

## Ground state search of interacting boson–fermion systems using variational Monte Carlo

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We study lattice QED in  $2 + 1$  dimensions coupled to Wilson fermions in the Hamiltonian formulation and develop a sign-problem-free variational Monte Carlo algorithm. Using a continuous basis to describe the gauge degrees of freedom and fermionic Gaussian states for the matter fields, we construct a variational ansatz for the ground state. The parameters of the ansatz are optimized using gradient descent and/or imaginary time evolution based on the time-dependent variational principle. For a lattice with  $N$  matter sites, the computational complexity for sampling a gauge configuration is  $O(N^2 \log N)$ , and the complexity for computing the energy per gauge configuration is  $O(N^4)$ . Comparing our method to results from exact diagonalization on small lattices, we demonstrate good agreement. In addition, we present preliminary results for the ground state for two fermion flavors,  $N_f = 2$ , in the presence of a non-zero chemical potential, a regime in which the conventional action-based Monte Carlo methods suffer from the sign problem.

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## 1. Introduction

Monte Carlo methods have been extremely successful for studying lattice field theories, in particular, for exploring phase diagrams, mass spectra, and many other (static) properties. However, the conventional action-based Markov chain Monte Carlo (MCMC) approach suffers from several limitations, the most notable one being the sign problem [1, 2]. It appears when the Euclidean action describing a theory becomes complex, for instance, for QCD at nonzero baryon chemical potential or in the presence of a topological term. For the same reason, real-time dynamics are not directly accessible with Monte Carlo methods, as the formulation in Minkowski spacetime leads to a complex action. Hence, these regimes, which are of great physical interest, remain largely inaccessible numerically. Additionally, conventional MCMC methods can suffer from critical slowing down [3] and topological freezing [4].

Hamiltonian-based methods for simulating quantum mechanical systems provide a promising alternative for overcoming the limitations of classical MCMC simulations. In recent years, tremendous progress has been made in applying quantum computing [5], tensor network methods [6], and quantum Monte Carlo [7] to lattice field theories. While most of these efforts have focused on (1+1)-dimensional models, first successful demonstrations have been made for theories in higher spatial dimensions.

In this work, we develop a Hamiltonian-based variational Monte Carlo (VMC) approach for lattice quantum electrodynamics (QED) in  $2 + 1$  dimensions coupled to fermions. Starting from the algorithm for staggered fermions developed in Ref. [8], we extend it to Wilson fermions, which allow the complete removal of fermion doublers in arbitrary spatial dimensions. We demonstrate ground-state preparation for the case of one and two fermion flavors and compare our results against exact diagonalization (ED) on small lattices. In addition, we study the phase structure of the model with two fermion flavors at nonzero isospin chemical potential, a regime in which conventional MCMC techniques generally suffer from the sign problem.

## 2. Lattice model

We consider the compact Hamiltonian formulation of QED in  $2 + 1D$  discretized on a square lattice with periodic boundary conditions. The pure gauge Hamiltonian can be written as [9]

$$H_G = \frac{g^2}{2} \sum_x (E_{x,1}^2 + E_{x,2}^2) + g_{\text{mag}} \sum_x (1 - \cos(aA_{x,\square})) \equiv H_E + H_B \quad (1)$$

where  $g$  is the coupling constant<sup>1</sup>,  $a$  the lattice spacing, and the sum  $\sum_x$  is over all the lattice sites. The gauge potential<sup>2</sup>  $A_{x,\mu}$  and the electric field  $E_{x,\mu}$  reside on the link emanating from site  $x$  in the direction  $\mu$  and satisfy the canonical commutation relation  $[aA_{x,\mu}, E_{y,\nu}] = i\delta_{\mu\nu}\delta_{xy}$ . We denote the lattice curl of the gauge potential at the site  $x$  as  $A_{x,\square} = A_{x,1} + A_{x+e_1,2} - A_{x+e_2,1} - A_{x,2}$ , where  $e_1, e_2$  are the unit vectors in the spatial directions 1, 2, respectively. To perform numerical simulations of the model, we work in the basis of gauge potentials  $\{A_{x,\mu}\}$ . Therefore, the basis

<sup>1</sup>In the standard formulation,  $g_{\text{mag}} = \frac{1}{g^2}$ . Here, however, we treat it as a general parameter.

