Variational low-depth preparation of correlated systems' ground states with the natural-orbitalization algorithm

QCMB workshop

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01. Strongly-correlated materials: what and why

Atos

Strongly-correlated materials

Or when electrons see each other and exotic behaviours emerge

Materials for which 1-particle theories fail

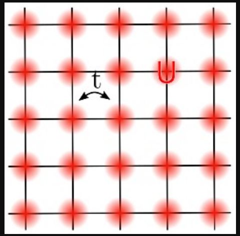
Perfect embodiments of the **particle/wave duality**: competition between electronic localization on atomic sites and tunneling

Minimal model : (Fermi-)Hubbard lattice

- Double occupancy of an atomic site comes with energy cost U
- Tunneling costs t

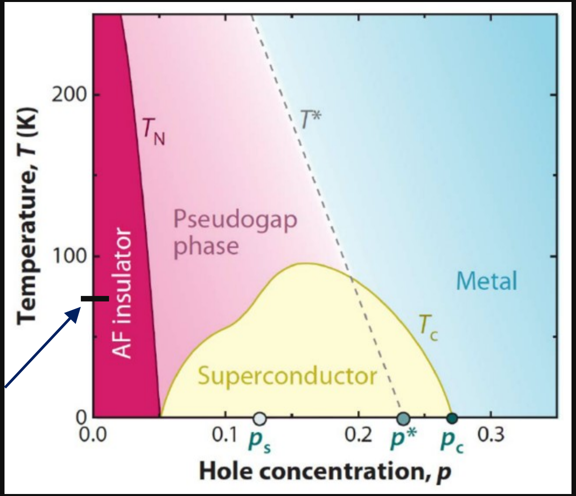
$$\hat{H}_{Hub} = U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + t \sum_{ij\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)$$

→ Different behaviours depending on the ratio U/t, tunable by P, T, V



Study boosted by the discovery of 'high' Tc superconductors in the 80s

Boiling point of liquid nitrogen

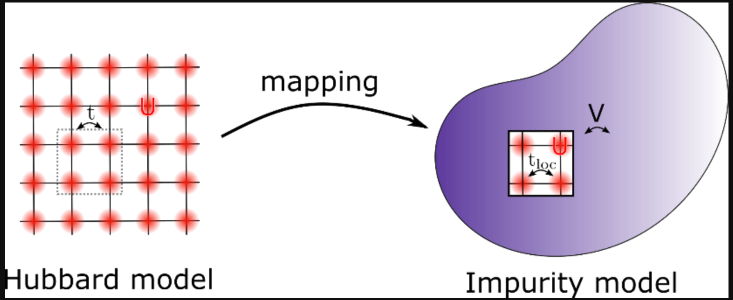


Phase diagram of a cuprate

Strongly-correlated materials

How can we solve the Hubbard model?

Self-consistent mapping to an 'impurity' model describing N_c correlated sites embedded in a fermionic bath:
(example: N_c =4)



Hamiltonian representation:

$$\hat{H}_{embedded} = \hat{H}_{imp}^{\{c_{i\sigma}^{\dagger}, c_{i\sigma}\}}(U, t_{loc}) + V \sum_{ij\sigma} (c_{i\sigma}^{\dagger} a_{j\sigma} + h.c.)$$

Requires to choose an embedding method (typically, Dynamical Mean-Field Theory [Georges, 1996])
+ an *impurity solver*
Impurity solving simpler, but definitely not simple:
- Bath truncation to a very low number of bath levels due to limited memory (Exact Diagonalization)

OR
- Keep the bath infinite but get fermionic sign problem (Monte-Carlo sampling)

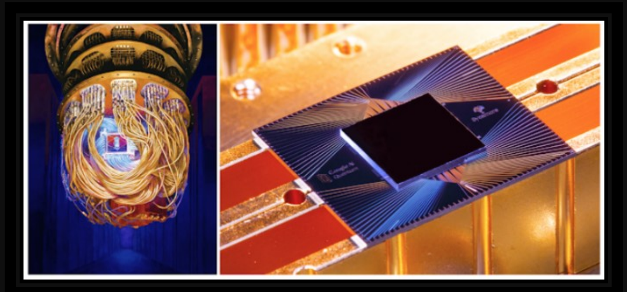
Quantum computing: Exponential speedup?

Strongly-correlated materials
Why could quantum computers help?

