Variational Simulation of the Hubbard Model using Majorana-based Fermion-to-Qubit Mapping

Ashutosh Tripathi

Department of Theoretical Physics
Tata Institute of Fundamental Research, Mumbai

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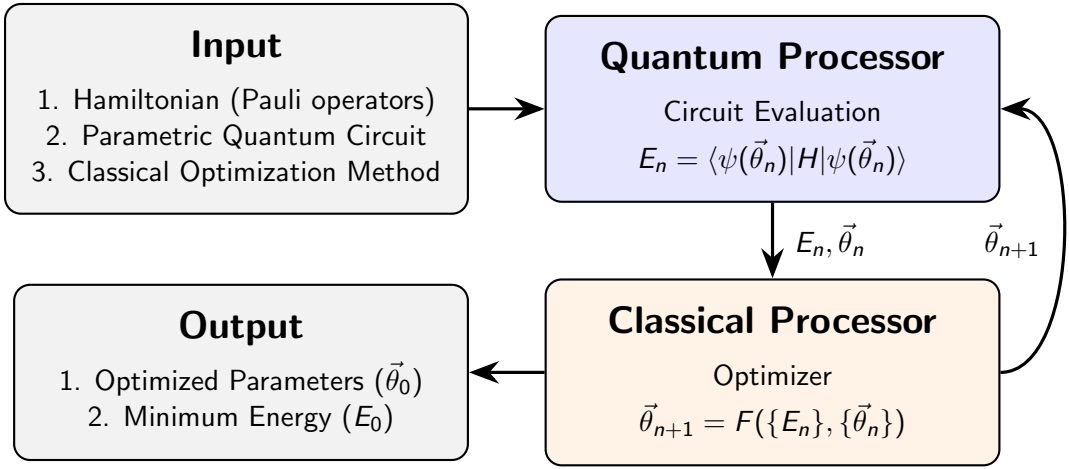
Collaborators
Debasish Banerjee Sandip Maiti Nilmani Mathur

Motivation

- Variational quantum algorithms provide a promising framework for near-term quantum devices.
- Efficient quantum simulation of fermionic systems remains a major challenge. Two broad approaches exist for fermionic quantum simulations.
- Native fermionic quantum hardware aims to directly encode fermionic statistics.
- Bosonization techniques map fermionic degrees of freedom onto qubits using fermion-to-qubit transformations.
- We study the spinless Hubbard model using the Variational Quantum Eigensolver (VQE) by employing the Derby–Klassen mapping [arXiv:2003.06939].

Variational Quantum Eigensolver



Jordan-Wigner mapping

Anti-commutation relation,

$$\{a_i, a_j\} = 0, \tag{1}$$
$$\{a_i^\dagger, a_j^\dagger\} = 0, \tag{2}$$
$$\{a_i, a_j^\dagger\} = \delta_{ij}. \tag{3}$$

Jordan–Wigner mapping [Eur. Phys. J. A 47, 631 (1928).],

$$a_j = \left(\prod_{k=1}^{j-1} Z_k\right) \frac{X_j + iY_j}{2}, \tag{4}$$
$$a_j^\dagger = \left(\prod_{k=1}^{j-1} Z_k\right) \frac{X_j - iY_j}{2}. \tag{5}$$

- Efficient in 1D.
- Long Pauli strings in 2D.
- More measurements needed.

Derby–Klassen Majorana Mapping

Majorana operators are defined as

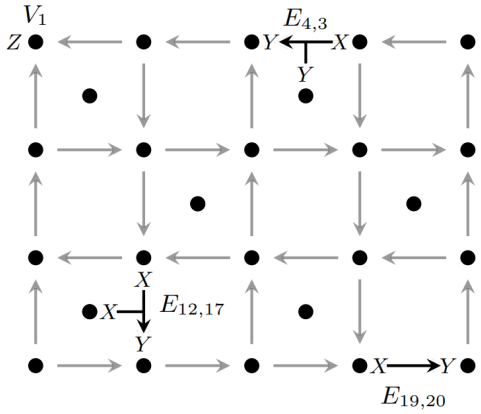
$$\bar{\gamma}_k = i(a_k^\dagger - a_k), \tag{6}$$

$$\gamma_k = a_k^\dagger + a_k. \tag{7}$$

Edge and vertex operators:

$$E_{jk} = -i\gamma_j\gamma_k, \tag{8}$$

$$V_j = -i\gamma_j\bar{\gamma}_j. \tag{9}$$



Source: [arXiv:2003.06939]

Advantages

- Preserves locality.
- Suitable for higher-dimensional lattices.

Vertex and Face Qubits

Edge and vertex operators:

$$E_{jk} = -i\gamma_j\gamma_k, \tag{10}$$
$$V_j = -i\gamma_j\bar{\gamma}_j. \tag{11}$$

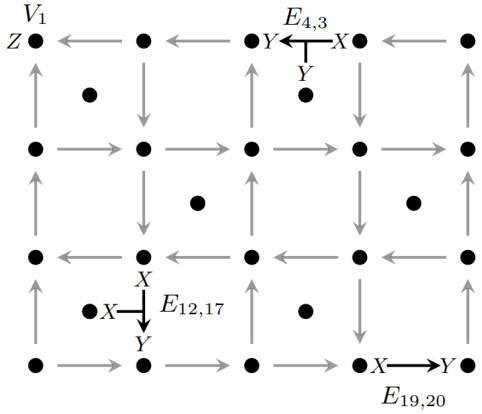
In mapped qubits, the vertex operators become

$$\tilde{V}_j = Z_j. \tag{12}$$

and the edge operators become

$$\tilde{E}_{jk} = \begin{cases} X_j Y_k X_{F(j,k)}, \\ -X_j Y_k X_{F(j,k)}, \\ X_j Y_k Y_{F(j,k)}, \end{cases} \tag{13}$$

where $F(j,k)$ denotes the face qubit associated with edge (j,k).



Source: [arXiv:2003.06939]

Physical Subspace

Not every state in the enlarged Hilbert space corresponds to a physical fermionic state.

Physical states satisfy the stabilizer constraints

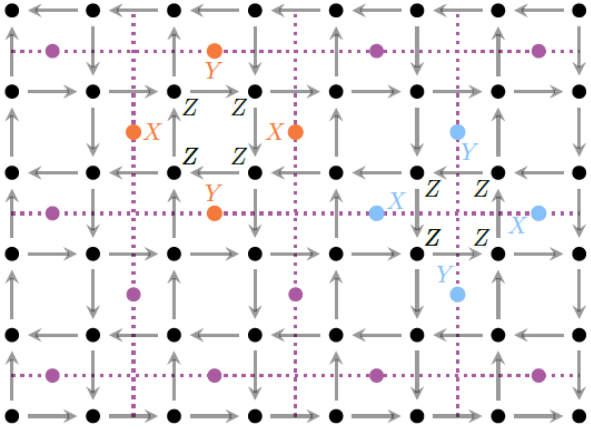
$$H_{\text{map}} = -\sum \Pi_s \otimes Z_s - \sum \Pi_p \otimes Z_p. \tag{14}$$

For a physical state

$$\langle H_{\text{map}} \rangle = -N_{\text{even}}, \tag{15}$$

where N_{even} denotes the number of even faces.

Hence every loop carries eigenvalue $+1$.



Source: [arXiv:2003.06939]

Penalty Hamiltonian

To suppress nonphysical states, we add a penalty term.

$$H_{\text{modified}} = H + \alpha \left(H_{\text{map}} + N_{\text{even}} \right). \tag{16}$$

- Penalty term raises the energies of nonphysical states.
- Restricts VQE optimization to the physical sector.
- Choose

  $$\alpha > E_n - E_0$$

  to obtain the lowest n eigenstates.

Spinless Hubbard Model

The charge-conjugation symmetric Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} \left(a_i^\dagger a_j + a_j^\dagger a_i \right) \tag{17}$$

$$- \mu \sum_i \left(n_i - \frac{1}{2} \right) + U \sum_{\langle ij \rangle} \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right). \tag{18}$$

- J : hopping strength.
- μ : chemical potential.
- U : nearest-neighbour interaction.

Local Qubit Hamiltonian

After the DK mapping, the spinless Hubbard model becomes

$$H = -\frac{J}{2}\sum_{\langle ij\rangle}(X_iX_jP_{ij} + Y_iY_jP_{ij}) + \frac{\mu}{2}\sum_i Z_i + \frac{U}{4}\sum_{\langle ij\rangle} Z_iZ_j, \tag{19}$$

where P_{ij} denotes the face-qubit operator associated with edge (i, j).

- The hopping terms remain local even in two dimensions.

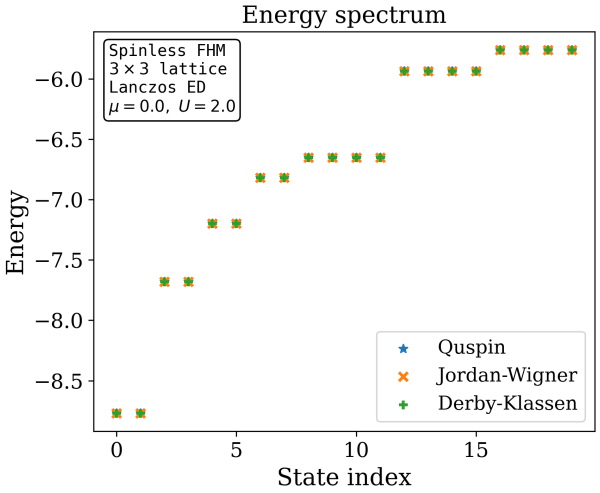
Spectrum Validation

The DK mapping enlarges the Hilbert space.

Physical states are selected through stabilizer constraints.

The resulting low-energy spectrum agrees with exact diagonalization.

- QuSpin [SciPost Phys. 7, 020 (2019)]
- Jordan–Wigner [Eur. Phys. J. A 47, 631 (1928).]
- Derby–Klassen [Phys. Rev. B 104, 035118 (2021)]



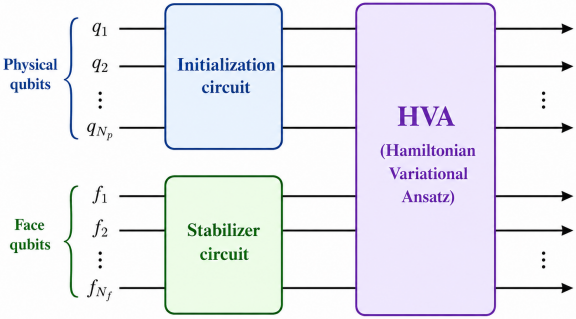
Hamiltonian Variational Ansatz

The ansatz is constructed directly from the Hamiltonian terms:

- Hopping terms
- Interaction terms
- Chemical potential terms

Advantages:

- Physically motivated
- Particle-number conserving
- Reduced search space



Variational Quantum Deflation (VQD)

Ground-state VQE can be extended to excited states.

The cost function becomes

$$C_n(\theta) = \langle H \rangle_\theta + \sum_{i<n} \beta_i \left| \langle \psi(\theta) | \psi_i \rangle \right|^2 . \tag{20}$$

- Orthogonality is enforced through overlap penalties.
- Ground and excited states are obtained sequentially.
- We compute the lowest three states.

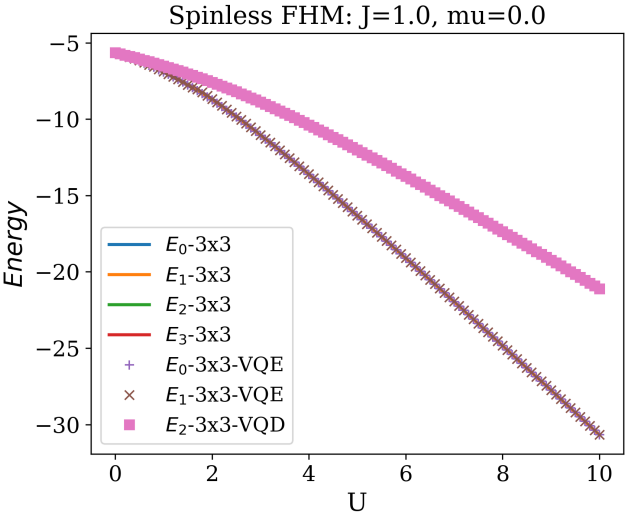
Ground and Excited-State Spectrum

We employ VQE and VQD to compute

- Ground state
- First excited state
- Second excited state

for the 3×3 spinless Hubbard model.

Good agreement with Quspin exact diagonalization is observed.



Comparison of JW and DK Mapping

Mapping	Ansatz	layers	Optimizer	E_0(VQE)	Fidelity	Time (min)
JW	SU2-full	8	LBFGS	-8.84520	0.96065	16.3
JW	SU2-linear	8	LBFGS	-8.95076	0.98504	16.6
DK	HVA	8	COBYLA	-8.92192	0.97983	2.3
JW	HVA	8	COBYLA	-8.92617	0.98082	38.4

Table: Single spin FHM 3x3 ($J = 1.0, \mu = 0.5, U = 2.0$,$E_0 = -9.01941$)

Mapping	Ansatz	layers	Optimizer	E_0(VQE)	Fidelity	Time (hr)
JW	SU2-full	8	COBYLA	-16.3853	0.4504	21.5
JW	SU2-linear	8	COBYLA	-14.3343	0.0003	19.4
DK	HVA	8	COBYLA	-16.2894	0.4384	0.5
JW	HVA	8	COBYLA	-13.38582	0.0049	7.3

Table: Single spin FHM 4x4 (even mapping) ($J = 1.0, \mu = 0.5, U = 2.0, E_0 = -16.8719$)

Resource Estimation

Mapping	Ansatz	parameters	CNOT gates	CNOT depth
JW	SU2-full	$2(N_l+1)L_xL_y$	$2N_lL_xL_y(L_xL_y-1)$	$N_l(L_xL_y+1)$
JW	SU2-linear	$2(N_l+1)L_xL_y$	$N_l(L_xL_y-1)$	$2N_l$
DK	HVA	$N_l(L_xL_y-L_x-L_y+2)$	$10N_l(2L_xL_y-L_x-L_y)+N_S$	$24N_l$
JW	HVA	$N_l(L_xL_y-L_x-L_y+2)$	$N_l(2L_x+4)(2L_xL_y-L_x-L_y)$	$(24+L_x)N_l$

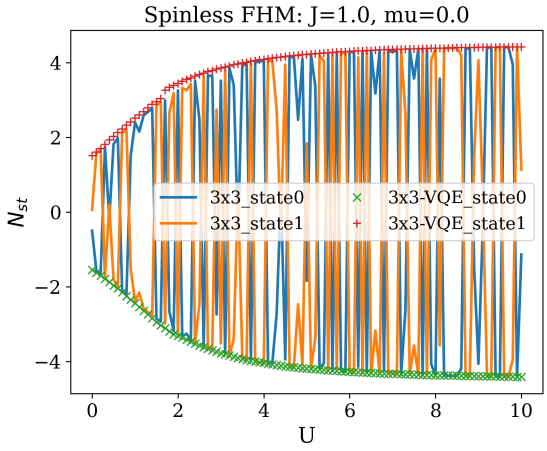
Table: Resource estimation

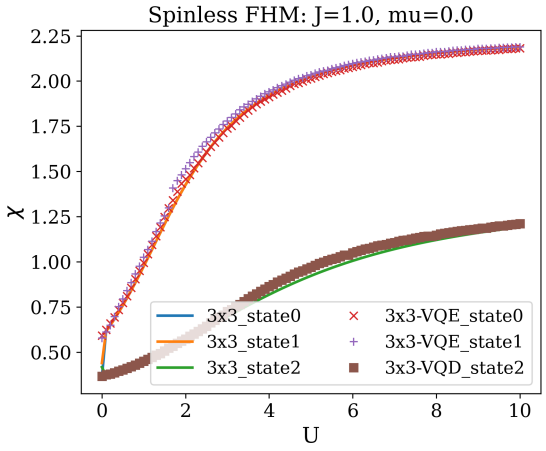
Tradeoff

- DK mapping introduces auxiliary qubits.
- DK mapping combined with HVA gives comparable performance while preserving locality.
- Circuit depth remains independent of system size.
- Locality is preserved in higher dimensions.

Staggered Occupation and Susceptibility

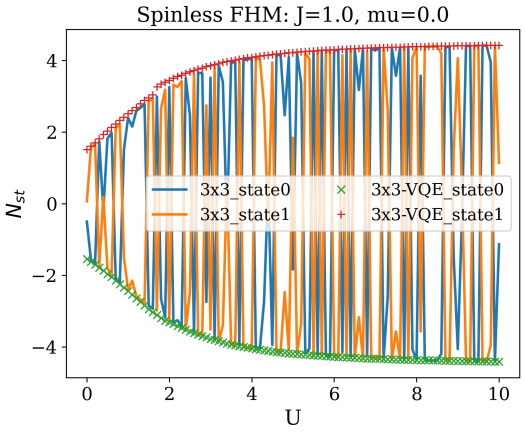
$$N_{\rm st} = \sum_r (-1)^r \left(n_r - \frac{1}{2} \right), \qquad \chi = \frac{\langle N_{\rm st}^2 \rangle}{V}. \tag{21}$$

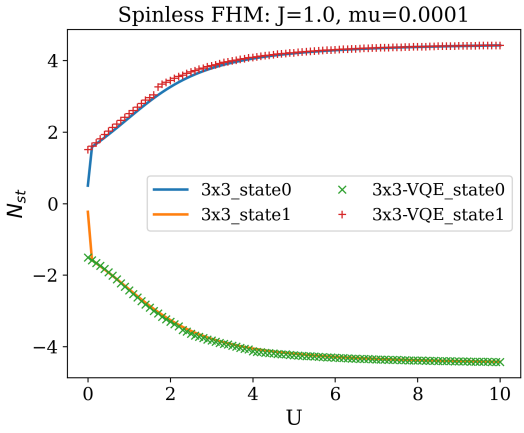




Lifting the Degeneracy

Introducing a small chemical potential lifts the degeneracy, resulting in good agreement between exact diagonalization (ED) and VQE results.





Conclusions

- The Derby–Klassen mapping preserves locality in higher dimensions.
- The Hamiltonian variational ansatz accurately reproduces low-lying spectra and observables.
- Locality preservation enables low-depth HVA circuits with reduced gate overhead.
- Comparison with the Jordan–Wigner mapping demonstrates the advantages of the DK mapping.
- The framework can be readily extended to larger lattices and multi-flavor Fermionic models.

Thank you!