<sup>2</sup>We work with the gauge potentials  $\{A_{x,\mu}\}$  on the links instead of the gauge fields  $\{U_{x,\mu}\}$ . The gauge field operator at link  $x, \mu$  has the form  $U_{x,\mu} = e^{iaA_{x,\mu}}$ .

states  $|A_{x,\mu}\rangle$  on the link  $x, \mu \forall x, \mu$ , are eigenstates of  $A_{x,\mu}$ . As we consider a  $U(1)$  compact theory, we have  $A_{x,\mu} \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right)$ . In this basis, the electric field operator has the form

$$E_{x,\mu} \equiv \frac{1}{ia} \frac{\partial}{\partial A_{x,\mu}} \equiv \frac{1}{ia} \partial_{A_{x,\mu}}. \quad (2)$$

Coupling the theory to Wilson fermions, the total Hamiltonian,  $H$ , in temporal gauge takes the form  $H = H_G + H_K + H_M$ , where the kinetic Hamiltonian and the mass term read

$$H_K = -\frac{a}{2} \sum_{f,x,\mu} \left[ \psi_{f,x}^\dagger \gamma_0 (i\gamma_\mu + r) e^{iaA_{x,\mu}} \psi_{f,x+e_\mu} + h.c. \right], \quad (3)$$

$$H_M = a^2 \sum_{f,x} \left( m + \frac{2r}{a} \right) \psi_{f,x}^\dagger \gamma_0 \psi_{f,x}. \quad (4)$$

Here,  $r$  is the Wilson parameter,  $\gamma_\mu$  are the  $\gamma$  matrices<sup>3</sup>, and  $\psi_{f,x}$  is two-component Dirac spinor at site  $x$  for flavor  $f$ , whose components satisfy the anti-commutation relations  $\{\psi_{f,x,i}^\dagger, \psi_{f',y,j}\} = \delta_{f,f'} \delta_{xy} \delta_{ij}$ , where  $i, j$  label the Dirac components. The charge at site  $x$  for Wilson fermions is  $q_{f,x} = \sum_i \psi_{f,x,i}^\dagger \psi_{f,x,i} - 1$ . The physical states have to satisfy Gauss' law,  $G_x |\text{physical}\rangle = 0$ , where

$$G_x = \sum_{\mu=1}^2 (E_{x,\mu} - E_{x-e_\mu,\mu}) - q_x. \quad (5)$$

Since we are interested in the regimes afflicted by the sign problem, we focus on two fermion flavors in the presence of isospin chemical potential. The corresponding chemical potential term that has to be added to  $H$  reads

$$H_\mu = a^2 \sum_{f,x} \mu_f \psi_{f,x}^\dagger \psi_{f,x}, \quad (6)$$

where  $\mu_f$  is the chemical potential for flavor  $f$ .

Lattice QED with two flavors of staggered fermions in the presence of the chemical potential has been shown to exhibit a rich phase structure with multiple first-order phase transitions [8, 10–13]. These transitions are characterized by discontinuous changes in the flavor imbalance

$$\Delta n = n_2 - n_1, \quad (7)$$

which serves as an order parameter distinguishing the different phases. Here,  $n_f = \sum_x \psi_{f,x}^\dagger \psi_{f,x}$  denotes the total particle number of flavor  $f$ . Since  $n_f$  is the spatial sum of local number operators with eigenvalue 0 or 1, it has an integer spectrum. Moreover, since  $H$  does not have any flavor mixing interactions,  $n_f$  is a conserved quantity. Thus, the Hilbert space decomposes into superselection sectors labeled by fixed particle numbers, and consequently  $\Delta n$  is also an integer-valued conserved quantity.