- N spinful sites → 2^N amplitudes: exponential scaling of classical resources to store the wavefunction $|\psi\rangle$
- Quantum computers: storage on N qubits
- Philosophy:

Feynman, 1982:

'Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy'



Google Sycamore superconducting quantum computer

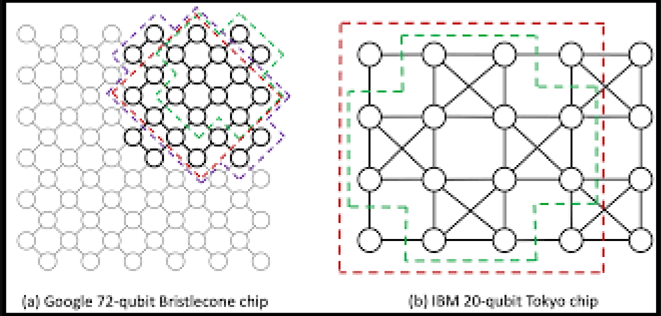
- Domain still in its infancy → for now, **test** noisy quantum computing on easy, small problem instances to lay the ground for improvement

02. Leveraging noisy quantum computers

Limitations of current hardware

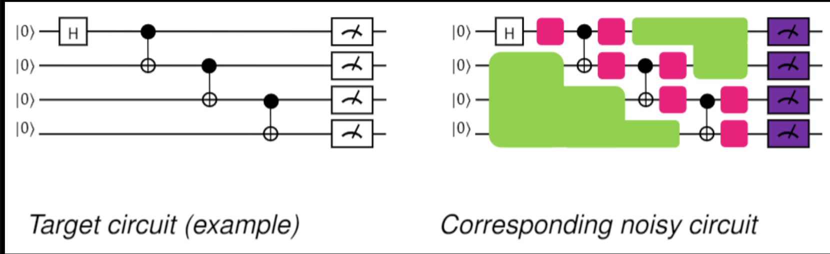
…and how it translates in terms of possible circuit architectures

- Low width = qubit count (a few tens)
- Limited connectivity of the chip → gate overhead due to operating swaps



(a) Google 72-qubit Bristlecone chip (b) IBM 20-qubit Tokyo chip

- Idle noise, gate errors, readout errors



Target circuit (example) *Corresponding noisy circuit*

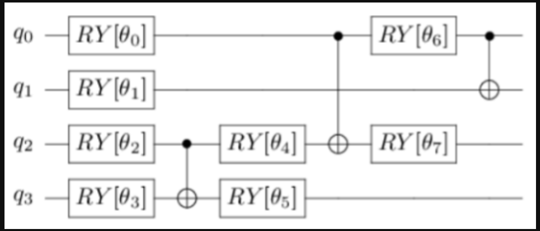
→ Impose limitations on the depth of the circuit = gate count

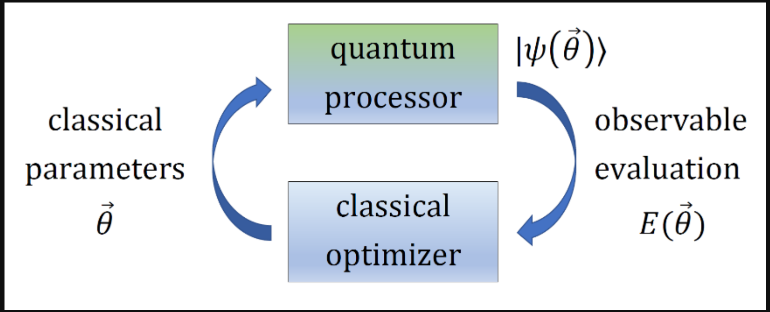
Strategy: develop **hybrid** algorithms (quantum-classical), letting CPU do what they're good at!

