Improved Fermion Hamiltonians for Quantum Simulation

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Outline

- Background
- Symanzik improvement for classical actions
  - ASQTAD, HISQ, Clover etc.
- Symanzik improvement for quantum Hamiltonians
  - Pure Gauge Theory
  - Inclusion of Matter (ASQTAD and HISQ)
- Toy Example Schwinger Model
- Outlook

Why do we need improved Hamiltonians?

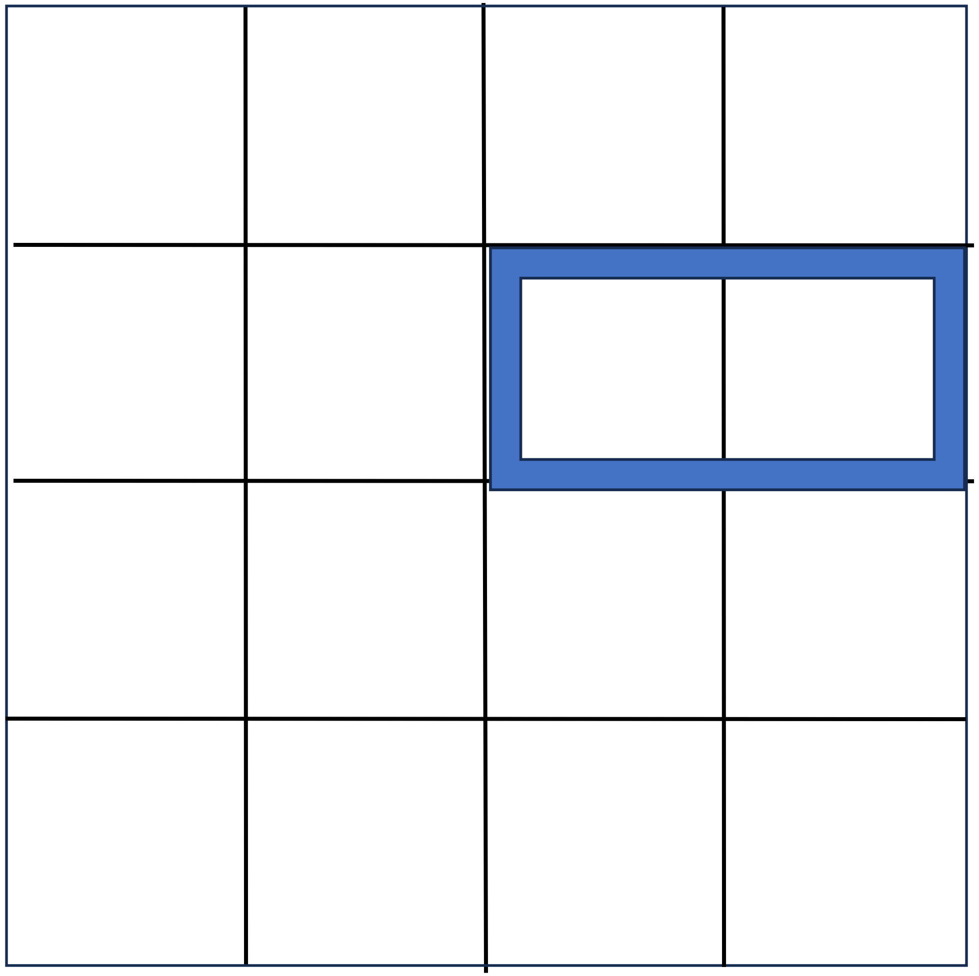
- Lattice actions and Hamiltonians have lattice spacing errors e.g $O(a^2)$
- Improved actions enabled cheaper determination of Hadronic spectra and other static quantities[1,2]
- Development of improved Hamiltonians should reduce qubit costs

[1] Follana et al. Phys.Rev.D75:054502,2007

[2] B. Sheikholeslami and R. Wohlert Nucl. Phys. B 259 (1985) 572.