As the chemical potentials are varied, the ground state may switch between different  $\Delta n$  sectors. The resulting discontinuous changes in  $\Delta n$  have been observed in  $1 + 1D$  [10–12, 14] and more

<sup>3</sup>We choose  $\gamma_0 = \sigma_z$ ,  $\gamma_1 = i\sigma_y$  and  $\gamma_2 = -i\sigma_x$ , such that  $\{\gamma_\mu, \gamma_\nu\} = 2\eta_{\mu\nu}$ .

recently in  $2 + 1D$  [8, 13], providing clear evidence for first-order transitions between sectors with different values of  $\Delta n$ .

In the action formulation, the severity of the Monte Carlo sign problem depends on the choice of chemical potentials. For two flavors, one can introduce  $\mu_{\pm} = \mu_1 \pm \mu_2$ . Choosing  $\mu_+ = 0$  ensures that the fermion determinant remains real and positive, thus allowing simulations without encountering a sign problem. At the same time, the phase diagram only depends on the chemical potential difference  $\mu_-$  [8, 10]. However, this simplification is specific to the two-flavor case. For more general cases — such as systems with more than two fermion flavors, or in the presence of additional topological terms — the fermion determinant generally becomes complex, making action-based Monte Carlo methods inefficient. In this work, we consider the more general setup with two flavors and nonvanishing  $\mu_+$  and  $\mu_-$ , thereby moving beyond the sign-problem-free regime.

### 3. Variational ansatz for the ground state

The total Hilbert space of the lattice model can be written as a tensor product of gauge Hilbert space with the fermionic one,  $\mathcal{H} = \mathcal{H}_G \otimes \mathcal{H}_F$ . Due to the tensor product structure of  $\mathcal{H}$ , a general state in the basis of  $\{A_{x,\mu}\}$  can be written as

$$|\Psi\rangle = \prod_{x,\mu} \int_0^{\frac{2\pi}{a}} dA_{x,\mu} \Psi_G(\{A_{x,\mu}\}) |\Psi_F(\{A_{x,\mu}\})\rangle |\{A_{x,\mu}\}\rangle \equiv \int DA \Psi_G(A) |\Psi_F(A)\rangle |A\rangle, \quad (8)$$

where we use the shorthand notation  $A \equiv \{A_{x,\mu}\}$  and  $\int DA = \prod_{x,\mu} \int_0^{2\pi/a} dA_{x,\mu}$ .  $\Psi_G(A) = \langle \{A_{x,\mu}\} | \Psi \rangle$  is the pure gauge wave function in the chosen basis, and  $|\Psi_F(A)\rangle$  is a general fermionic state defined for every gauge field configuration. The gauge invariance can be incorporated in  $|\Psi\rangle$  through the choice of the ansatz  $\Psi_G$ , which is constructed as a function of the gauge invariant variables  $A_{x,\square}$  and the global loops<sup>4</sup>, and  $|\Psi_F\rangle$  constructed using gauge invariant terms  $\psi_x^\dagger \psi_y U_{y \rightarrow x}$ .

A good trial wave function for the pure gauge ground state is a periodic Gaussian distribution, as studied in [15–19], which has been shown to exhibit the confinement properties of the compact model. We use the same form of the wave function  $\Psi_G(A)$  as in [8], which is approximated from an infinite sum of Gaussian distributions to a more compact form as<sup>5</sup>

$$\Psi_G(A) = e^{-\frac{1}{2}b(A)^T \alpha b(A) - \beta^T b(A)}, \quad (9)$$

where,  $b(A) = (\cos(aA_{1,\square}), \dots, \cos(aA_{N,\square}), \sin(aA_{1,\square}), \dots, \sin(aA_{N,\square}))$ , and  $\alpha$  ( $\beta$ ) is a matrix (vector) containing the variational parameters. Taking into account translation invariance, the total variational parameters in  $\alpha$  and  $\beta$  scales linearly with the total lattice sites.