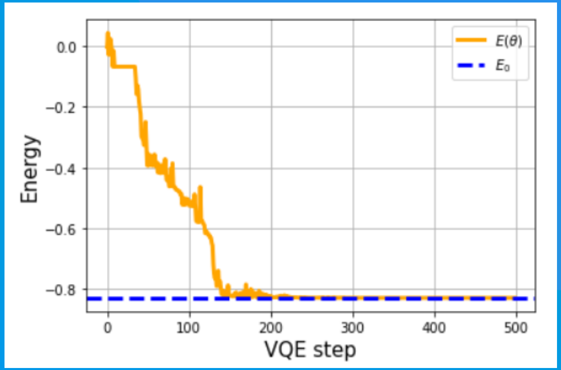
The Variational Quantum Eigensolver (VQE) algorithm

Or how to get away with small circuits by tuning them

Idea : Minimize energy over instances of a parametrized circuit [Peruzzo 2014]
CPU and QPU work hand in hand







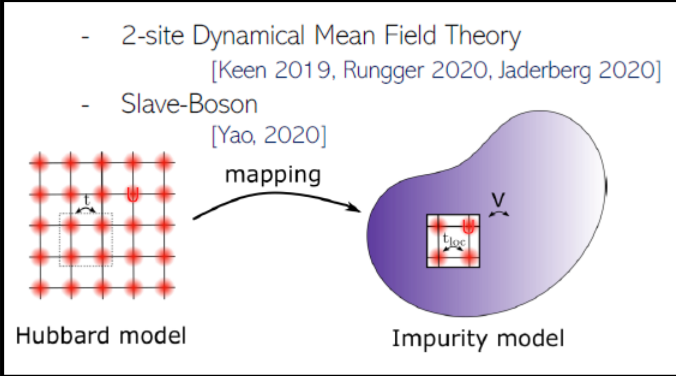
One must find a **trade-off** between expressivity and circuit depth

$$\theta^* = \mathrm{argmin}\langle\psi(\theta)|\widehat{H}_{embedded}|\psi(\theta)\rangle:\ |\psi(\theta^*)\rangle \approx |\psi_{GS}\rangle$$

State of the art

A few baby steps, scalability issue

- 4-qubit circuits only, corresponding to 1 correlated site coupled to 1 bath site



- Not scalable to more sites
- Yet, it is crucial to increase the number of embedded impurity sites in the model → control parameter for the embedding error!
- Use small, very specific circuits → no variational ansatz to go to N_c=2, except 'LDCA' [Dallaire-Demers 2019], which is too big to handle noise

03. Our work: towards a scalable hybrid framework to solve the Hubbard model

Our proposal to increase N_c

An embedding method that accomodates hardware limitations

The Rotationally-Invariant Slave Boson method…

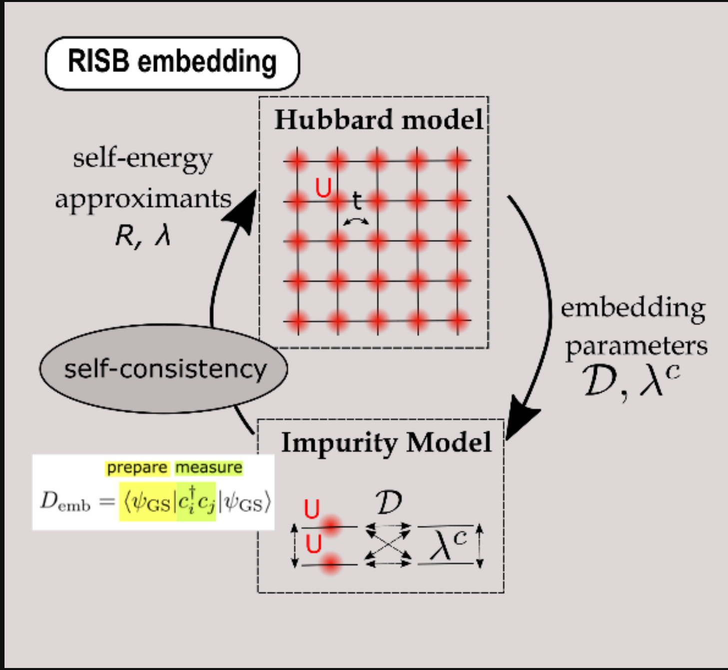
- Caps the number of qubits with #bath sites=#impurity sites
- Does not imply lengthy time evolution circuits: only monitor static correlators

$$D_{emb} = \langle \psi_{GS} | c_i^\dagger c_j | \psi_{GS} \rangle$$

- Gives access to the low-energy physics: self-energy parametrized as

$$\Sigma(\omega) = \omega \left(1 - \left(R^\dagger R\right)^{-1}\right) + \mathrm{R}^{-1} \lambda \left(R^\dagger\right)^{-1}$$