Symanzik improvement: add terms to action to cancel lattice errors

- Pure Gauge Theories: add rectangular plaquettes
- Fermions:
  - add Naik Term (staggered),
  - Clover Term (wilson),
  - Four Fermion Contact Terms



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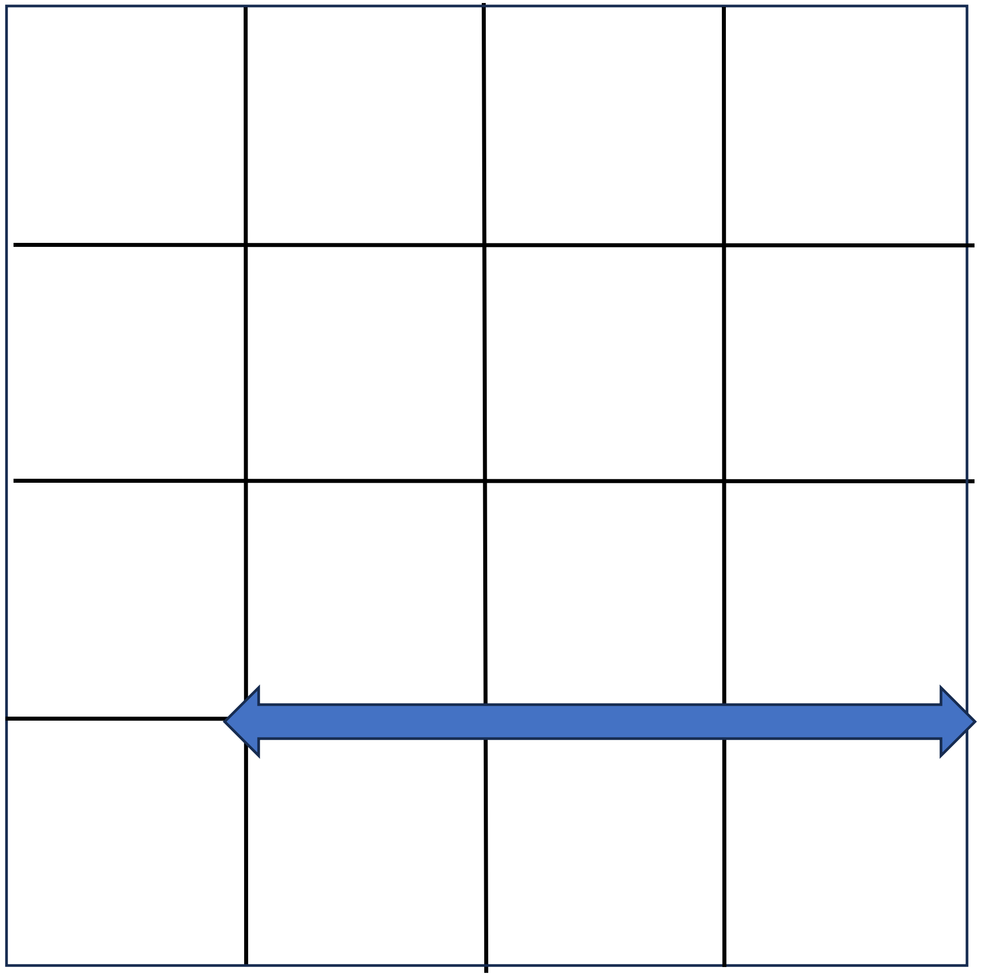