Turning to the fermionic state  $|\Psi_F(A)\rangle$ , there are different possible ways to approximate the ansatz for the fermionic state  $|\Psi_F(A)\rangle$ . Here we follow [8], where it is approximated as a fermionic Gaussian state (f.g.s.). This allows us to compute the expectation values of fermionic observables,  $\langle \Psi_F | O | \Psi_F \rangle$ , analytically, since a fermionic Gaussian state is completely characterized

<sup>4</sup>Global loops refer to the sum of the gauge potential along a loop wrapping the periodic lattice.

<sup>5</sup>An infinite sum of Gaussian distributions is required for periodicity of  $A$  and the approximation is done by taking into account the Villain approximation [20].

by its covariance matrix or the two-point fermionic correlations. One can write an f.g.s.  $|\Psi_F(A)\rangle$  as

$$|\Psi_F(A)\rangle = \exp\left(\frac{i}{2} \sum_{x,y} \psi_x^\dagger \psi_y \xi(A)_{xy}\right) |\Psi_0\rangle \equiv U_{GS}(A) |\Psi_0\rangle \quad (10)$$

where  $U_{GS}(A)$  is a parametrized Gaussian unitary transformation acting on a Gaussian reference state  $|\Psi_0\rangle$ . Under such transformations, the covariance matrix,  $\Gamma_0$ , of the reference state,  $|\Psi_0\rangle$ , transforms as  $\Gamma_F(A) = e^{i\xi(A)} \Gamma_0 e^{-i\xi(A)}$ .

The generator  $\xi(A)_{xy}$  is constructed using gauge invariant terms  $\psi_x^\dagger \psi_y U_{y \rightarrow x}$  which are parameterized in a translationally invariant manner as

$$\xi(A)_{xy} = \frac{\eta_{|x-y|}}{\|x-y\|} \sum_{y \rightarrow x} U_{y \rightarrow x}, \quad (11)$$

where the variational parameters  $\eta_{|x-y|}$  depend on the lattice distance  $|x-y| \equiv (|x_1-y_1|, |x_2-y_2|)$  and  $\|x-y\| = |x_1-y_1| + |x_2-y_2|$  is the norm of the distance. The sum  $\sum_{y \rightarrow x}$  is over all paths on the lattice from the site  $y$  to  $x$ . Furthermore, we can apply multiple unitaries to increase the expressivity of the parameterized state.

Our parameterization of the Gaussian unitary is different from that used for staggered fermions in [8]. In that work, the generator  $\xi(A)$  was expressed in the eigenbasis of the hopping Hamiltonian  $H_K$ , exploiting the bipartite sublattice symmetry of staggered fermions. This symmetry ensures that the spectrum of  $H_K$  is symmetric about zero, with eigenvalues paired as  $(-\epsilon_k, +\epsilon_k)$ . Performing a similar analysis for Wilson fermions is not straightforward, since this symmetry is absent in that case. Furthermore, computing the expectation values of the operators involving derivatives, such as  $\partial_{A_{x,\mu}}$ , with respect to the state  $|\Psi_F(A)\rangle$  requires differentiating the eigenvectors of  $H_K$ . This procedure is problematic when  $H_k$  is nearly degenerate, as the derivatives of its eigenvectors are then ill-conditioned.

As a consequence of this parameterization, the computational complexity differs between the two cases. For Wilson fermions, the cost of evaluating the energy scales as  $O(N^4)$  per gauge-field configuration, whereas for staggered fermions it scales as  $O(N^3)$ .