R: quasiparticle weight renormalization, λ: energy shift



Our proposal to increase N_c

A basis change to lower circuit requirements on the VQE ansatz

$$|\psi_{GS}\rangle = \sum_j a_j |\phi_j\rangle$$

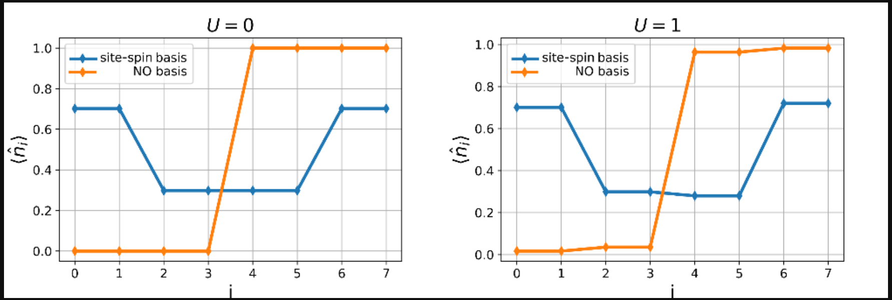
Correlation entropy: $$S_{corr} = -\sum_i n_i \ln(n_i)$$

minimal in the 'Natural Orbitals' (NO) basis

= diagonalization basis of $D_{emb} = \langle\psi_{GS}|c_i^\dagger c_j|\psi_{GS}\rangle$,

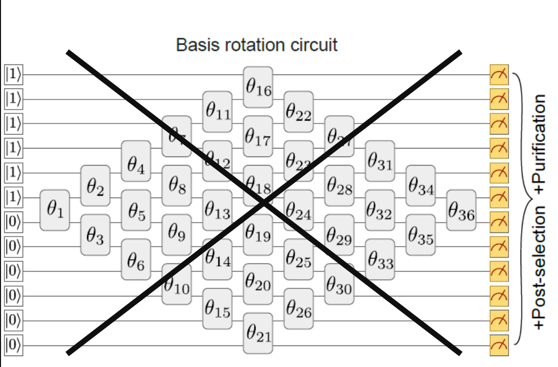
$N \times N$ matrix

→ minimal number of $|\phi_j\rangle$ in decomp. of $|\psi_{GS}\rangle$



Spin-orbital occupations of the ground state in NO VS site-spin basis

Idea: working in NO avoids carrying out basis rotation on the chip



Circuit from *'Hartree-Fock on a superconducting qubit quantum computer'* [Arute, 2020]

Our proposal to increase N_c

A basis change to lower circuit requirements on the VQE ansatz

'Natural Orbitals' (NO) basis = diagonalization basis of $D_{emb} = \langle \psi_{GS} | c_i^\dagger c_j | \psi_{GS} \rangle$:

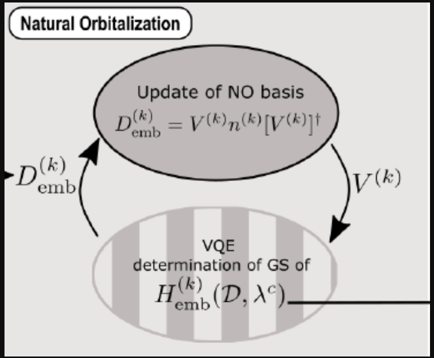
$$V^\dagger D_{emb} V = diag(n_1, n_2, \ldots, n_N)$$

Orbital rotation $\tilde{c}^\dagger{}_k = \sum_l V_{lk} c_l^\dagger$

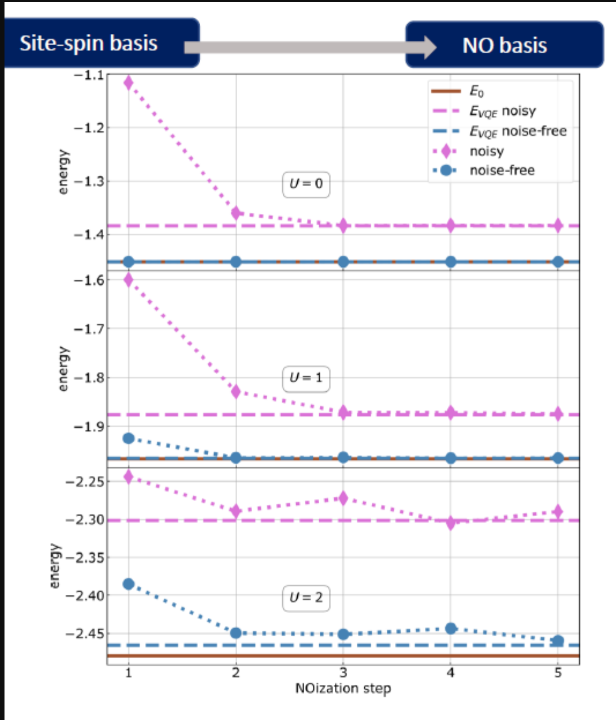
Transformation of the Hamiltonian $\widetilde{H} = \sum \left(V h_1 V^\dagger\right)_{pq} c_p^\dagger c_q + \sum \left(V V h_2 V^\dagger V^\dagger\right)_{pqrs} c_p^\dagger c_q \, c_r^\dagger c_s$

