, 104 (2021) 3 034504)

- Topological term from divergence of chiral current $(\hat{j}_5^\mu = \hat{\bar{\psi}}\gamma^\mu\gamma^5\hat{\psi})$

$$\sum_\mu \partial_\mu \hat{j}_5^\mu = \frac{g^2}{8\pi^2}\sum_{\mu,\nu}\hat{F}^{\mu\nu}\hat{\tilde{F}}_{\mu\nu}$$

  - tensor network calculations
  - quantum computations
- relation between θ-term and (complex) mass term

  under chiral rotation $\hat{\psi} \rightarrow e^{i\alpha\gamma^5}\hat{\psi}$

$$m\hat{\bar{\psi}}\hat{\psi} \rightarrow m\hat{\bar{\psi}}e^{2i\alpha\gamma^5}\hat{\psi}$$

$$\hat{H} \rightarrow \hat{H} + \alpha\sum_\mu \partial_\mu \hat{j}_5^\mu = \hat{H} + \frac{\alpha g^2}{8\pi^2}\sum_{\mu,\nu}\hat{F}^{\mu\nu}\hat{\tilde{F}}_{\mu\nu} + m\hat{\bar{\psi}}e^{2i\alpha\gamma^5}\hat{\psi}$$

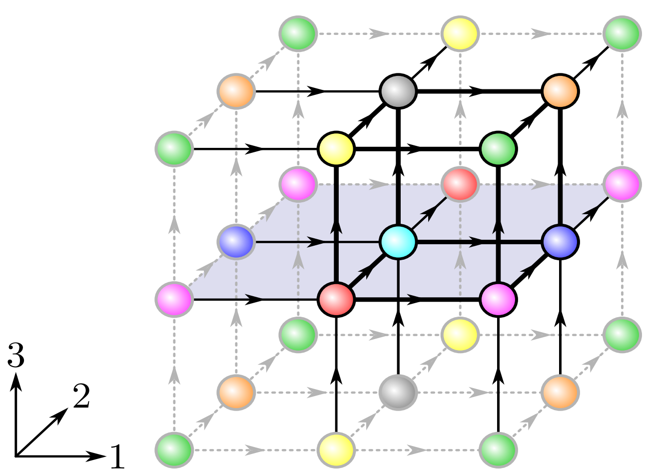
$\rightarrow$ negative mass $(-m, \theta = 0) \leftrightarrow (+m, \theta = \pi)$

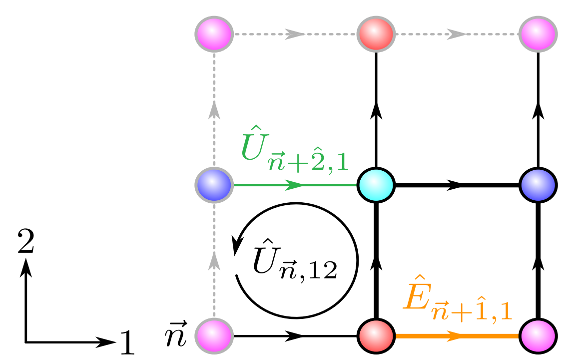
Lattice version of topological terms

- abelian and non-abelian lattice version of $\hat{F}^{\mu\nu}\hat{\tilde{F}}_{\mu\nu}$:

$$\theta\hat{Q} = -\frac{ig^2\theta}{8\pi^2 a}\sum_{\vec{n},b}\sum_{(i,j,k)\in\,\text{even}} \mathrm{Tr}\left[\left(\hat{E}^b_{\vec{n}-\hat{\imath},i} + \hat{E}^b_{\vec{n},i}\right)\lambda^b\left(\hat{U}_{\vec{n},jk} - \hat{U}^\dagger_{\vec{n},jk}\right)\right]$$

- alternative ways:
  - transfer matrix (arxiv:2105.06019)
  - θ-term as perturbation (arXiv:2104.02024)
- here: look at single periodic cube with exact diagonalization





Lattice Hamiltonian and observables

- lattice Hamiltonian $\hat{H} = \hat{H}_E + \hat{H}_B + \theta\hat{Q}$

$$\hat{H}_E = \frac{1}{2\beta}\sum_{\vec{n}}\sum_{j=1}^{3}\hat{E}^2_{\vec{n},j},$$

$$\hat{H}_B = -\frac{\beta}{2}\sum_{\vec{n}}\sum_{j,k=1;k>j}^{3}\left(\hat{U}_{\vec{n},jk} + \hat{U}^\dagger_{\vec{n},jk}\right)$$

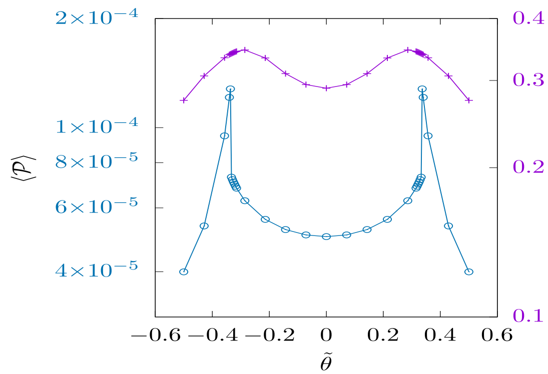
$$\theta\hat{Q} = -i\frac{\tilde{\theta}}{\beta}\sum_{\vec{n}}\sum_{(i,j,k)\in\,\text{even}}\left(\hat{E}_{\vec{n}-\hat{\imath},i} + \hat{E}_{\vec{n},i}\right)\left(\hat{U}_{\vec{n},jk} - \hat{U}^\dagger_{\vec{n},jk}\right)$$

- observables

$$\langle\mathcal{P}\rangle = -\frac{1}{V\beta}\left\langle\Psi_0\left|\hat{H}_B\right|\Psi_0\right\rangle\,(\text{plaquette})\;\langle\mathcal{Q}\rangle = -\frac{\beta}{V}\left\langle\Psi_0|\hat{Q}|\Psi_0\right\rangle\,(\text{topological charge})$$

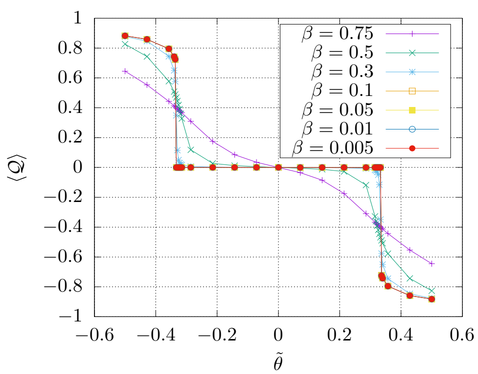
$$\left\langle E^2\right\rangle = \frac{\beta}{V}\left\langle\Psi_0\left|\hat{H}_E\right|\Psi_0\right\rangle\,(\text{electric energy})\;\langle\mathcal{E}\rangle = \left\langle\Psi_0\left|\sum_{\vec{n},j}\hat{E}_{\vec{n},j}\right|\Psi_0\right\rangle\,(\text{electric field})$$

Results: plaquette, electric energy and topological charge



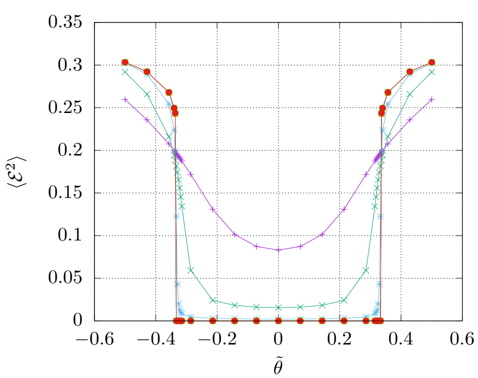
plaquette at $\beta = 0.01$ and $\beta = 0.75$

$\rightarrow$ weakening of transiton



topological charge

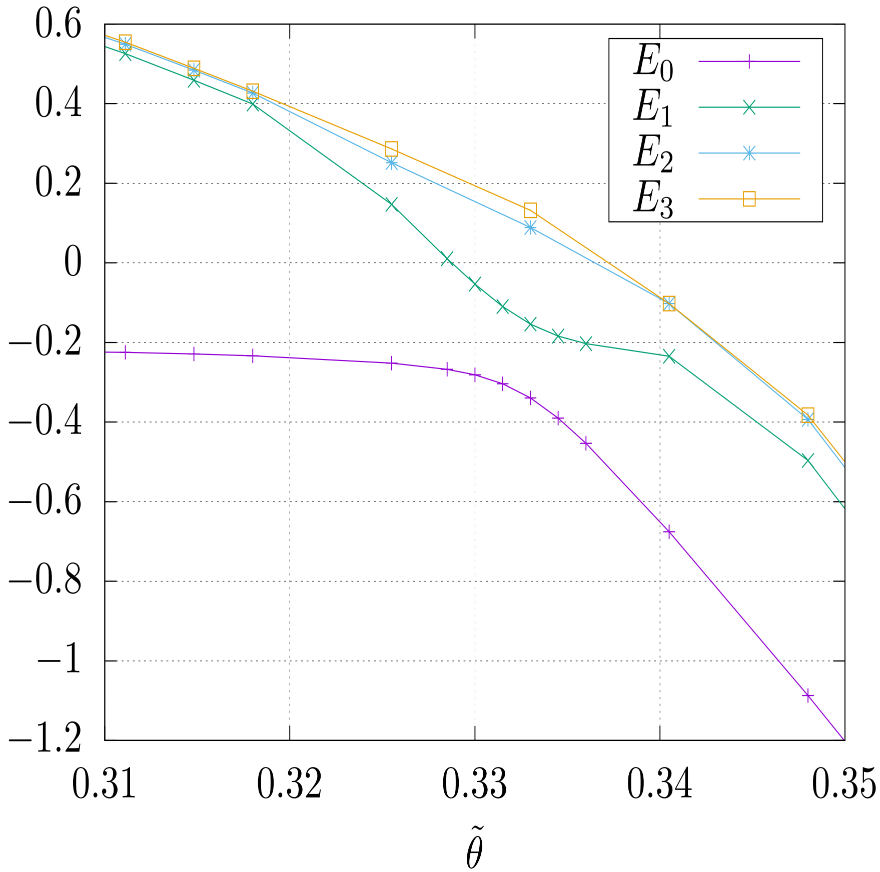
$\rightarrow$ signs of phase transition for $\beta \ll 1$



electric field

$\rightarrow$ signs of phase transition for $\beta \ll 1$

Results: avoided level crossing



energy spectrum
calculation at $\beta = 0.3$
$\rightarrow$ avoided level crossing
2nd order phase transition?

- check finding with tensor networks on larger lattices
- investigate larger β and Coulomb phase
- explore the nature of the phases close to phase transition

Conclusion: topological terms in lattice gauge theories

- 2+1-dimensional gauge theory
  - developed resource effcient formulation for quantum simulations and tensor network calculations
  - allows to perform computations at all values of the coupling
    $\rightarrow$ demonstrated at example of d=2+1 dimensional QED
    $\rightarrow$ signature of phase transition at negative fermion mass
  - can be generalized to higher dimensions
  - ready for simulations with topological term
- Outlook
  - Hamiltonian formulation of topological term in d=2+1 and d=3+1 dimensional QED

  * classical calculations: tensor networks
  * quantum calculations: quantum computer

Steps towards quantum simulation of LGT
VI: Finding ground state: Variational Quantum Simulation

- start with some initial state $|\Psi_{\rm init}\rangle$
- apply succesive gate operations $\equiv$ unitary operations $e^{iS\theta}$
- examples for S: Pauli matrices σ_x, σ_y, σ_z, parametric CNOT

$$|\Psi(\vec{\theta}_{\rm init})\rangle = e^{iS_{(n)}\theta_n^{\rm init}} \dots e^{iS_{(1)}\theta_1^{\rm init}} |\psi_{\rm init}\rangle$$

- with $R_j := e^{iS_{(j)}\theta_j}$ cost function evaluated on quantum computer

$$C(\vec{\theta}_{\rm init}) := \left\langle \psi_{\rm init} \left| \left(\prod_{j=1}^n R_j\right)^\dagger H \prod_{j=1}^n R_j \right| \psi_{\rm init} \right\rangle$$

- Hamiltonian expressed in terms of Pauli matrices (generally possible)
  $\rightarrow$ measure result of Pauli matrix operation on $|\Psi(\vec{\theta}_{\rm init})\rangle$

Finding ground state: Variational Quantum Simulation

(0) evaluate cost function for initial parameters $\vec{\theta}_{\text{init}}$ on *quantum computer*

$$C(\vec{\theta}_{\text{init}}) := \left\langle \psi_{\text{init}} \middle| \left(\prod_{j=1}^{n} R_j(\vec{\theta}_{\text{init}})\right)^{\dagger} H \prod_{j=1}^{n} R_j(\vec{\theta}_{\text{init}}) \middle| \psi_{\text{init}} \right\rangle$$

$\downarrow$

(1) give to *classical computer* $\rightarrow$ optimize over $\vec{\theta}_{\text{init}}$
e.g. gradient descent, baysean optimization, ...
$\rightarrow$ obtain new set of parameters $\vec{\theta}_{\text{new}}$

$\downarrow$

(2) give to *quantum computer* evaluate new cost function

$$C(\vec{\theta}_{\text{new}}) := \left\langle \psi_{\text{init}} \middle| \left(\prod_{j=1}^{n} R_j(\vec{\theta}_{\text{new}})\right)^{\dagger} H \prod_{j=1}^{n} R_j(\vec{\theta}_{\text{new}}) \middle| \psi_{\text{init}} \right\rangle$$

$\downarrow$

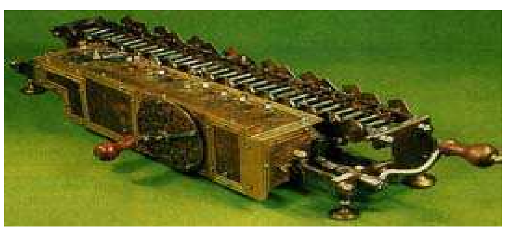
(3) give to *classical computer* $\rightarrow$ optimize over $\vec{\theta}_{\text{init}}$ and $\vec{\theta}_{\text{new}}$, ...
$\rightarrow$ obtain new set of parameters $\vec{\theta}_{\text{new}}$

(4) go to (2) until converge, i.e. find minimum

Variational quantum simulation

- evaluate cost function $\langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$
  on quantum device

- feedback loop



- optimize over parameters $\vec{\theta}$
  on classical computer
  $\rightarrow$ give back new set of $\vec{\theta}$

The Schwinger model with topological θ-term

(L. Funcke, S. Kühn, KJ, Phys.Rev.D 101 (2020) 5, 054507)

- Lagrangian of Schwinger model with topological θ-term

$$\mathcal{L} = \bar{\psi}(i \not{\partial} - gA - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{\theta}{4\pi}\varepsilon^{\mu\nu}F_{\mu\nu}$$

- Hamiltonian

$$\mathcal{H} = -i\bar{\psi}\gamma^1 (\partial_1 - igA_1)\psi + m\bar{\psi}\psi + \frac{1}{2}\left(\mathcal{F} + \frac{g\theta}{2\pi}\right)^2$$

- θ-term shifts electric field operator
  (derivation on operator level in Phys.Rev.D 101 (2020) 5, 054507)

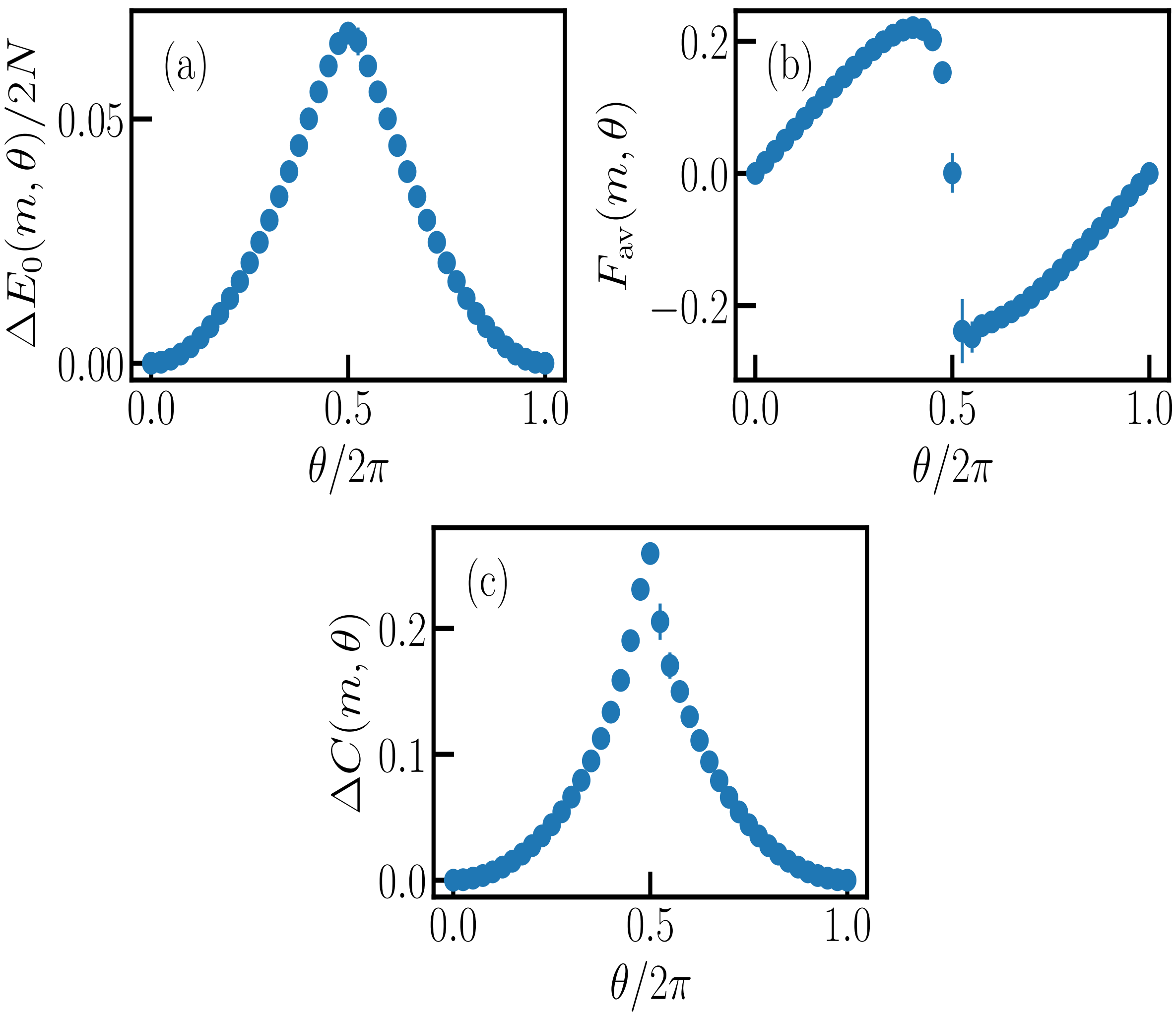
- Lattice formulation

$$H = -\frac{i}{2a}\sum_n \left(\phi_n^\dagger e^{i\vartheta_n}\phi_{n+1} - \text{h.c.}\right) + m\sum_n (-1)^n \phi_n^\dagger \phi_n + \frac{ag^2}{2}\sum_n F_n^2$$

- integrating out gauge fields and Jordan-Wigner transform $(x = 1/a^2g^2)$

$$W = x\sum_n \left(\sigma_n^+\sigma_{n+1}^- + \text{h.c.}\right) + \frac{\mu}{2}\sum_n (-1)^n \left(\mathbb{1} + \sigma_n^z\right) + \sum_n \left(\sum_{k=0}^n Q_k + \frac{\theta}{2\pi}\right)^2$$

Phase transition at $\theta = \pi$



ground state energy,
electric field

chiral condensate

$\frac{\Delta E_0, \mathcal{C}(m,\theta)}{g^2} = \frac{E_0, \mathcal{C}(m,\theta) - E_0, \mathcal{C}(m,\theta_0)}{g^2}$, θ_0 reference value

θ dependence of physical Observables

- perturbative formulae for $m/g \ll 1$ (C. Adams, Ann. Phys. 259, 1 (1997))
- Ground state energy ($\mathcal{E}_+$, $\mathcal{E}_-$ numerical constants)

$$\frac{E_0(m,\theta)g^2}{2L} = -\frac{m\Sigma}{g^2}\cos(\theta) - \pi\left(\frac{m\Sigma}{2g^2}\right)^2 \times \left(\mu_0^2\mathcal{E}_+\cos(2\theta) + \mu_0^2\mathcal{E}_-\right)$$

- Electric field density

$$\frac{\mathcal{F}(m,\theta)}{g} = 2\pi\frac{m\Sigma}{g^2}\sin(\theta) + \pi^2\left(\frac{m\Sigma}{g^2}\right)^2 \mu_0^2\mathcal{E}_+\sin(2\theta)$$

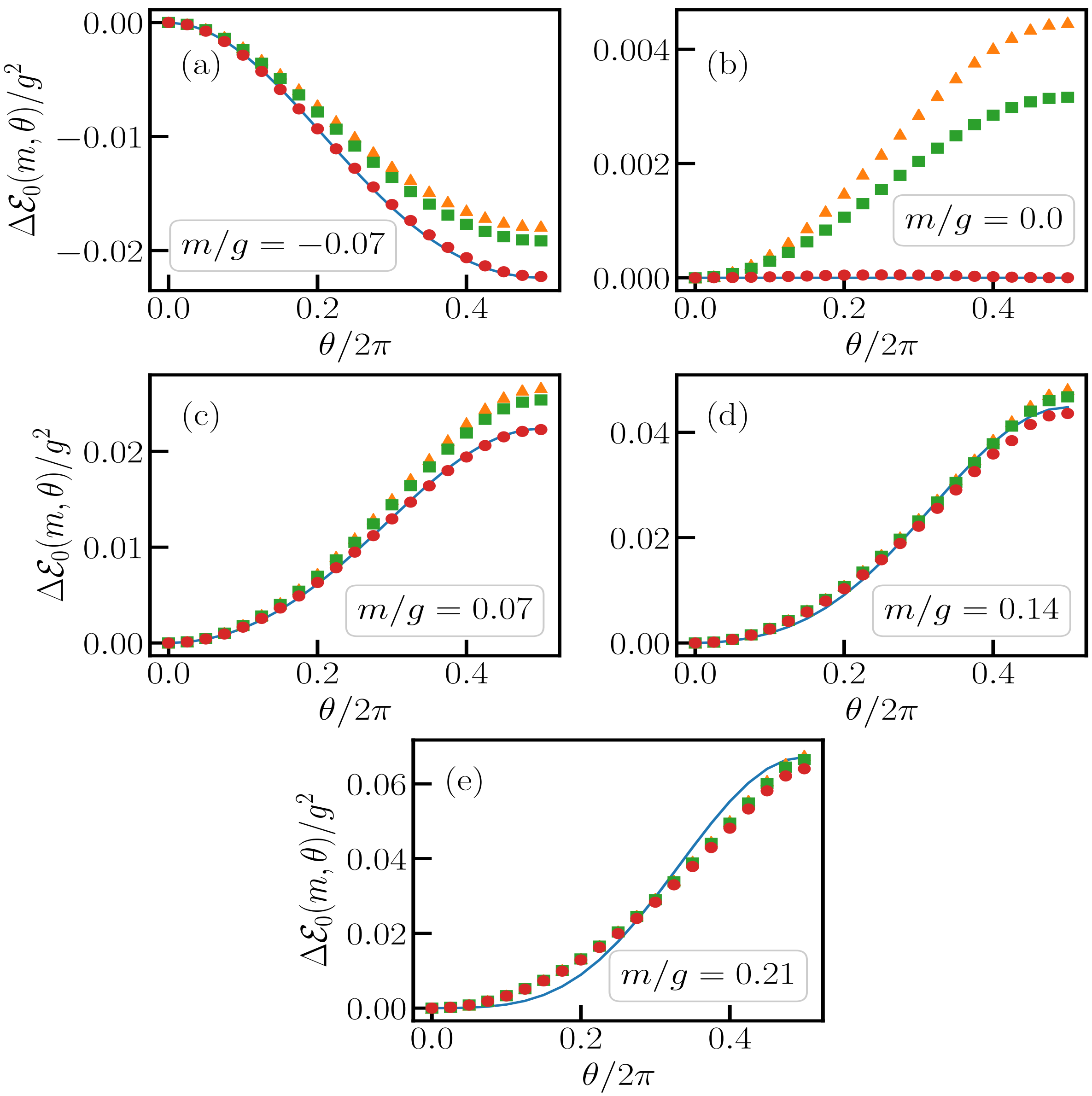
- topological susceptibiliy

$$\frac{\chi_{\text{top}}(m,\theta)}{g} = -\frac{m\Sigma}{g^2}\cos(\theta) - \pi\left(\frac{m\Sigma}{g^2}\right)^2 \mu_0^2\mathcal{E}_+\cos(2\theta)$$

- chiral condensate

$$\frac{\mathcal{C}(m,\theta)}{g} = -\frac{\Sigma}{g}\cos(\theta) - \frac{\pi m}{2g}\left(\frac{\Sigma}{g}\right)^2 \times \left(\mu_0^2\mathcal{E}_+\cos(2\theta) + \mu_0^2\mathcal{E}_-\right)$$

Small mass regime: ground state energy



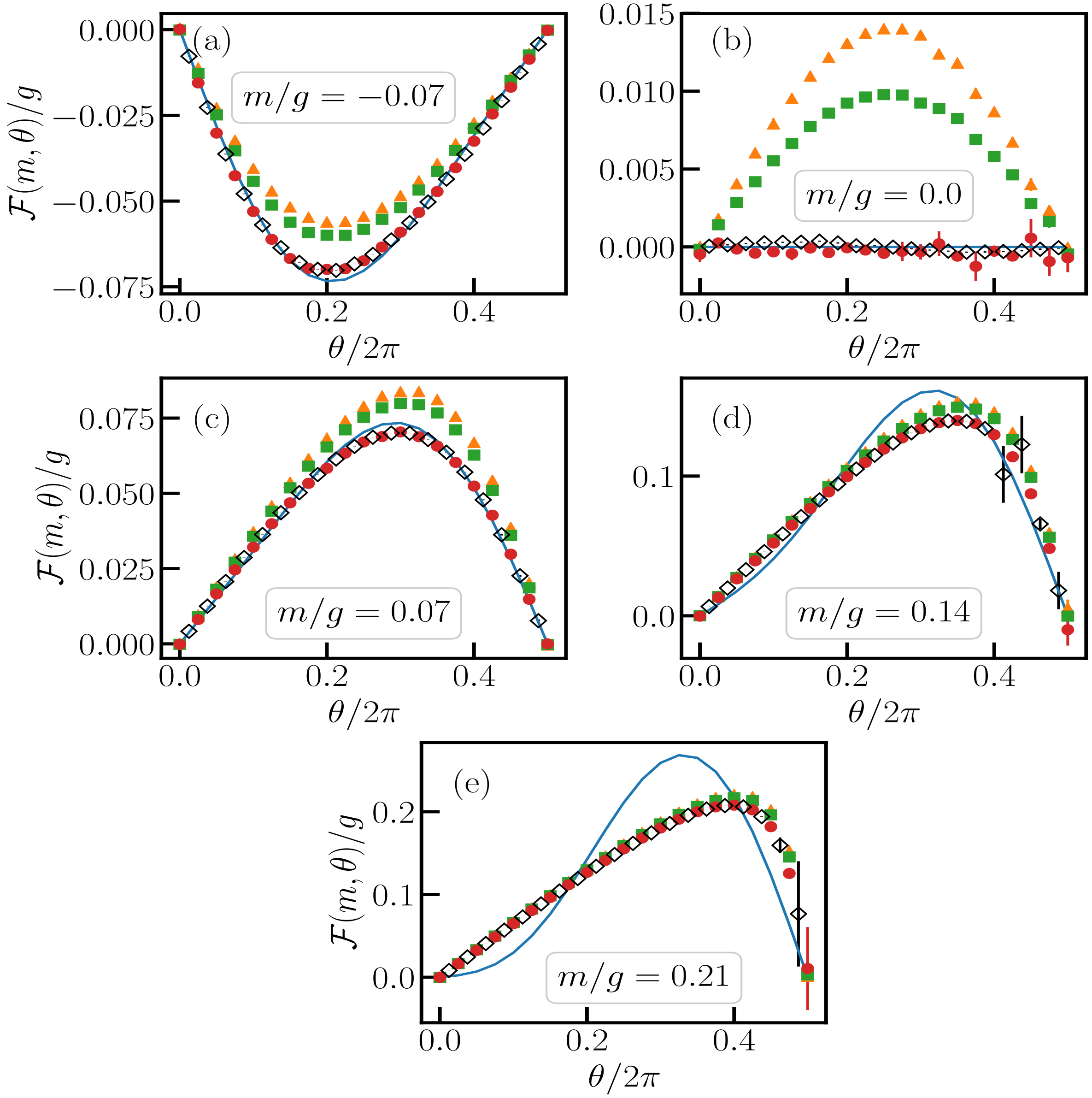
triangle: coarsest lattice spacing

square: finest lattice spacing

circle: continuum limit

$\frac{\Delta\mathcal{E}_0(m,\theta)}{g^2} = \frac{\mathcal{E}_0(m,\theta)-\mathcal{E}_0(m,\theta_0)}{g^2}$, $\theta_0 = 0$ reference value $\rightarrow$ ultra-violet finite

Small mass regime: electric field density



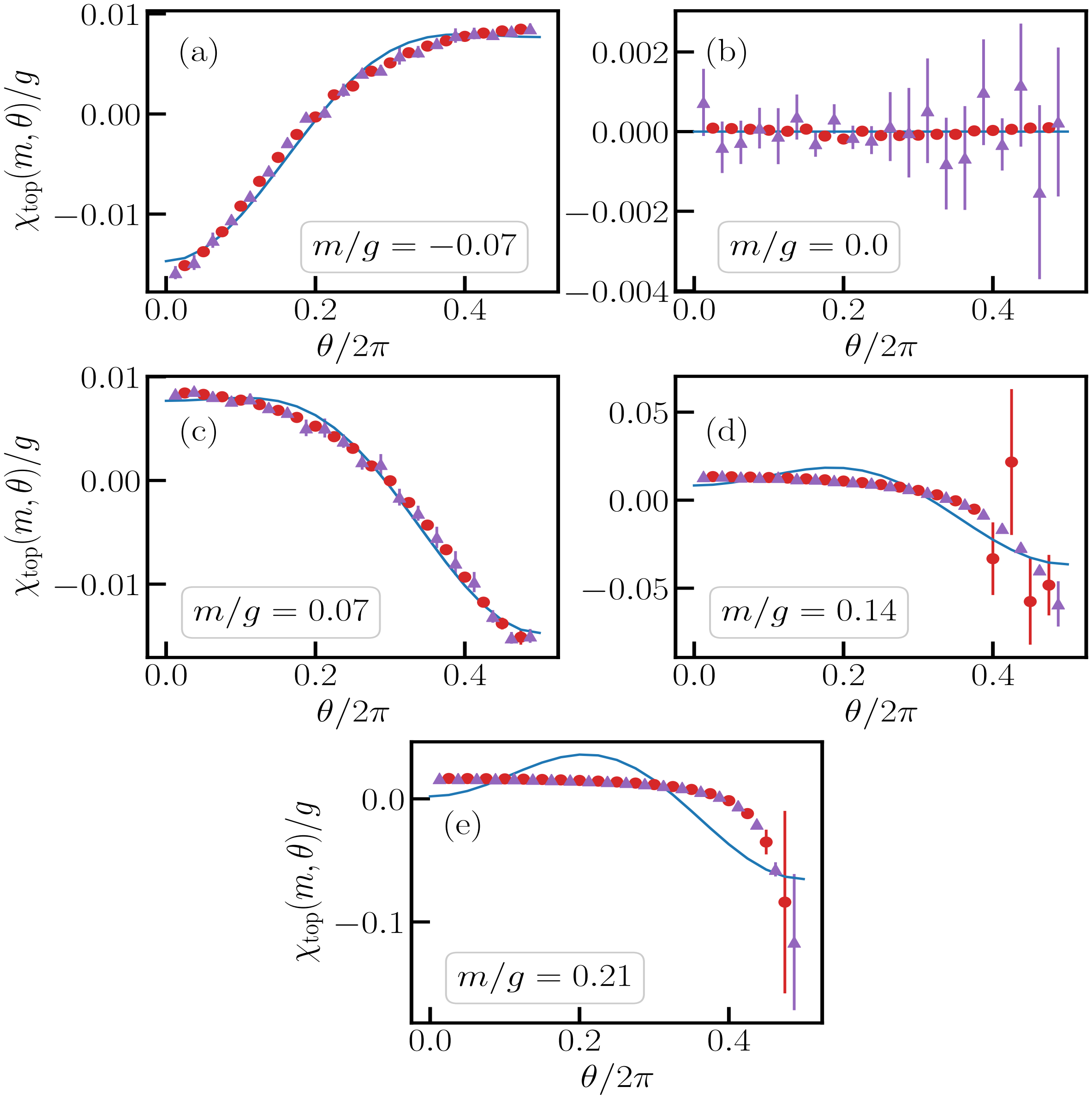
triangle: coarsest lattice spacing

square: finest lattice spacing

circle: continuum limit

$\frac{\Delta\mathcal{F}(m,\theta)}{g^2} = \frac{\mathcal{F}(m,\theta)-\mathcal{F}(m,\theta_0)}{g^2}$, θ_0 reference value

Small mass regime: topological susceptibility



at $m/g = 0 \rightarrow \chi/g = 0$
$\rightarrow$ CP invariance

triangle: coarsest lattice spacing

square: finest lattice spacing

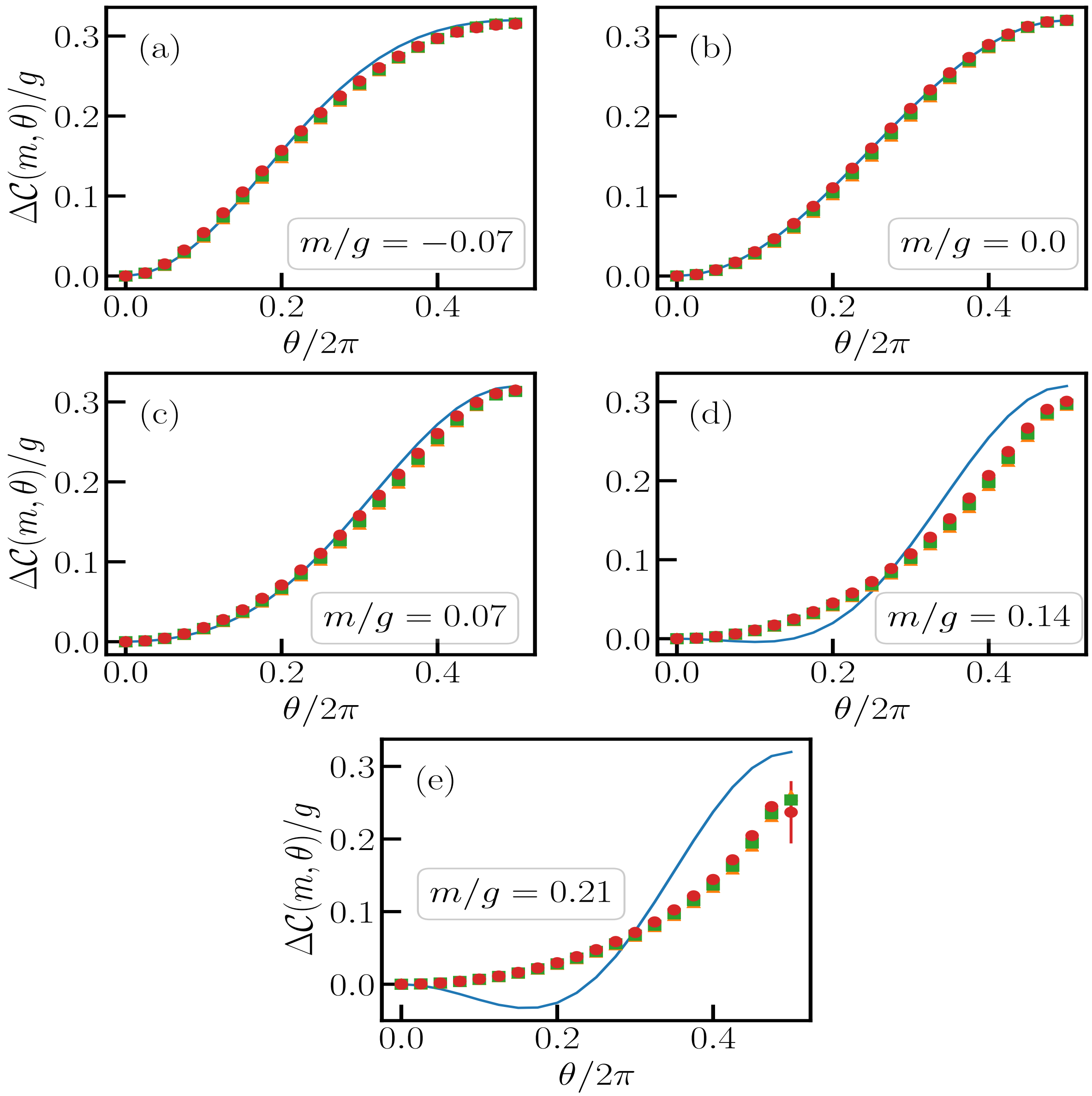
circle: continuum limit

derivative of electric field

2nd derivative of E_0

$\frac{\Delta\chi(m,\theta)}{g^2} = \frac{\chi(m,\theta)-\chi(m,\theta_0)}{g^2}$, θ_0 reference value

Small mass regime: chiral condensate



triangle: coarsest lattice spacing

square: finest lattice spacing

circle: continuum limit

$\frac{\Delta\mathcal{C}(m,\theta)}{g^2} = \frac{\mathcal{C}(m,\theta)-\mathcal{C}(m,\theta_0)}{g^2}$, θ_0 reference value

Summary for 1+1 dimensional QED with θ-term

- MPS allows for controlled computations for $m/g \leq 0$
  $\rightarrow$ not accessible for MCMC

- mass perturbation theory breaks down for $|m/g| \gtrsim 0.14$

Outlook

- 1+1-dimensional QED with many flavours

- 2+1-dimensional and 3+1-dimensional QED
  - develop Hamiltonian for θ-term
  - augmented tree tensor networks,
    (arxiv:2011.10658 and Phys.Rev.X 10 (2020) 4, 041040
  - quantum computation $\rightarrow$ truncation effects

- non-abelian theories