#### 4. Computing expectation values

In order to estimate the expectation value of an operator  $O$ , one writes

$$\langle O \rangle = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\int DA \overline{\Psi_G(A)} \langle \Psi_F(A) | O \Psi_G(A) | \Psi_F(A) \rangle}{\int DA |\Psi_G(A)|^2} \equiv \int DA O_{loc}(A) p(A) \quad (12)$$

where  $O_{loc}(A)$  and  $p(A)$  are given by

$$O_{loc}(A) = \frac{\langle \Psi_F(A) | O \Psi_G(A) | \Psi_F(A) \rangle}{\Psi_G(A)}, \quad p(A) = \frac{|\Psi_G(A)|^2}{\int DA |\Psi_G(A)|^2}. \quad (13)$$

The integral in Eq. (12) can be computed using MCMC with  $p(A)$  as the probability distribution from which gauge field configurations are sampled. Therefore, the estimator for the expectation value  $\langle O \rangle$  becomes

$$\langle O \rangle \approx \frac{1}{N_s} \sum_{s=1}^{N_s} O_{loc}(A), \quad (14)$$

averaged over the total number of configurations  $N_s$ . We emphasize that the Monte Carlo procedure is free from a sign problem. This follows from the fact that the fermionic degrees of freedom are integrated out analytically, which is possible due to the Gaussian form of  $|\Psi_F(A)\rangle$ . Moreover, the sampling is performed with respect to the probability distribution  $|\Psi_G|^2$ , which is manifestly real and non-negative.

## 5. Calculating energy and gradient

The expectation value of the total Hamiltonian can be computed as

$$\langle H \rangle = \langle H_E \rangle + \langle H_B \rangle + \langle H_K \rangle + \langle H_M \rangle + \langle H_\mu \rangle. \quad (15)$$

Firstly, for the expectation value  $\langle H_B \rangle$ , since we are working in the basis of  $\{A_{x,\mu}\}$ , we simply obtain

$$\langle H_B \rangle = \int DA p(A) \frac{1}{g^2} \sum_x (1 - \cos(aA_{x,\square})) \equiv \int DA p(A) H_{B,loc}(A). \quad (16)$$

The expectation value of the electric Hamiltonian,  $\langle H_E \rangle$ , can be written as

$$\langle H_E \rangle = -\frac{g^2}{2a^2} \int DA p(A) \frac{1}{\Psi_G(A)} \langle \Psi_F(A) | \sum_{x,\mu} \frac{\partial^2}{\partial A_{x,\mu}^2} \Psi_G(A) | \Psi_F(A) \rangle. \quad (17)$$

In the above equation, the second derivatives of  $\Psi_G(A) | \Psi_F(A) \rangle$  w.r.t.  $A_{x,\mu}$  can be reduced to first derivatives by a simple integration by parts, which gives

$$\begin{aligned} \langle H_E \rangle = & \frac{g^2}{2a^2} \sum_{x,\mu} \int DA p(A) \left\{ |\partial_{A_{x,\mu}} \log \Psi_G(A)|^2 + |\partial_{A_{x,\mu}} | \Psi_F(A) \rangle|^2 \right. \\ & \left. + 2 \operatorname{Re} \left[ i (\partial_{A_{x,\mu}} \log \overline{\Psi_G(A)}) \langle \Psi_F(A) | \partial_{A_{x,\mu}} | \Psi_F(A) \rangle \right] \right\}. \end{aligned} \quad (18)$$

Here, the expectation value of the derivative operator  $\partial_{A_{x,\mu}}$  with respect to the fermionic state  $|\Psi_F(A)\rangle$  involves taking the derivative of the matrix exponentials as

$$\langle \Psi_F(A) | \partial_{A_{x,\mu}} | \Psi_F(A) \rangle = \langle \Psi_0 | \vec{\psi}^\dagger (e^{-i\xi} \partial_{A_{x,\mu}} e^{i\xi}) \vec{\psi} | \Psi_0 \rangle \equiv \langle \Psi_0 | \vec{\psi}^\dagger f_{x,\mu}(A) \vec{\psi} | \Psi_0 \rangle, \quad (19)$$

where  $\vec{\psi} = (\psi_0, \psi_1, \dots, \psi_{2N_f N})^T$  is the vector of all the fermionic annihilation operators, including all flavor, site, and Dirac components. The term containing the two derivatives becomes

$$\begin{aligned} |\partial_{A_{x,\mu}} | \Psi_F(A) \rangle|^2 &= \langle \Psi_0 | [\partial_{A_{x,\mu}} U_{GS}^\dagger(A)] [\partial_{A_{x,\mu}} U_{GS}(A)] | \Psi_0 \rangle \\ &= \langle \Psi_0 | \vec{\psi}^\dagger f_{x,\mu}(A) \vec{\psi} \vec{\psi}^\dagger f_{x,\mu}(A) \vec{\psi} | \Psi_0 \rangle \end{aligned} \quad (20)$$

Now, the expectation value of the operators of the form  $\vec{\psi}^\dagger h \vec{\psi}$ , where  $h$  is some  $2N_f N \times 2N_f N$  matrix, can be written as

$$\langle \Psi_0 | \vec{\psi}^\dagger h \vec{\psi} | \Psi_0 \rangle = \sum_{mn} h_{mn} \langle \Psi_0 | \psi_m^\dagger \psi_n | \Psi_0 \rangle = \operatorname{Tr}[(\mathbb{I} - \Gamma_0)h], \quad (21)$$

where  $(\Gamma_0)_{nm} = \langle \Psi_0 | \psi_n \psi_m^\dagger | \Psi_0 \rangle$ . Since the fermionic operators  $H_K$ ,  $H_M$ , and  $H_\mu$  are of this form, their expectation values can be computed using Eq. (21).

The expectation value of a quartic fermionic operator (a 2-body operator, as in Eq. (20)) is

$$\langle \Psi_0 | \vec{\psi}^\dagger h_1 \vec{\psi} \vec{\psi}^\dagger h_2 \vec{\psi} | \Psi_0 \rangle = \sum_{mnm'n'} (h_1)_{mn} (h_2)_{m'n'} \langle \Psi_0 | \psi_m^\dagger \psi_n \psi_{m'}^\dagger \psi_{n'} | \Psi_0 \rangle, \quad (22)$$

where  $h_1$  and  $h_2$  are again  $2N_f N \times 2N_f N$  matrices. For a Gaussian  $|\Psi_0\rangle$ , the four-point correlator can be written in terms of two-point correlators using Wick's theorem, and it reduces to

$$\langle \Psi_0 | \vec{\psi}^\dagger h_1 \vec{\psi} \vec{\psi}^\dagger h_2 \vec{\psi} | \Psi_0 \rangle = \text{Tr}[(\mathbb{I} - \Gamma_0)h_1] \text{Tr}[(\mathbb{I} - \Gamma_0)h_2] + \text{Tr}[(\mathbb{I} - \Gamma_0)h_1 \Gamma_0 h_2]. \quad (23)$$

Once we have  $H_{loc}(A)$ , the gradient w.r.t. the parameters in  $|\Psi\rangle$ , say  $\eta_i$ 's, can be computed as

$$\frac{\partial E}{\partial \eta_i} = \frac{\partial}{\partial \eta_i} \langle H \rangle = \int DA p(A) \left( \frac{\partial}{\partial \eta_i} H_{loc}(A) + (H_{loc}(A) - \langle H \rangle) \frac{\partial}{\partial \eta_i} \log |\Psi_G(A)|^2 \right), \quad (24)$$

which can be estimated like any other observable after the gauge configurations are obtained.

Sampling from the distribution  $p(A)$  for some given parameter values in  $\alpha$ ,  $\beta$ , and  $\xi$ , one can compute the energy expectation value and the gradient. The gradient can then be used to update the parameters for the variational procedure, and iteratively find the optimal parameters that minimize the energy of the state  $|\Psi\rangle$  w.r.t. the total Hamiltonian.

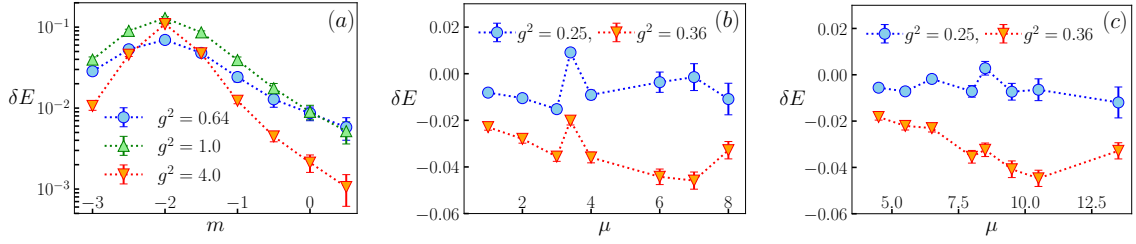
We optimize the parameters using a simple gradient descent and/or imaginary time evolution (ITE). For ITE, we first construct the quantum geometric tensor (QGT) [21, 22],  $S$ , with elements given as  $S_{ij} = \langle \Psi_{\eta_i} | \Psi_{\eta_j} \rangle$ , where  $|\Psi_{\eta_i}\rangle = \partial_{\eta_i} |\Psi\rangle - \langle \Psi | \partial_{\eta_i} |\Psi\rangle |\Psi\rangle$ . Consequently, the parameters are updated as (with  $\Delta\tau$  the discrete time step used in the Euler discretization below)

$$\dot{\eta}_i = -\frac{1}{2} \sum_j [\text{Re}(S)^{-1}]_{ij} \frac{\partial E}{\partial \eta_j} \Rightarrow \eta'_i = \eta_i - \frac{\Delta\tau}{2} \sum_j [\text{Re}(S)^{-1}]_{ij} \frac{\partial E}{\partial \eta_j}. \quad (25)$$

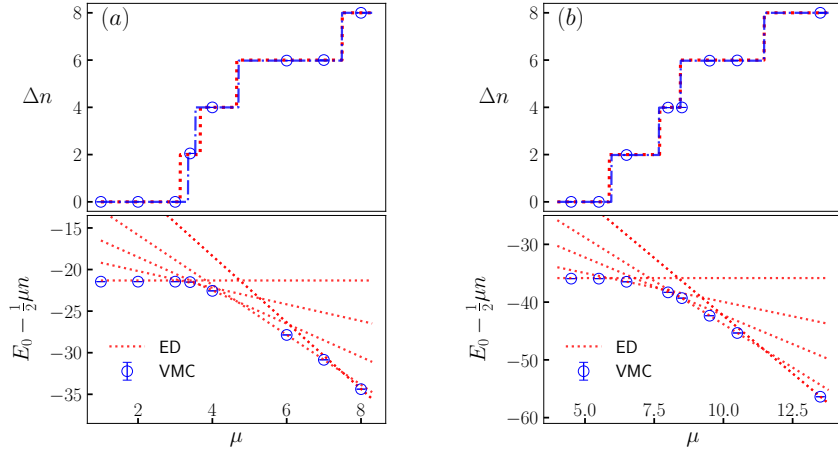
## 6. Numerical results

In our current simulations, we consider a Gaussian reference state for the fermionic part. To benchmark the algorithm, we compare the variational energies to the energies obtained from ED on a small lattice of  $2 \times 2$  with a single fermion flavor in Fig. 1(a), and with two fermion flavors in Fig. 1(b), (c). The Hamiltonian for ED is constructed in the electric basis (which has an integer spectrum) and the electric states are truncated up to  $l$  states [13]. Here  $l$  is an integer, so the allowed basis states are  $|-l\rangle, |-l+1\rangle, \dots, |0\rangle, \dots, |l\rangle$ . The results show good agreement with ED when the coefficient of the on-site term,  $m + 2r/a$ , is large (Fig. 1(a)). In contrast, the variational energies exhibit increasing deviations from ED as  $m + 2r/a \rightarrow 0$ , with the largest discrepancy occurring at  $m = -2r$ . Although the variational ansatz introduces some non-Gaussianity upon summation over gauge-field configurations, the intrinsic non-Gaussianity of the true ground state at  $m = -2r$  is substantially greater than what the current ansatz can capture. This likely accounts for the observed discrepancies in the vicinity of  $m = -2r$ .

To show that the algorithm is free of the sign problem, we consider the case of  $N_f = 2$  fermion flavors with non-zero isospin chemical potential. We choose  $\mu_1 = \mu$  and  $\mu_2 = 0$  such that  $\mu_\pm \neq 0$ .



**Figure 1:** Relative energy difference,  $\delta E$ , between the variational energy—optimized using imaginary-time evolution—and the energies obtained from ED on a  $2 \times 2$  periodic lattice. (a) shows  $\delta E$  as a function of the fermion mass  $m$  with  $N_f = 1$ , for  $g^2 = 0.64, 1, 4$  and  $g_{\text{mag}} = 1/g^2$ . The ED basis is truncated at  $l = 3$  for  $g^2 = 0.64, 1$  and at  $l = 2$  for  $g^2 = 4$ . (b), (c) show  $\delta E$  as a function of chemical potential  $\mu$  with  $N_f = 2$ , for  $g^2 = 0.25, 0.36$  and  $g_{\text{mag}} = 1$  and  $1/g^2$ , respectively. The fermion mass,  $m = 0$  in (b), and  $m = 2$  in (c). The ED basis has  $l = 2$  truncation for all the  $N_f = 2$  cases. In all cases,  $a = 1, r = 1$ .



**Figure 2:** Rescaled energy,  $E_0 - \frac{1}{2}\mu n$ , (bottom) and flavor imbalance,  $\Delta n$ , (top) in the ground state as a function of the isospin chemical potential  $\mu$  on a  $2 \times 2$  lattice with  $a = 1, r = 1, g^2 = 0.25$  and  $g_{\text{mag}} = 1$ . In (a),  $m = 0$ . In (b),  $m = 2$ . VMC (blue circles) denotes the data obtained using variational optimization. The red dotted lines are obtained using ED in different  $\Delta n = 0, 2, \dots, 8$  sectors with  $l = 2$  truncation. In the  $\Delta n$  plots, the blue curve (dash dotted), is obtained by extrapolating the variational energies and determining their intersection points.

Figure 2 shows the rescaled energy  $E_0 - \mu n/2$  obtained after the variational optimization on a  $2 \times 2$  lattice. Here,  $n = n_1 + n_2$  is the total particle number of the two flavors combined and is fixed to be  $N_f N$ . To understand the plot we can rewrite the total Hamiltonian as

$$H = H_E + H_B + H_K + H_M + \mu \frac{-\Delta n}{2} + \mu \frac{n}{2}. \quad (26)$$

Since  $n$  is fixed,  $\langle H - \mu n/2 \rangle$  depends linearly on  $\mu$ , with slope  $-\Delta n/2$  [12]. The resulting slopes (i.e., the flavor imbalance) obtained from the variational optimization for different  $\mu$  (Fig. 2) are in good agreement with those extracted from ED. As  $\mu$  increases, the ground state exhibits first-order phase transitions to sectors with larger  $\Delta n$ . The transition points are also consistent with ED.

## 7. Conclusion

We have developed a sign-problem-free variational algorithm to prepare the ground state of lattice QED in  $2 + 1D$  coupled to Wilson fermions by extending the algorithm originally developed for staggered fermions in [8]. In our approach, the complexity of evaluating the energy and its gradient is  $O(N^4)$  per gauge configuration, and the complexity of generating configurations from the distribution  $p(A)$  is  $O(N^2 \log N)$ .

The initial results that we have obtained show good agreement with exact diagonalization in the regimes of large on-site potential for single fermion flavor. For two fermion flavors, we observe discrete jumps of the flavor imbalance in the ground state as the isospin chemical potential is varied, which are also in close agreement with the transition points computed using exact diagonalization.

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