Finding the optimal basis
Topping VQE with Natural Orbitalization

Idea: Use approximate ground state to rotate basis, reach approximate NO basis iteratively



Hamiltonian-learning philoshophy as within Caroline Robin's algorithm, but state optimization separate from orbital basis optimization

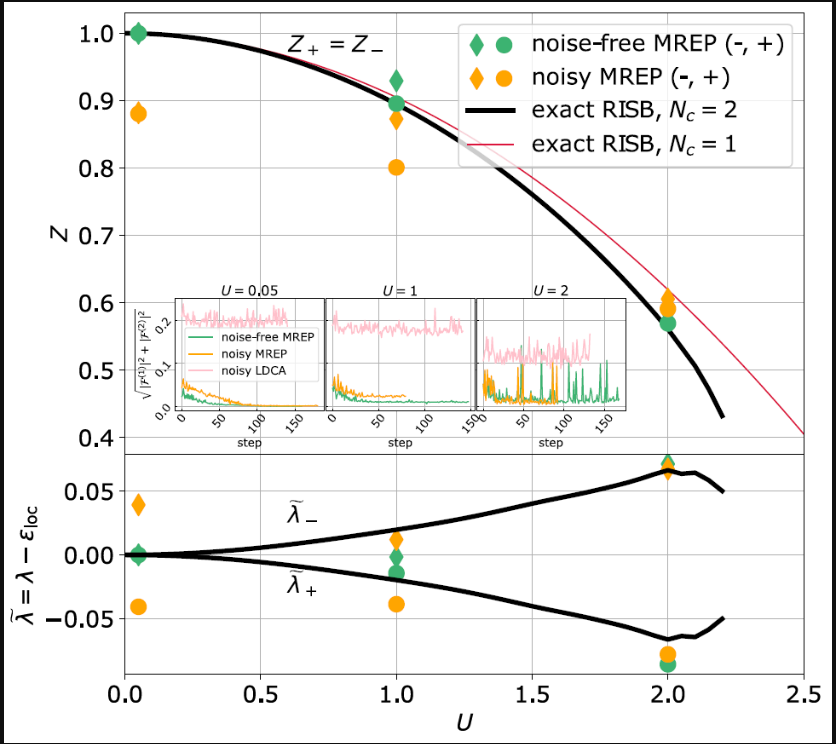


→ The NOization procedure works as expected.

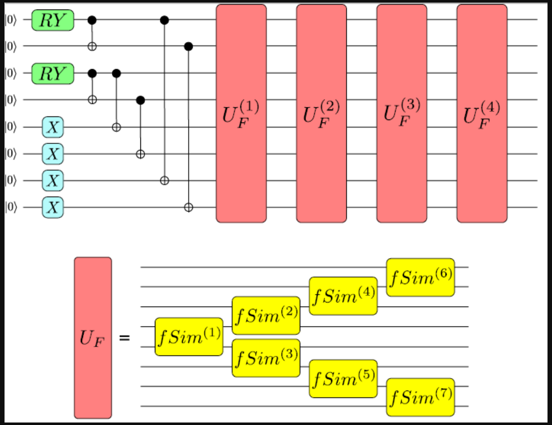
Results

Convergence of 2-impurity RISB - half-filled, paramagnetic model

'metallicity'



Intensity of correlations



The 'MREP' circuit we proposed and used.

58 parameters
56 fSim gates, native in Google hardware
6 CNOT gates
6 one-qubit gates

LDCA: 112 CNOT gates, 148 parameters

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Thank you!

Article available on arXiv at: