Variational Monte Carlo Algorithm for Hamiltonian Lattice QED in $2+1D$ Coupled to Wilson Fermions

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Introduction

This poster presents an application of the sign-problem-free, Hamiltonian-based variational Monte Carlo algorithm to search for the ground state of compact lattice QED in $2+1D$ with Wilson fermion discretization. We aim to tackle the sign-problem-afflicted regime of non-zero isospin chemical potential for two fermion flavors and develop a scalable algorithm to prepare the ground state of the system.

Simulation Basis

Define a basis state $|A_{x,\mu}\rangle$ on the link at site x in μ direction:

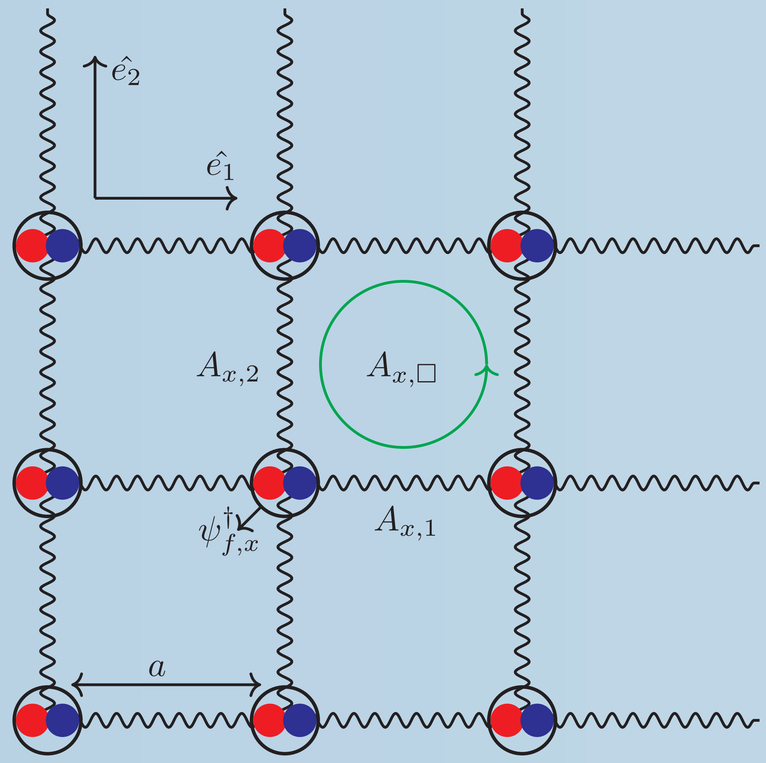
$$\hat{A}_{x,\mu}\,|A_{x,\mu}\rangle = A_{x,\mu}\,|A_{x,\mu}\rangle\,,\ \forall x,\mu$$

Compact QED : $aA_{x,\mu} \in [-\pi,\pi)$

Plaquette angle: $A_{x,\Box} = A_{x,1} + A_{x+\hat{e}_1,2} - A_{x+\hat{e}_2,1} - A_{x,2}$

Electric fields : $E_{x,\mu} \equiv \dfrac{-i}{a}\partial_{A_{x,\mu}}$

Gauge fields : $U_{x,\mu} \equiv \exp(iaA_{x,\mu})$



Lattice Hamiltonian

$$H = \underbrace{\frac{g^2}{2}\sum_{x,\mu}\hat{E}^2_{x,\mu}}_{H_E} \underbrace{- g_m \sum_x \cos\left(a\hat{A}_{x,\Box}\right)}_{H_B} + \underbrace{a^2\sum_{f,x}\left(m+\frac{2r}{a}\right)\psi^\dagger_{f,x}\gamma_0\psi_{f,x}}_{H_M} + \underbrace{\frac{a}{2}\sum_{f,x,\mu}\left[\psi^\dagger_{f,x}\gamma_0(i\gamma_\mu + r)\hat{U}_{x,\mu}\psi_{f,x+\hat{e}_\mu} + h.c.\right]}_{H_K} + \underbrace{a^2\sum_{x,f}\kappa_f\psi^\dagger_{f,x}\psi_{f,x}}_{H_\kappa}$$

g : electric coupling strength, a : lattice spacing, r : Wilson parameter, γ_μ: gamma matrices,
g_m: magnetic coupling, m: lattice fermion mass, $\psi_{f,x}$: two comp. Dirac spinor, κ_f: flavor chemical potential.

Variational Monte Carlo

1. State

General state $|\Psi(\gamma)\rangle \in \mathcal{H}_G \otimes \mathcal{H}_F$ in the basis:

$$|\Psi(\gamma)\rangle = \int DA\ \underbrace{|\Psi_F(A,\gamma_F)\rangle}_{\text{fermionic state}}\ \underbrace{\Psi_G(A,\gamma_G)\,|A\rangle}_{\text{gauge part}}$$

γ_G, γ_F: variational parameters.

Wavefunction for gauge fields

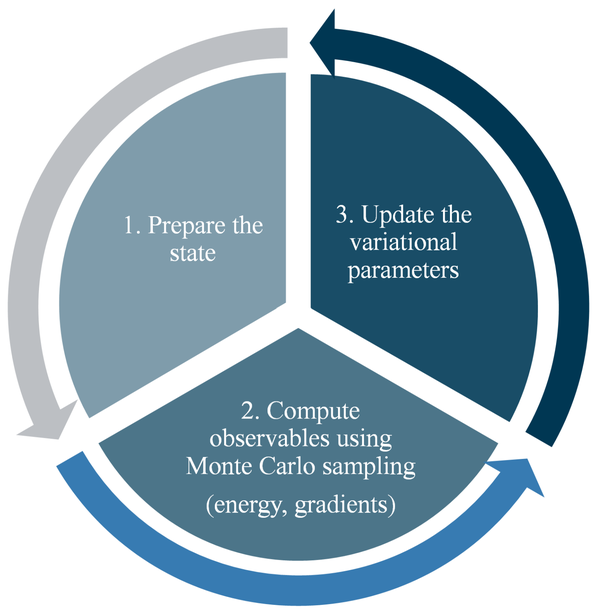
$$\Psi_G(A) = \exp\left\{-\tfrac{1}{2}\vec{P}(A).\gamma_1.\vec{P}(A) - \vec{\gamma}_2.\vec{P}(A)\right\}$$

$\vec{P}(A)$: Vector of compact gauge invariant variables constructed with plaquette and global loop angles.

Fermionic state

$$|\Psi_F(A,\gamma_F)\rangle = \underbrace{\exp\left(\frac{i}{4}\vec{\psi}^\dagger.K(A,\gamma_F).\vec{\psi}\right)}_{\text{Gaussian unitary}}|\Psi_0\rangle$$

- $|\Psi_0\rangle$: Initial fermionic reference state.
- $\vec{\psi}^\dagger K\vec{\psi} \equiv \sum_{xy}(\gamma_F)_{xy}\psi^\dagger_x\psi_y U_{y\to x} + h.c.$



2. Observables

$$\langle O\rangle = \int DA\ p(A)\ O_{loc}(A)$$

- Local observable:

$$O_{loc}(A) = \frac{\langle\Psi_F(A)|\hat{O}\Psi_G(A)|\Psi_F(A)\rangle}{\Psi_G(A)}$$

- Sampling distribution for Monte Carlo

$$p(A) = \frac{|\Psi_G(A)|^2}{\int DA\,|\Psi_G(A)|^2}$$

- Estimated expectation value

$$\langle O\rangle \approx \frac{1}{N_s}\sum_{s=1}^{N_s} O_{loc}(A)$$

3. Optimiztion

Gradients w.r.t. the parameters, γ_i:

$$(\nabla E)_i = \frac{\partial\langle H\rangle}{\partial\gamma_i} = \int DA\ p(A)G_{i,loc}(A)$$

$$G_{i,loc}(A) = \partial_{\gamma_i}H_{loc}(A) + (H_{loc}(A) - \langle H\rangle)\partial_{\gamma_i}\log|\Psi_G(A)|^2$$

Gradient descent

$$\gamma_i' = \gamma_i - \frac{\Delta\tau}{2}(\nabla E)_i$$

Imaginary time evolution

Compute the metric: $S_{ij} = \langle\partial\gamma_i\Psi|\partial\gamma_j\Psi\rangle$

$$\gamma_i' = \gamma_i - \frac{\Delta\tau}{2}\sum_j[\mathrm{Re}(S)^{-1}]_{ij}(\nabla E)_j$$

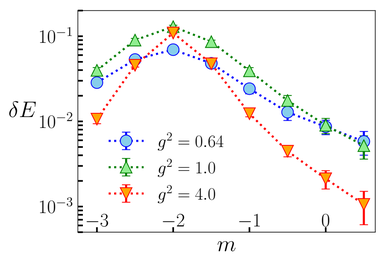
$\Delta\tau$: imaginary time step

Benchmark: Relative Energies

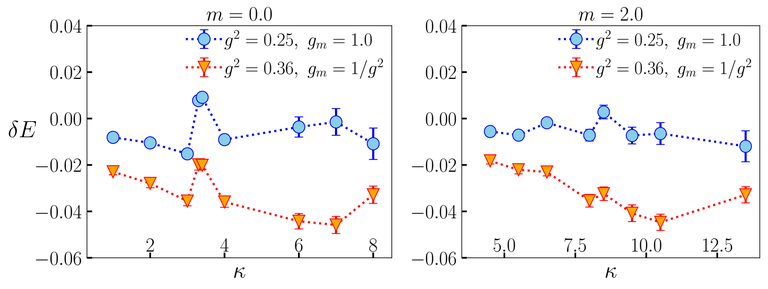
Relative ground-state energy difference, δE, as compared to exact diagonalization (ED) on a 2×2 lattice at different coupling strengths.

$$\delta E = \frac{\langle H\rangle - E_{ED}}{|E_{ED}|}$$

$N_f = 1$

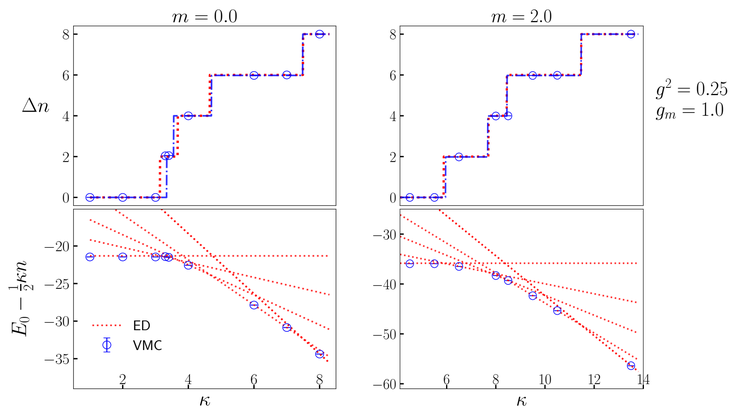


$N_f = 2$



Benchmark: Phase Transitions

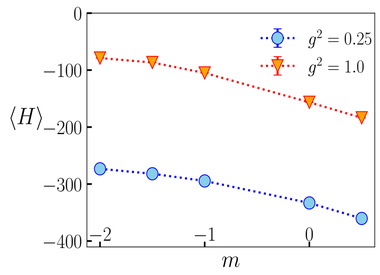
- $H = H_0 + H_\kappa = H_0 - \dfrac{\kappa}{2}\Delta n + \dfrac{\kappa}{2}n.$
- $n_f := \sum_x \psi^\dagger_{f,x}\psi_{f,x},\ \ n := n_1 + n_2,\ \ \text{and}\ \Delta n := n_2 - n_1.$
- Action-based MCMC methods suffer from the sign problem when $\kappa_1 + \kappa_2 \neq 0$, so we set $\kappa_1 = \kappa$ and $\kappa_2 = 0$.
- As $[H, \Delta n] = 0$, ground state lies in one of the Δn sectors.



Results

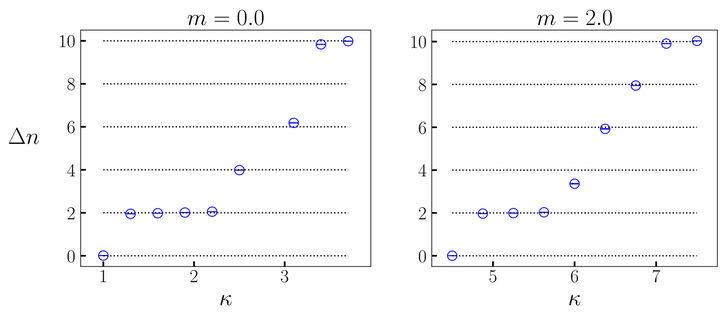
$N_f = 1$

Energy expectation value after optimization as a function of mass for a single fermion flavor on an 8×8 lattice with $a = 1.0$ and $r = 1.0$.



$N_f = 2$

Flavor imbalance, $\langle\Delta n\rangle$, in the optimized state as a function of κ on a 4×4 lattice with $g^2 = 0.25, g_m = 1$.



Summary and Conclusions

- Successfully implemented a scalable, sign-problem-free variational Monte Carlo framework to determine the ground state.
- The complexity to compute $H_{loc}(A)$ and the gradients per gauge field configuration is $\mathcal{O}(N_f^4 N^4)$ for N lattice sites.
- For $N_f = 1$, the variational energies from VMC show good convergence to exact diagonalization for large fermion mass.
- The variational energies start to deviate when the coefficient of the on-site term, H_M, namely, $m + 2r/a \to 0$.
- For $N_f = 2$, the algorithm has no sign problem for non-zero $(\kappa_1 + \kappa_2 \neq 0)$ isospin chemical potential.
- Ground-state particle imbalances and the critical points in the $\Delta n - \kappa$ plots agree with ED benchmarks on the 2×2 lattice.

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