Matching Quantum Computing with Markov Chain Monte Carlo*

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Motivations and Goal

- As for QCD in 3+1 dimensions, the behaviour of QED in 2+1 dimensions shows the phenomena of *confinement* and *asymptotic freedom*.
- Quantum simulations are based on the Hamiltonian formulation $\longrightarrow$ they have no **sign problem**, contrary to Monte Carlo calculations.
- Provides a path to address topological terms, chemical potential or real time simulations.

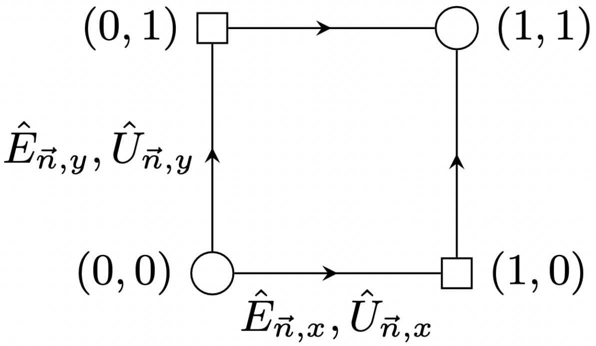
Goal of present work:

- Setup of (2+1)-dimensional QED for quantum computation as a basis for these extensions.
- Compute the running of the coupling and calculate the Λ-parameter (analogous to QCD) by making contact with perturbation theory and matching MC simulations for scale setting.

QED Kogut-Susskind Hamiltonian

- Electric

$$\hat{H}_E = \frac{g^2}{2} \sum_{\vec{n}} \left(\hat{E}^2_{\vec{n},x} + \hat{E}^2_{\vec{n},y} \right)$$



- Mass

$$\hat{H}_m = m \sum_{\vec{n}} (-1)^{n_x+n_y} \hat{\phi}^\dagger_{\vec{n}} \hat{\phi}_{\vec{n}}$$

- Magnetic

$$\hat{H}_B = -\frac{1}{2g^2} \sum_{\vec{n}} \left(\hat{P}_{\vec{n}} + \hat{P}^\dagger_{\vec{n}} \right)$$

with $\hat{P}_{\vec{n}} = \hat{U}_{\vec{n},x} \hat{U}_{\vec{n}+x,y} \hat{U}^\dagger_{\vec{n}+y,x} \hat{U}^\dagger_{\vec{n},y}$ ($\hat{U} = \mathrm{e}^{iag\hat{A}_\mu(\vec{n})}$
measures the phase proportional to g acquired by a unit charge moved along the link)

- Kinetic

$$\hat{H}_{kin} = \Omega \sum_{\vec{n}} \sum_{\mu=x,y} (-1)^x (\hat{\phi}^\dagger_{\vec{n}} \hat{U}^\dagger_{\vec{n},\mu} \hat{\phi}_{\vec{n}+\mu} + H.c.)$$

Haase, Dellantonio, Celi, Paulson, Kan, Jansen, Muschik, Quantum 5 (2021)

Electric/Magnetic Basis

- **Strong coupling:** $\hat{H}_E = \frac{g^2}{2}\sum_{\vec{n}}\left(\hat{E}^2_{\vec{n},x} + \hat{E}^2_{\vec{n},y}\right)$

  Electric Hamiltonian dominant, electric field operators are diagonal $\longrightarrow$ ELECTRIC BASIS

  - Discretisation of *U(1)*:

    U(1) discretised to $\mathbb{Z}_{2L+1}$ (L indicates the size of Hilbert space) $\longrightarrow$ $(-\infty, +\infty) \rightarrow [-L, L]$

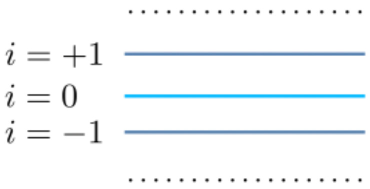
    but difference in cyclic property of lowering (raising) operator, $|-L\rangle \leftrightarrow |L\rangle$

  - Truncation (*l<L*):

    cyclic property lost.

    Truncated electric field and link operator:

$$\hat{E} = \sum_{i=-l}^{l} i\,|i\rangle_{\text{phys.}}\,\langle i|_{\text{phys.}}\,,\hat{U} = \sum_{i=-l+1}^{l} |i-1\rangle_{\text{phys.}}\,\langle i|_{\text{phys.}}$$



Electric/Magnetic Basis

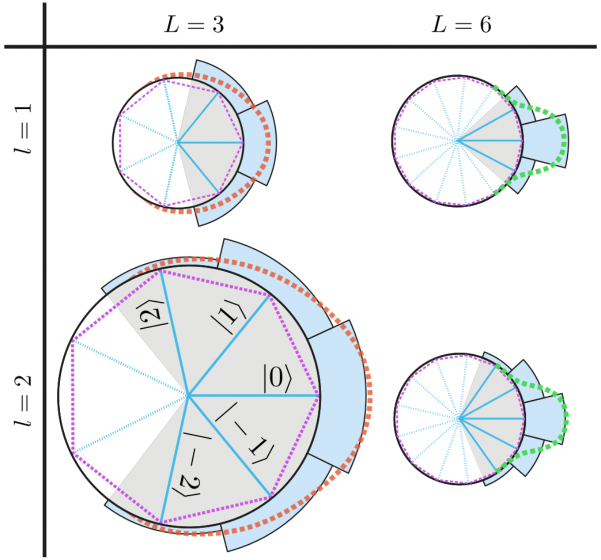
- Weak coupling: $\hat{H}_B = -\frac{1}{2g^2}\sum_{\vec{n}}\left(\hat{P}_{\vec{n}} + \hat{P}^{\dagger}_{\vec{n}}\right)$

Magnetic Hamiltonian dominant, plaquette operators are diagonal ⟶ MAGNETIC BASIS

- Discretization and truncation of *U(1)* :

  Discretization and truncation as seen before,

  but now *L* parameter affects the accuracy of the simulation



Setting the scale and renormalized coupling

Goals:

- Compute the energy gap in the scalar sector: $\Delta E = E_1 - E_0$
- Compute static force: $F(r) = \partial_r V(r)$

$\longrightarrow$ Match with MC

- Compute exp.val. of the plaquette operator and define[1]: $g^2_{\mathrm{boosted}} = \dfrac{g^2}{\langle \Box \rangle}$

$\longrightarrow$ Scale dependence in perturbation theory

- Compute the static potential of a particle-antiparticle pair: $V(r)$

$\longrightarrow$ Running coupling with *step-scaling* approach[2]

[1]Booth et al. Physics Letters B 519 (2001)

[2] Lüscher, Weisz, Wolff Nucl. Phys. B 359 (1991)

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→ Running coupling with *step-scaling* approach[2]

Method: **Variational Quantum Algorithm**

[1]Booth et al. Physics Letters B 519 (2001)

[2] Lüscher, Weisz, Wolff Nucl. Phys. B 359 (1991)

Encoding on a quantum circuit

- Fermions

Mapped to spins using a *Jordan-Wigner transformation*

$$\phi_{\vec{n}} = \Big[\prod_{\vec{k}<\vec{n}} (i\sigma^z_{\vec{k}})\Big]\sigma^-_{\vec{n}}\,, \qquad \phi^\dagger_{\vec{n}} = \Big[\prod_{\vec{k}<\vec{n}} (-i\sigma^z_{\vec{k}})\Big]\sigma^+_{\vec{n}}$$

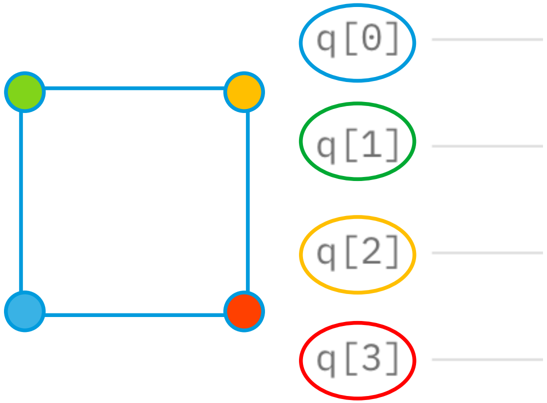
where the relation $\vec{k} < \vec{n}$ is defined by $(0,0) < (0,1) < (1,1) < (1,0)$.

For example:

$$\hat{H}_m = m\sum_{\vec{n}}(-1)^{n_x+n_y}\hat{\phi}^\dagger_{\vec{n}}\hat{\phi}_{\vec{n}} = m/2\sum_{\vec{n}}(1+(-1)^{n_x+n_y}\sigma^z)$$

- Since we are interested in zero-charge sector for the mass-gap, for 4 sites we have 6 states with combination of vacuum and e-p pairs

$$|vvvv\rangle\,,|epvv\rangle\,,|vpev\rangle\,,|vvep\rangle\,,|evvp\rangle\,,|epep\rangle \longrightarrow$$ 4 qubits: $|q_0\rangle\ldots|q_3\rangle$



Encoding on a quantum circuit

- ## Gauge fields

Gray Encoding

Minimum number of qubits required per gauge variable: $q_{\min} = \lceil \log_2 [N(2l+1)] \rceil$

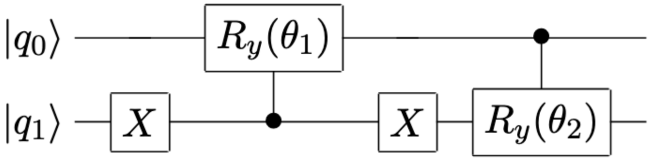
Neighbour physical states differ only by 1 bit.

Example *l=1*:

$$|-1\rangle_{\text{ph.}} \mapsto \ |00\rangle \,, \ |0\rangle_{\text{ph.}} \mapsto \ |01\rangle \,, \ |1\rangle_{\text{ph.}} \mapsto \ |11\rangle$$

$$\boxed{(|10\rangle \ \ \text{unphysical})}$$

Quantum Circuit:



Excited states: Variational Quantum Deflation

- Variational Quantum Deflation (VQD)

Extends VQE to compute excited states by optimizing the cost function

$$E(\theta_k) = \langle\psi(\theta_k)|H|\psi(\theta_k)\rangle + \sum_{i=0}^{k-1}\beta_i \left|\langle\psi(\theta_k)|\psi(\theta_i^*)\rangle\right|^2$$

where β is a real-valued coefficient (must be larger than mass gap).

1) Perform VQE and obtain optimal parameters and an approximate ground state $|\psi(\theta_0^*)\rangle$
2) For E_1 define $H_1 = H + \beta\,|\psi(\theta_0^*)\rangle\langle\psi(\theta_0^*)|$
3) Perform the VQE with the Hamiltonian H_1 to find an approximation of the first excited state $|\psi(\theta_1^*)\rangle$.

Ansatz and Penalty Term

- ## Method

Instead of constraining reachable states to the physical ones in the ansatz, we define a **penalty term** in *H* that suppresses unphysical contributions on the final states

$$\Delta H_{\text{suppr.}} = \lambda \Big[\sum_{p \in \text{gauge}} \Pi_p^{(u)} + \Pi_{\text{ferm.}}^{(Q_{\text{tot}} \neq 0)} \Big]$$

Assess how much the optimal state reached is *unphysical* by computing the expectation value

$$u(\theta_k^*) \equiv \langle \psi(\theta_k^*) | \Pi_{\text{unph.}} | \psi(\theta_k^*) \rangle$$

of the projector into $\mathcal{H}_{unph.}$,e.g.

Fermions: $|0011\rangle_{ph.}, |0101\rangle_{ph.}, |0110\rangle_{ph.}, |1010\rangle_{ph.}, |1100\rangle_{ph.}, |1001\rangle_{ph.},$

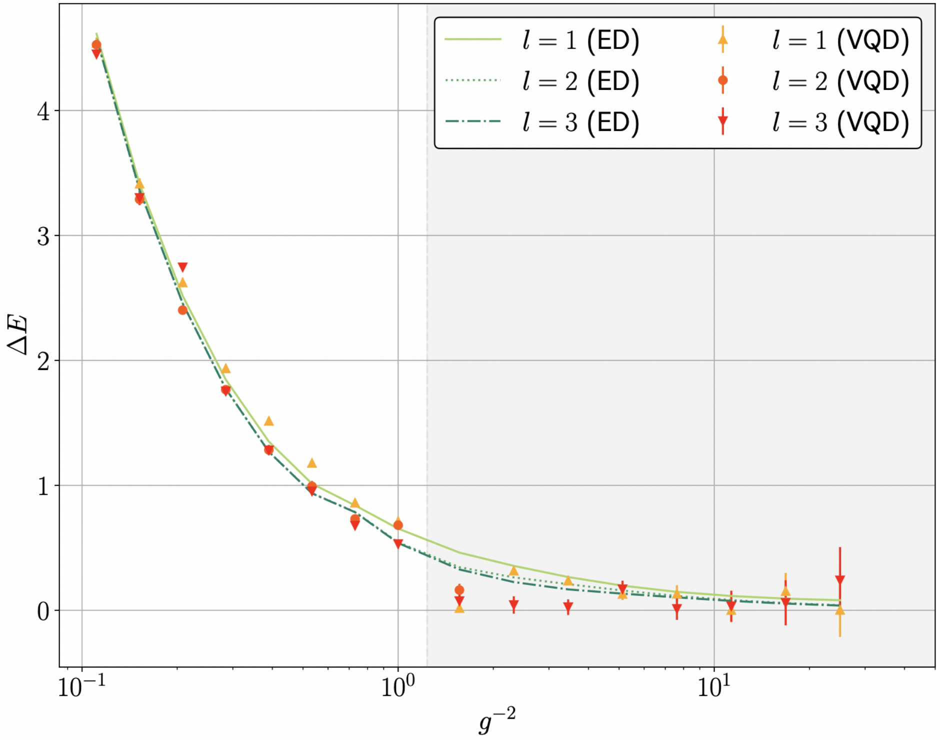
Gauge fields: $|00\rangle_{ph.}, |01\rangle_{ph.}, |11\rangle_{ph.}, |10\rangle_{unph.}$

Results for fermionic system

- Energy gap

- Comparison between VQD and exact diagonalization results for range $0.2 < g < 3$

- With the penalty term method we obtained reliable values for energy gap for MC match



Matching proposal

- Energy gap

Measure energy gap with QC and MC

Compare the values of the coupling at which we obtain the same gap.

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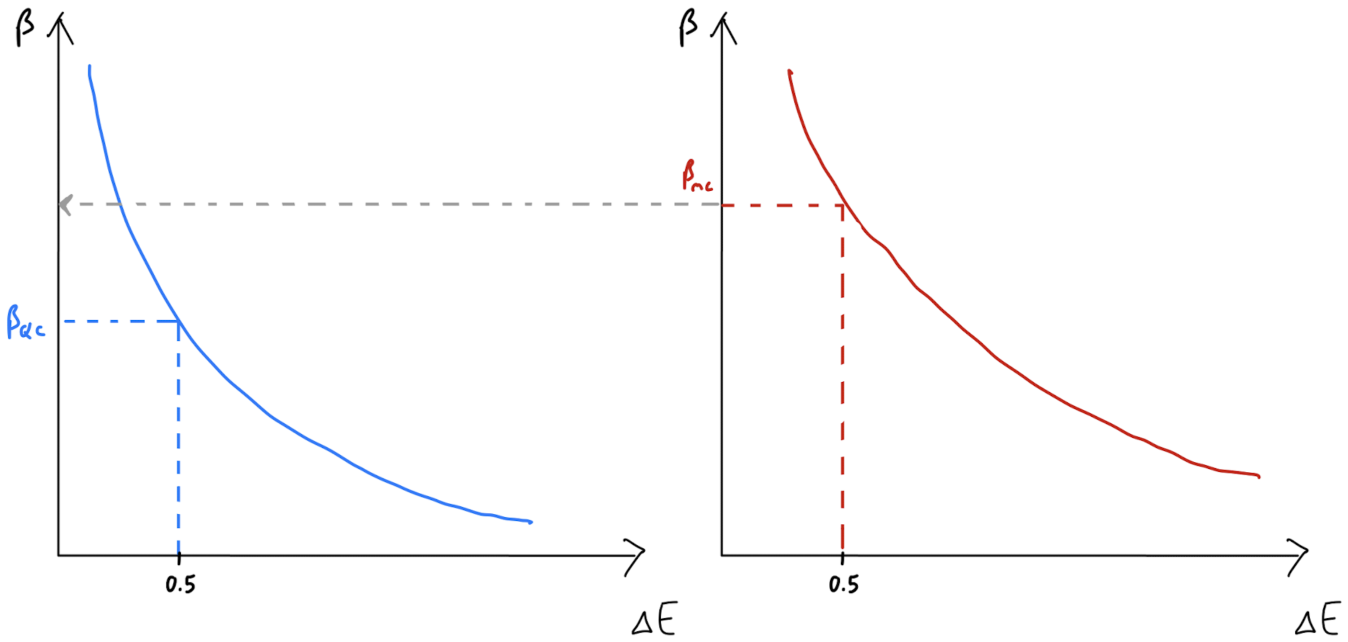
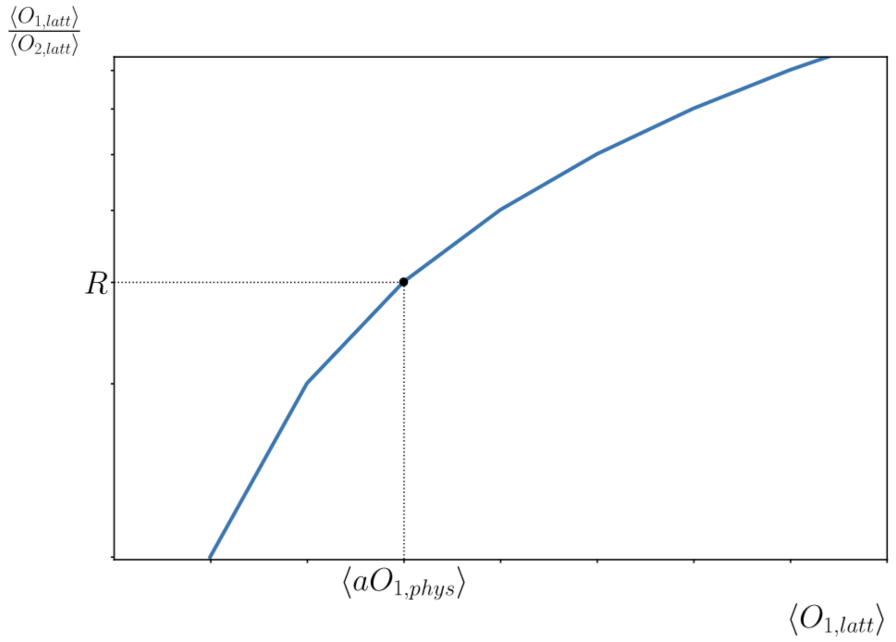
Find relation between couplings.



Scale setting

- Extract ratio $R = \langle O_1 \rangle \, / \, \langle O_2 \rangle$ from experiments (e.g. $O_1 = m_\pi$ and $O_2 = m_p$)
- Tune the parameters of the theory such that at a certain value of $\langle O_{1,\mathrm{latt}} \rangle$, *R* is reproduced.
- At this value of $\langle O_{1,\mathrm{latt}} \rangle$ the lattice spacing can be determined by the relation $aO_{1,\mathrm{phys}} = O_{1,\mathrm{latt}}$.



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Boosted coupling

The calculation of $\Lambda_{\overline{MS}}$ proceeds in four steps:

1) Compute the average plaquette, obtain $g_{\text{boosted}} \equiv g_{\Box}$
2) Use relation between coupling in continuum and on the lattice

$$g^2_{\overline{MS}}(\mu) = g^2_{\Box}(a) + \left(\tilde{t}_2^{\Box} - \frac{b_1}{b_0}\tilde{t}_1^{\Box}\right) g^6_{\Box}(a) + O(g^8)$$

to calculate $g_{\overline{MS}}$ at the scale μ. Putting this value into the solution of renormalization group equation,

$$\mu\frac{\partial g_{\overline{MS}}}{\partial \mu} = \beta(g_{\overline{MS}}(\mu))$$

gives us $\mu/\Lambda_{\overline{MS}}$.

3) Use the conversion factor $a\mu = \exp\left(\frac{\tilde{t}_1^{\Box}}{2b_0}\right)$ to set the scale and turn this into a value for $a\Lambda_{\overline{MS}}$.

4) To find the lattice spacing and convert the results to a physical scale, use e.g. the force parameter r_0 .

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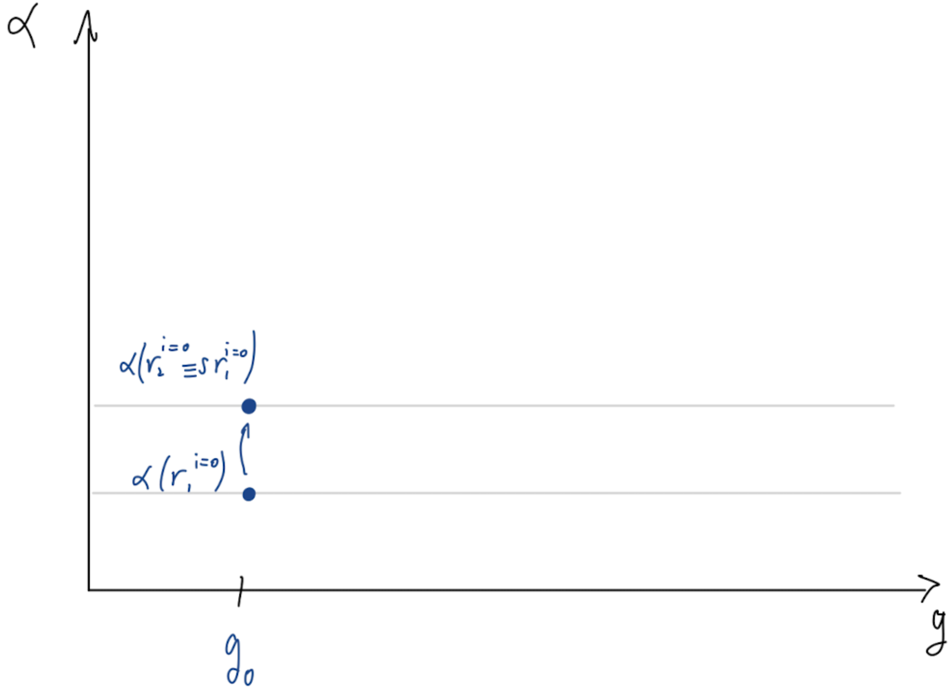
Step-scaling: Coulomb potential $V(r) = \alpha(r)/r$

- *i=0:* compute $\alpha_{ren}(r_1^{i=0}, g_0)$ and $\alpha_{ren}(r_2^{i=0}, g_0)$, at a fixed value of the bare coupling and at **two scales** r_1, r_2, related by a scale factor *s*: $r_2^{i=0} = s r_1^{i=0}$, e.g. *s=2.*



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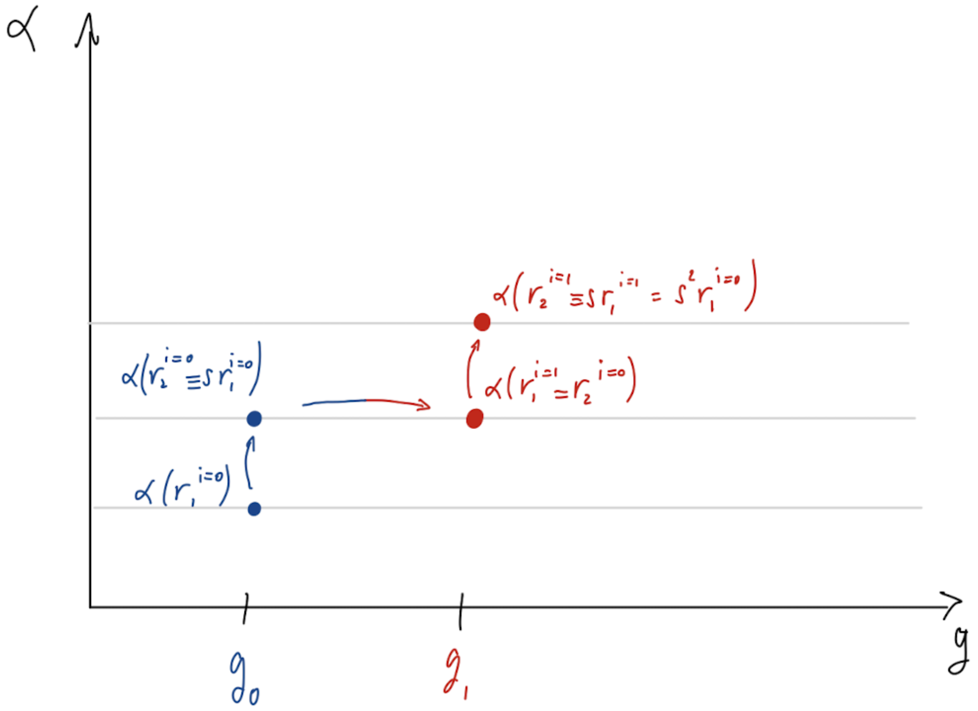
- *i=1:* g^2 tuned $\longrightarrow$ $\alpha_{ren}(r_1^{i=1}, g) = \alpha_{ren}(r_2^{i=0}, g_0)$ with $g^2 \equiv g_1^2$ the renormalized couplings agree, so scales match and apply: $r_2^{i=1} = s r_1^{i=1} = s^2 r_1^{i=0}$.



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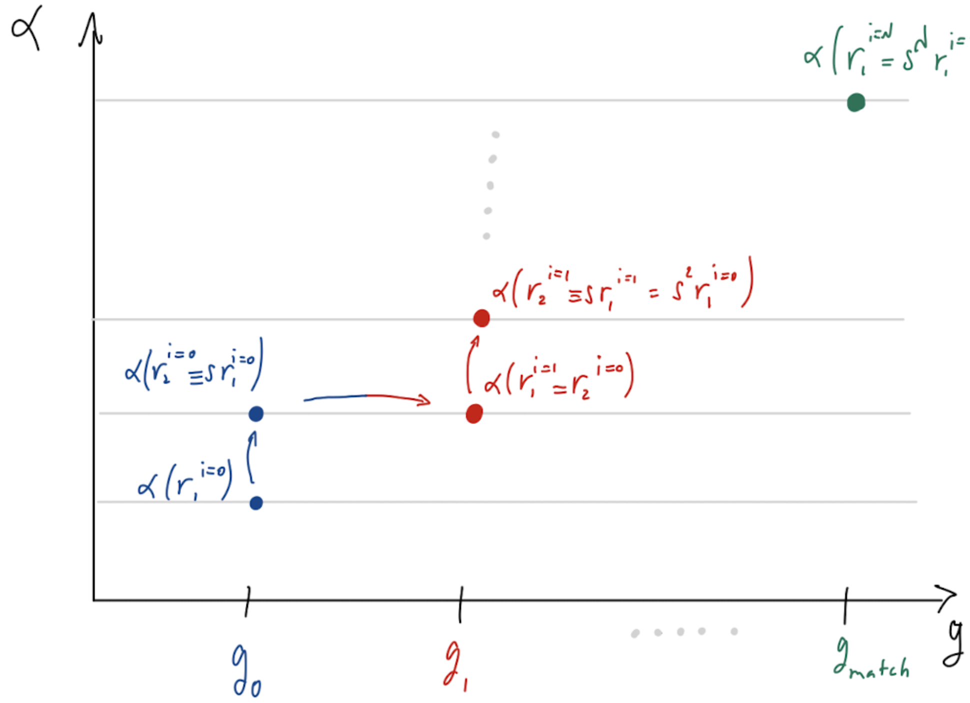
- i=*N:* obtain the scale dependence of the coupling where the scale changes by the factor *s* in each step arriving at $\alpha_{ren}(s^N r_1^{i=0}, g_{\text{match}})$ with g_{match} for MC matching.



Step-scaling: Coulomb potential $V(r) = \alpha(r)/r$

- From MC we have $a \longrightarrow$ scale converted to physical units: $r_{\rm phys} = a s^N r_1^{i=0}$ given thus the **renormalized coupling** $\alpha_{ren}(r_{\rm phys}, g_{\rm match})$.
- Invert sequence by changing the scale by *s*:

$$r_{\rm phys}^{i=N} \to r_{\rm phys}^{i=N-1} = r_{\rm phys}^{i=N}/s$$
$$\to r_{\rm phys}^{i=N-2} = r_{\rm phys}^{i=N-1}/s, \; ..., \to r_{\rm phys}^{i=0}$$

- Obtain renormalized coupling in physical scale, contact with **perturbation theory**: Λ parameter.

Summary

- Discuss the discretization of (2+1)-dimensional QED and comment on the two possible bases (electric and magnetic) via exact diagonalization.
- The resource efficient encoding can eventually be used to bring (2+1)-dimensional QED on a quantum computer.
- Demonstrate that suppression terms can be used to avoid unphysical states.
- Describe matching proposals: energy gap and *step-scaling* approach with static potential.
- Describe strategy to determine scale dependence of the running coupling using perturbation theory

Future perspectives

- Automatization of Hamiltonian definition
- Study the **static force** for the OBC system (*step-scaling* approach).
- Accurate results for **energy gap** in intermediate range of the coupling can make contact to **MC** simulations.
- Accurate results for **plaquette operator** in broad range of coupling can assess the renormalized coupling.
- Setup is a basis for extensions: adding topological terms, chemical potential or real time simulations.

Thank you.

*Phys. Rev. D 106, 114511

Check our paper for more info on this work:

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Sommer parameter

- Static force

From the static potential we can find static force and the relation

$$r^2 \frac{\partial V(r)}{r} = c$$

Choose *c* such that one can agree with experimental results of static potential

$$c^{QCD} = 1.65 \Longrightarrow r_0$$

we find the Sommer parameter with a phenomenological value $r_0^{QCD} = 0.5$ fm.

Electric/magnetic basis: comparison with ED

- Weak coupling: **convergence** in *l* at fixed *L* is generally faster in the **magnetic basis**.
- Strong coupling: **electric basis** performs better, due to the relative dominance of the E/M terms in H.

Matching with MCMC results can be done for the couplings of *O(1)* or larger

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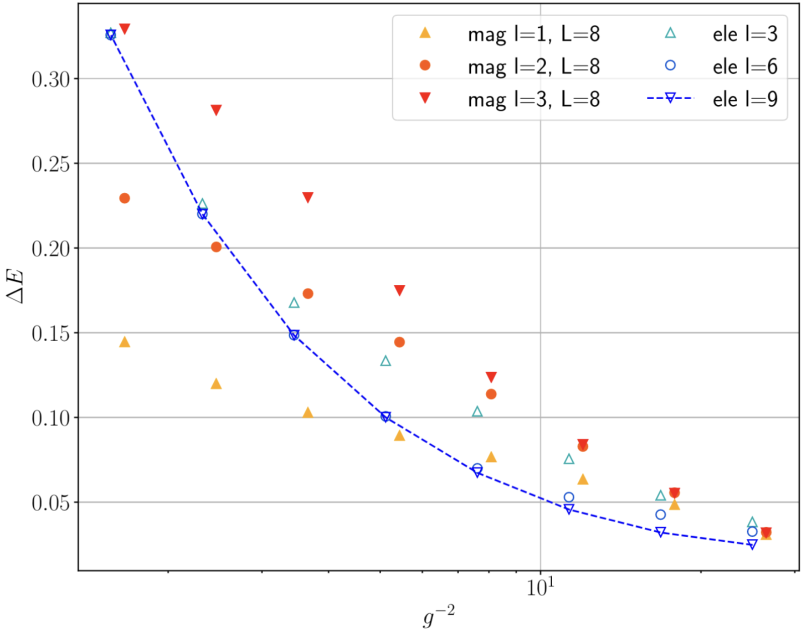
use electric basis for the QC analysis



Encoding on a quantum circuit

- Gauge fields

One-hot Encoding[1]

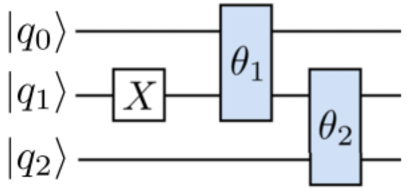
Maps the gauge physical states onto (*2l+1)* qubits

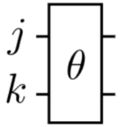
$$|-l+j\rangle_{\text{ph.}} \mapsto |\overbrace{0\ldots0}^{j}\,1\,\overbrace{0\ldots0}^{2l-j}\rangle$$

Example *l=1:*

$$|-1\rangle_{\text{ph.}} \mapsto \ |100\rangle\,,\ |0\rangle_{\text{ph.}} \mapsto \ |010\rangle\,,\ |1\rangle_{\text{ph.}} \mapsto \ |001\rangle$$

Quantum Circuit:





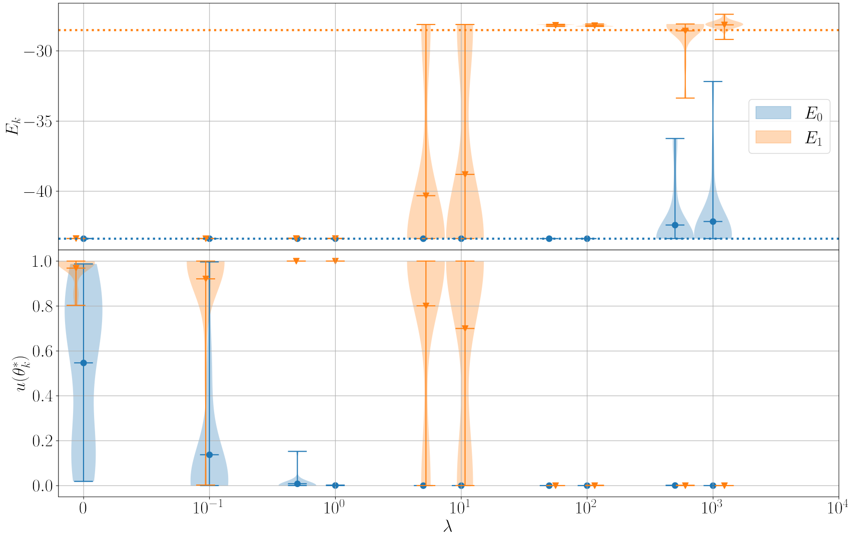
$$\equiv i\text{SWAP}_{j,k}(\theta) \equiv \exp(-i\frac{\theta}{2}[\hat{\sigma}_j^+\hat{\sigma}_k^- + \hat{\sigma}_j^-\hat{\sigma}_k^+])$$

NOT resource efficient: needs $(2l+1)N$ qubits for *N* gauge variables

[1]D. Paulson, L. Dellantonio, J. F. Haase, A. Celi, A. Kan,A. Jena, C. Kokail, R. van Bijnen, K. Jansen, P. Zoller,and C. A. Muschik, PRX Quantum, vol. 2,2021

Pure gauge test

- 200 iterations, 20 runs



As λ increases the % of unphysical states decreases, until we can reach an accurate solution

- 800 iterations, 20 runs