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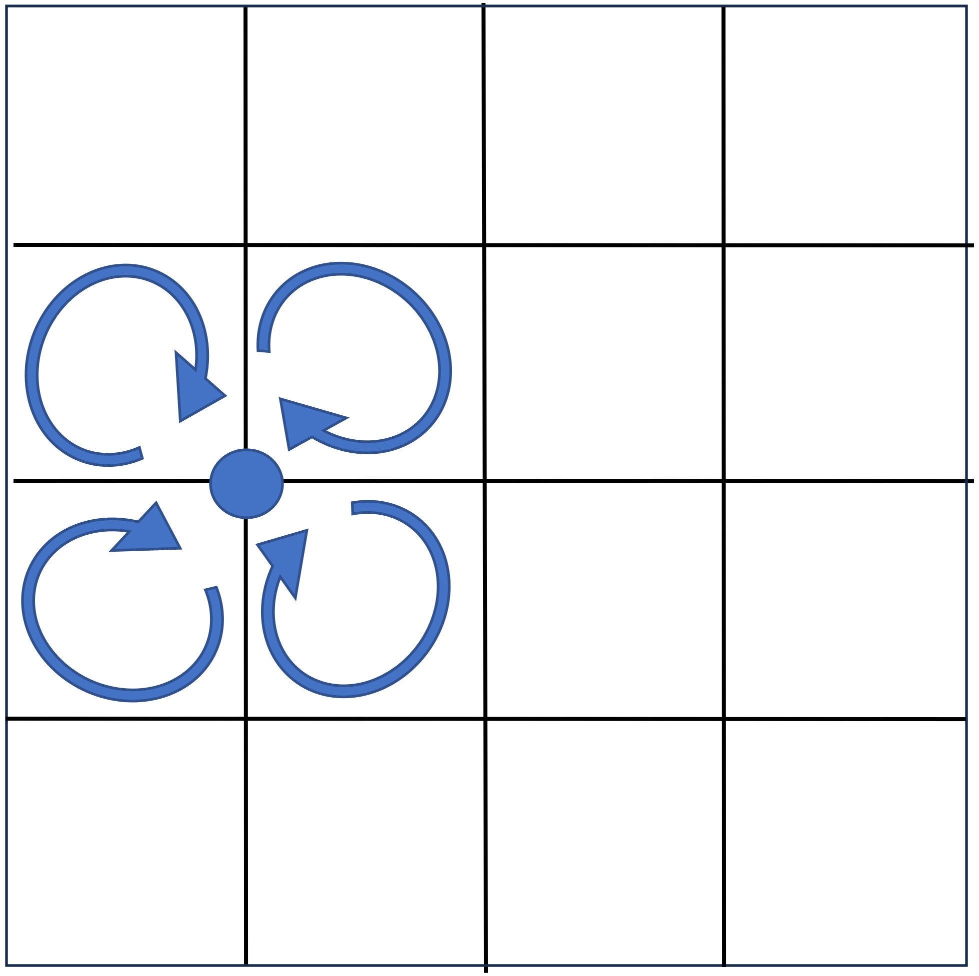

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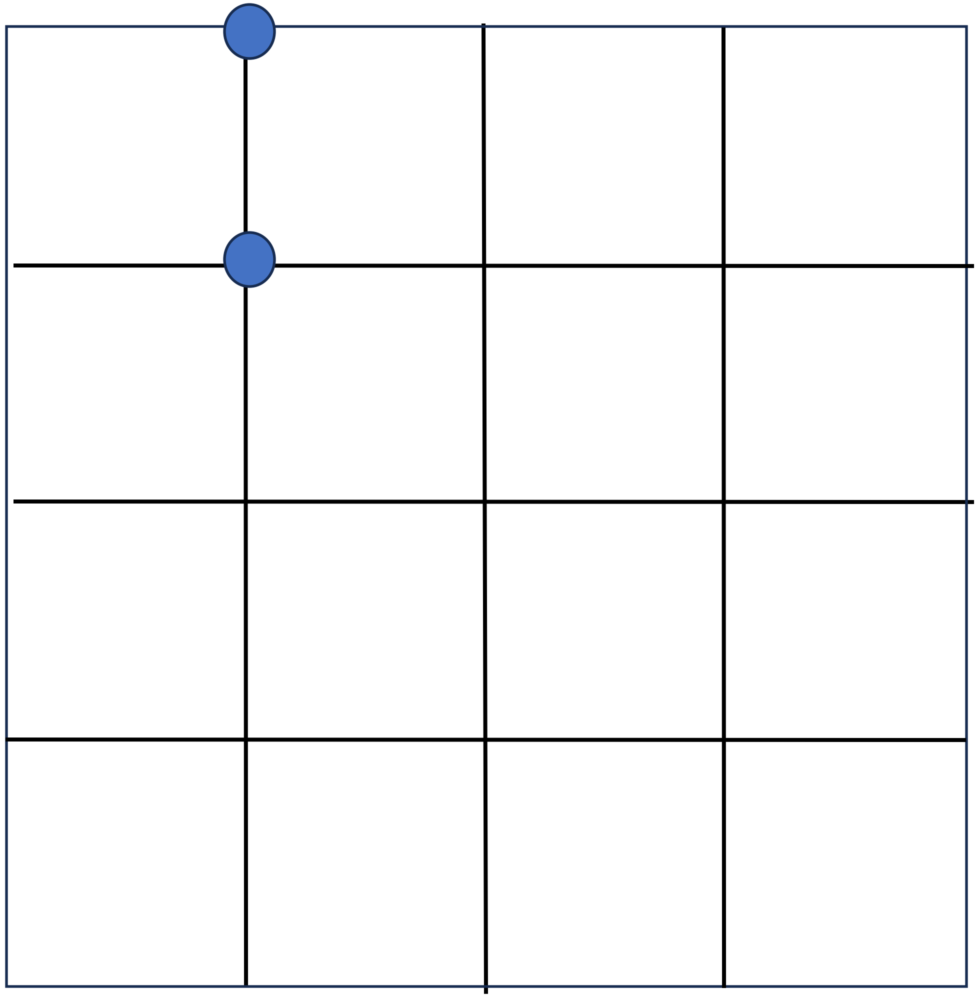

Hamiltonian improvement follows similarly

- Time continuum from euclidean action[1,2]
- Introduce terms which cancel $O(a^2)$ errors[1,2]
- Pure Gauge Theory:
    - Rectangular Plaquettes
    - Extended Electric Field $Tr(E_x U_x E_{x+m} U_x^{+})$
- Fermionic Theories:
    - Depends on choice of fermions

[1] X.-Q. Luo et al PRD59 (1999) 034503,
[2] J. Carlsson and McKellar PRD 64 (2001) 094503

[3] Carena et al. PRL 129.051601
[4] Ciavarella arxiv:2307.05593

ASQTAD Hamiltonian

Two sources of $O(a^2)$ error

Partial derivative -> Lattice Derivative

Taste Splitting

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"Naik" Term: $\Delta \; -> \Delta - \frac{1}{6}\Delta^3$

$\psi^+ U \; U U \psi$

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Additional Terms or Smearing

Four Quark Operator Complicated New Primitive Trotter terms. Or Smearing

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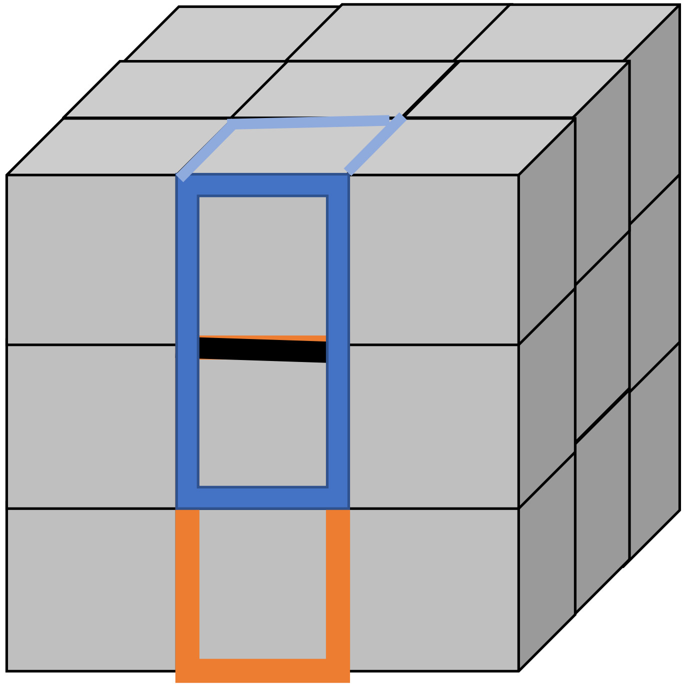
ASQTAD Operator Smears Links

$$\mathcal{F}_\mu^{\mathrm{ASQTAD}}[U] = \left(\prod_{\rho\neq\mu} (1 + \frac{a^2\delta_\rho^{(2)}}{4})|_{\mathrm{symm.}} \right) - \sum_{\rho\neq\mu} \frac{a^2(\delta_\rho)^2}{4}$$

- Average over the links and project back onto the group space
- Smearing is done only to the nearest neighbor operator



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  - This is solved in Gustafson arXiv:2211.05607
- How do we tackle "smearing" the electric fields?
  - Just use these terms as additions to Hamiltonian

The ASQTAD Hamiltonian

$$\mathcal{F}_j^{\text{ASQTAD}}[U] = \left(\prod_{k\neq j}(1+\frac{a^2\delta_k^{(2)}}{4})|_{\text{symm.}}\right) - \sum_{k\neq j}\frac{a^2(\delta_k)^2}{4}$$

$$\hat{H}^{\text{ASQTAD}} = -\frac{1}{2a}\sum_{\vec{n},\hat{j}}\left(\eta_j(\vec{n})\psi_{\vec{n}}^\dagger\left(\left(\mathcal{F}_{\hat{j}}^{\text{ASQTAD}}[U_{\vec{n},\hat{j}}]\psi_{\vec{n}+\hat{j}}\right) - \frac{1}{48}\left[\left(\prod_{x=0}^{2}U_{\vec{n}+x\hat{j}}\right)\psi_{\vec{n}+3\hat{j}} - 3U_{\vec{n}}\psi_{\vec{n}+\hat{j}} - \left(\prod_{x=1}^{3}U_{\vec{n}-x\hat{j}}\right)\psi_{\vec{n}-3\hat{j}} + 3U_{\vec{n}-\hat{j}}^\dagger\psi_{\vec{n}-\hat{j}}\right]\right) + h.c.\right)$$

$$+\frac{1}{2a}\sum_{\vec{n},\hat{j}}\left(\eta_j(\vec{n})\psi_{\vec{n}}^\dagger\left(\sum_{b=1}^{2}(c_{1,b}E_{\vec{n},\hat{j}}^{2b}U_{\vec{n},\hat{j}}\psi_{\vec{n}+\hat{j}}) + c_2E_{\vec{n},\hat{j}}^2\sum_{\hat{k}\neq\hat{j}}S_{\vec{n},(\hat{j},\hat{k})}^{(3)}\psi_{\vec{n}+\hat{j}} + c_3\sum_{\hat{k}\neq\hat{i}\neq\hat{j}}S_{\vec{n},(\hat{j},\hat{k},\hat{i})}^{(5)}\psi_{\vec{n}+\hat{j}} + h.c.\right)\right) + \sum_{\vec{n}}\rho(\vec{n})\psi_{\vec{n}}^\dagger\psi_{\vec{n}} + \hat{H}_{\text{gauge improved}}$$

- To form the HISQ Hamiltonian
    - ASQTAD Smear the links that appear in the Naik Term
    - ASQTAD Smear again the links that appear in the Kogut Susskind Term

Gate Costs for Trotterization

Gate	Naive Kogut Susskind	$O(a^2)$ gauge	ASQTAD NR	Asqtad RE	HISQ
$\mathfrak{U}_{G.M.}$	1	0	$14(d-1)-11$	2	2
$\mathfrak{U}_{-1}$	$3(d-1)$	$2+8(d-1)$	$52(d-1)-48$	$52(d-1)-48$	$104(d-1)-96$
$\mathfrak{U}_{\times}$	$6(d-1)$	$4+20(d-1)$	$132d-256$	$132d-256$	$264d-512$
$\mathfrak{U}_{\text{phase}}$	1	1	0	0	0
$\mathfrak{U}_{Tr}$	$\frac{d-1}{2}$	$d-1$	0	0	0
$\mathfrak{U}_{F}$	2	2	0	0	0
$\mathfrak{U}_{U}$	0	0	0	2	4

Toy Example: Schwinger Model

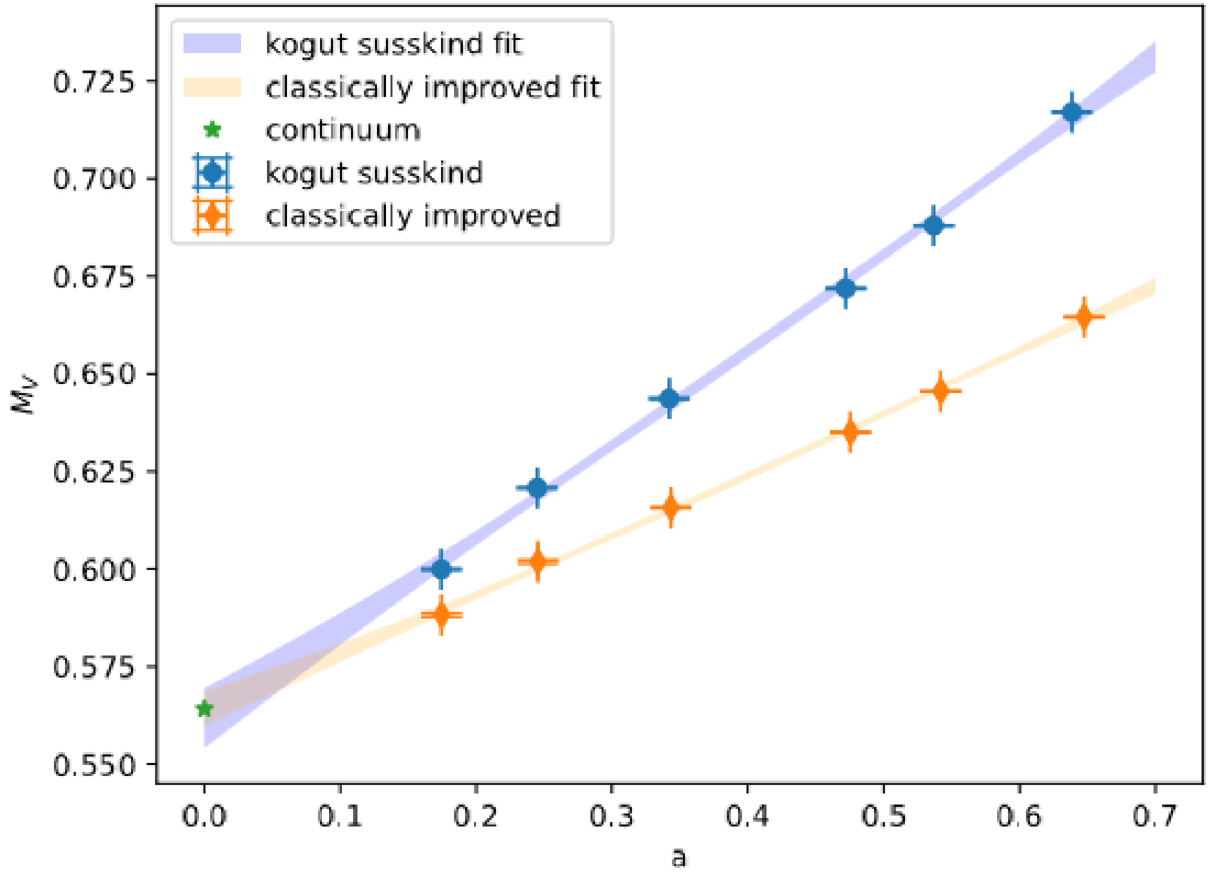
$$\hat{H}_{K.S.} = \frac{1}{2}\sum_n (\psi_n^\dagger U_n \psi_{n+1} + h.c.) + m\sum_n (-1)^n \psi_n^\dagger \psi_n + \frac{g^2}{2}\sum_n E_n^2$$

All c's have been set to 0

$$\hat{H} = \sum_n (\frac{9}{16}\hat{\psi}_n^\dagger U_n \hat{\psi}_{n+1} - \frac{1}{48}\hat{\psi}_n^\dagger U_n U_{n+1} U_{n+2}\hat{\psi}_{n+3} + h.c.) + m\sum_n \hat{\psi}_n^\dagger \hat{\psi}_n + g^2 \sum_n (\frac{5}{6}\hat{E}_n^2 + \frac{1}{6}\hat{E}_n \hat{E}_{n+1})$$

Continuum Limit Comparison for Vector Mass: m=0

- Same Continuum Limit!
- Some lattice errors removed
- One loop errors are likely still present



Outlook

- Developed an ASQTAD and HISQ like Fermion Hamiltonian
- Shown that inclusion of some of the terms reduce lattice errors
- Investigate effects with non-zero mass
- Consider using classical coupled cluster theory to study problems for U(1) and SU(2) in 2+1d
- Examine efficient methods to determine coefficients to remove one loop errors

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