

Title: Gate-Based Quantum Simulation of Strongly Correlated Fermions - Philipp Preiss

Speakers: Philipp Preiss

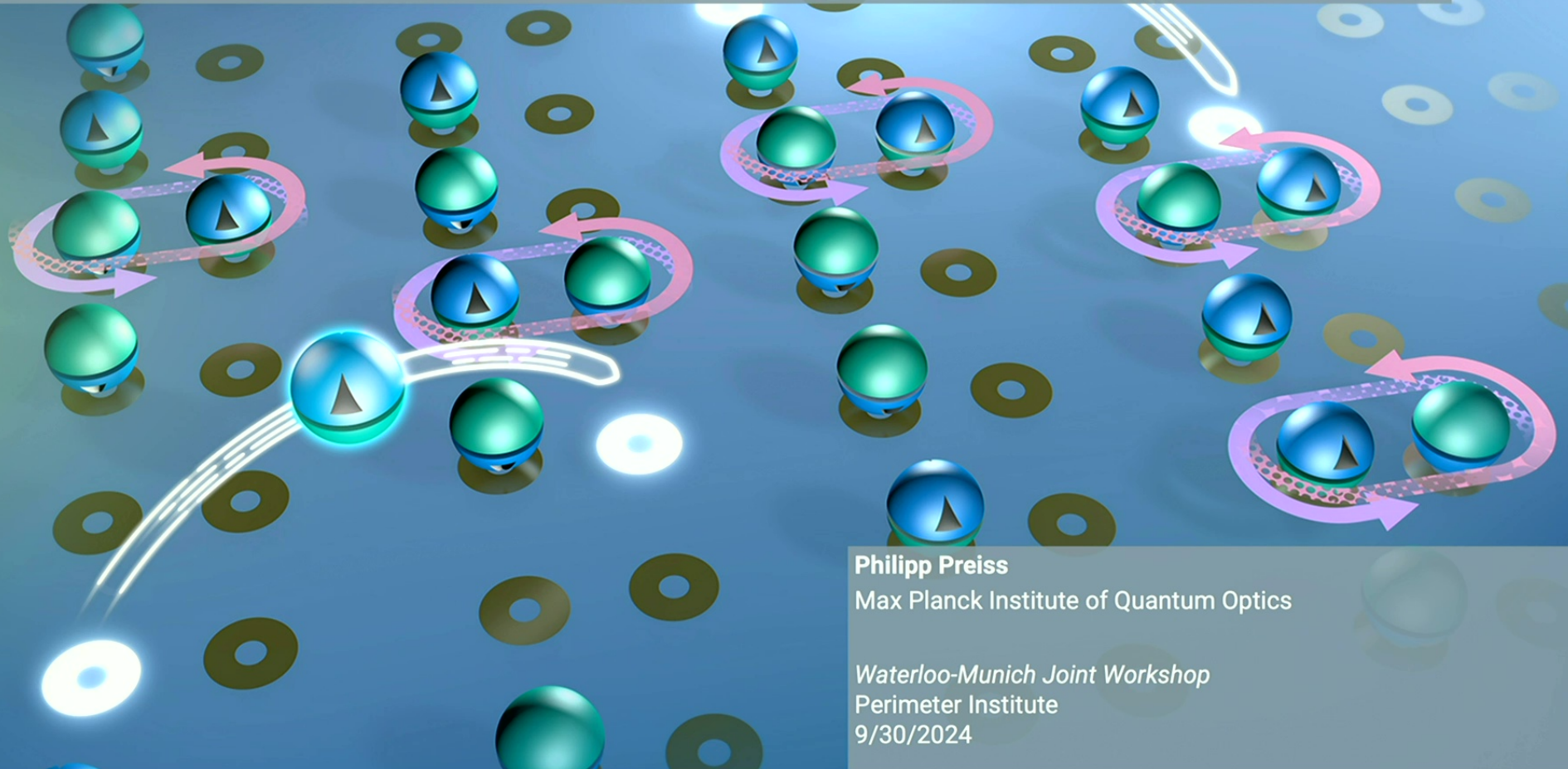
Collection/Series: Waterloo-Munich Joint Workshop

Subject: Quantum Information

Date: September 30, 2024 - 11:00 AM

URL: <https://pirsa.org/24090181>

Gate-Based Quantum Simulation of Strongly Correlated Fermions



Philipp Preiss

Max Planck Institute of Quantum Optics

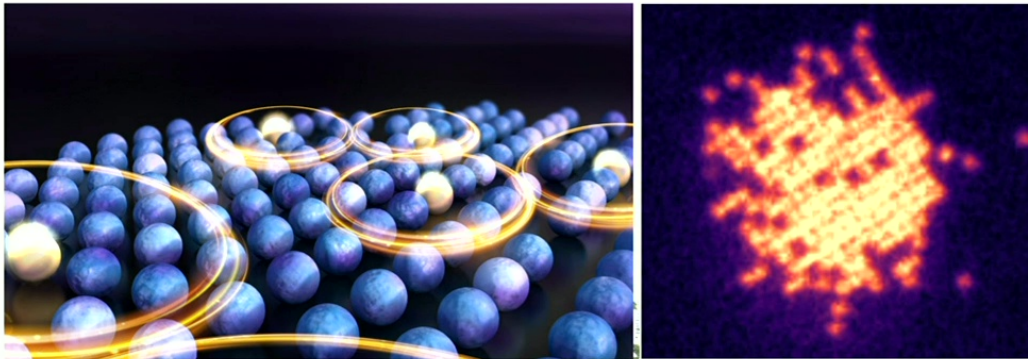
Waterloo-Munich Joint Workshop

Perimeter Institute

9/30/2024



Quantum Many Body Division



Ultracold atoms in optical lattices

- Quantum simulation
- Bose- and Fermi-Hubbard models
- Quantum computing



See also
Johannes Zeiher's talk on Thursday:
Rydberg simulation and computation

<https://www.quantum-munich.de/>

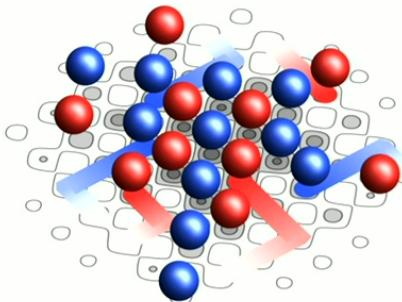
Immanuel Bloch



Ultracold Fermions @ MPQ

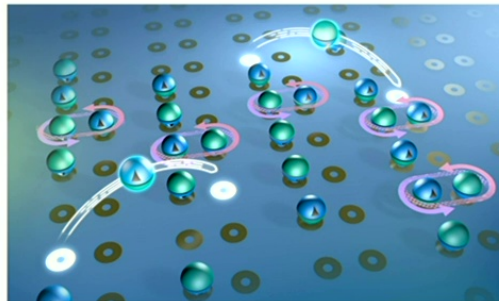
Two new Fermi microscope experiments

UniRand
Random unitaries in lattices



- Optical lattice assembly
- Combine tweezers + lattice

FermiQP
Hybrid digital/analog simulator
with Titus Franz



- Fermi Hubbard systems
- Gate-based simulation

Li 1.0
Fermion Microscope
Titus Franz & Timon Hilker



- Fermi Hubbard simulation
- Gate-based approach to fermions

Teams@MPQ



UniRand



Naman Jain



Daniel Dux



Jin Zhang



Xinyi Huang



Marcus Culemann

FermiQP



Liyang Qiu



Luca Muscarella



Janet Qesja



Andreas v Haaren



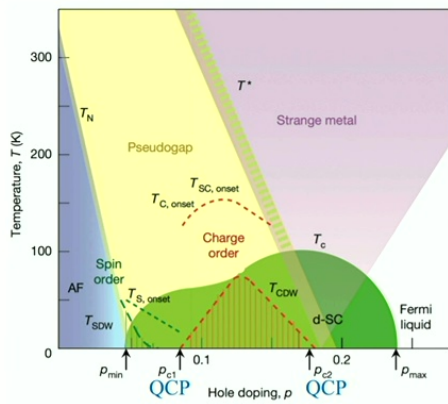
Robin Groth

Lithium 1.0





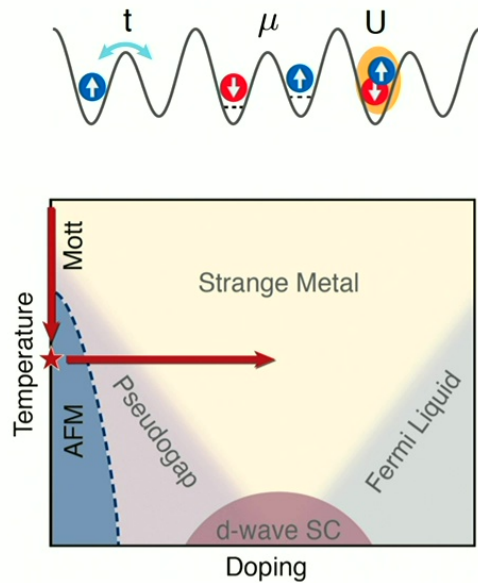
Many-fermion problems



Condensed matter physics



Quantum Simulation of the Fermi-Hubbard model

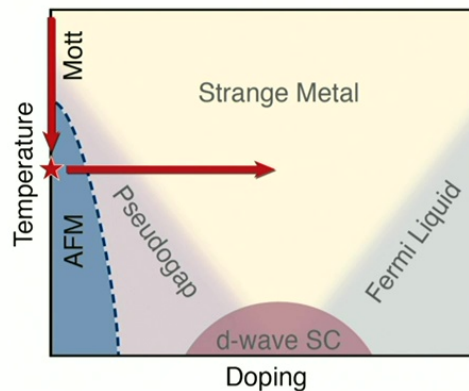
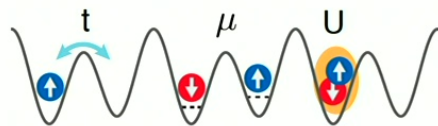


- Minimalistic model for solid state systems
- Relation to cuprates, high T_c superconductors

M. Qin ... S. Zhang, *Phys. Rev. X* **10**, 031016 (2020)
H. Xu, C.-M. Chung ... S. Zhang, *arxiv* 2303.08376 (2023)



Quantum Simulation of the Fermi-Hubbard model



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 H. Xu, C.-M. Chung ... S. Zhang, arxiv 2303.08376 (2023)

PHYSICAL REVIEW X **10**, 031016 (2020)

Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model

Mingpu Qin^{1,2,*} Chia-Min Chung^{3,4,*} Hao Shi,⁵ Ettore Vitali,^{6,2} Claudius Hubig⁷
 Ulrich Schollwöck^{3,4} Steven R. White⁸ and Shiwei Zhang^{5,2}

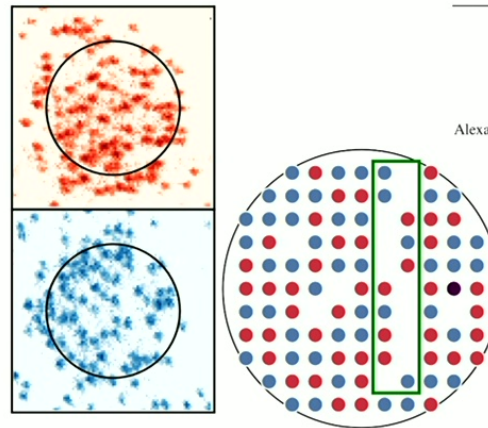
PHYSICAL REVIEW X **11**, 031007 (2021)

Stripes, Antiferromagnetism, and the Pseudogap in the Doped Hubbard Model at Finite Temperature

Alexander Wietek^{1,7} Yuan-Yao He,¹ Steven R. White² Antoine Georges^{1,3,4,5} and E. Miles Stoudenmire¹
¹Center for Computational Quantum Physics, Flatiron Institute,
 162 Fifth Avenue, New York, New York 10010, USA

²Department of Physics and Astronomy, University of California, Irvine, California 92697-4575 USA
³Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France
⁴CPHT, CNRS, École Polytechnique, IP Paris, F-91128 Palaiseau, France
⁵DQMP, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève, Switzerland

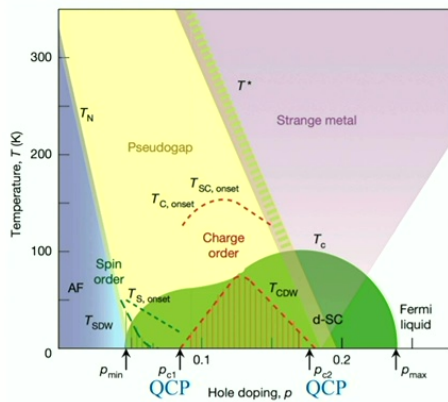
(Received 12 October 2020; revised 24 March 2021; accepted 11 May 2021; published 12 July 2021)



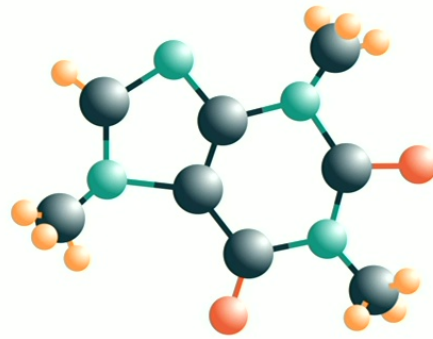
S. Hirthe ... T. Hilker, Nature **613**, 463 (2023)
 D. Bourgund ... T. Hilker, arxiv 2212.14156 (2023)



Many-fermion problems



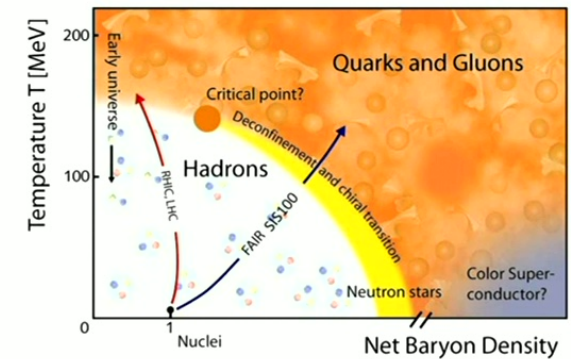
Condensed matter physics



Quantum chemistry



Material science



High energy physics

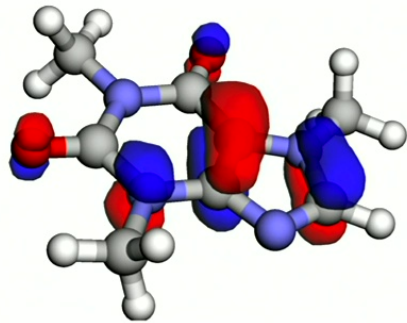
$$\mathcal{H} = \sum_{ij} h_{ij}^{(1)} c_i^\dagger c_j + \sum_{ijkl} h_{ijkl}^{(2)} c_i^\dagger c_j^\dagger c_k c_l$$

Fermions are everywhere in nature: electrons, neutrons, protons etc.

- Exchange statistics make the many-body problem particularly hard
- Monte Carlo methods suffer from the “sign problem”



Quantum Chemistry with quantum devices



$$\mathcal{H} = \sum_{ij} h_{ij}^{(1)} c_i^\dagger c_j + \sum_{ijkl} h_{ijkl}^{(2)} c_i^\dagger c_j^\dagger c_k c_l$$

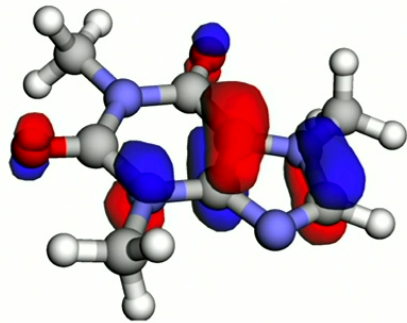
State of the art:

Simulation of few fermionic modes with ions/SCqubits

A. Kandala ... J.M. Gambetta, Nature **549**, 242 (2017)
C. Hempel ... C. Roos, PRX **8**, 031022 (2018)
P.J.J. O'Malley ... J.M. Martinis, PRX **6**, 031007 (2016)
... and many more



Quantum Chemistry with quantum devices



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... and many more

Electron to qubit mapping

Jordan-Wigner or Bravyi-Kitaev transformation

$$c_j^\dagger = \sigma_j^+ e^{(-i\pi \sum_{k=1}^{j-1} \sigma_k^+ \sigma_k^-)}$$

Hydrogen molecule in spin form:

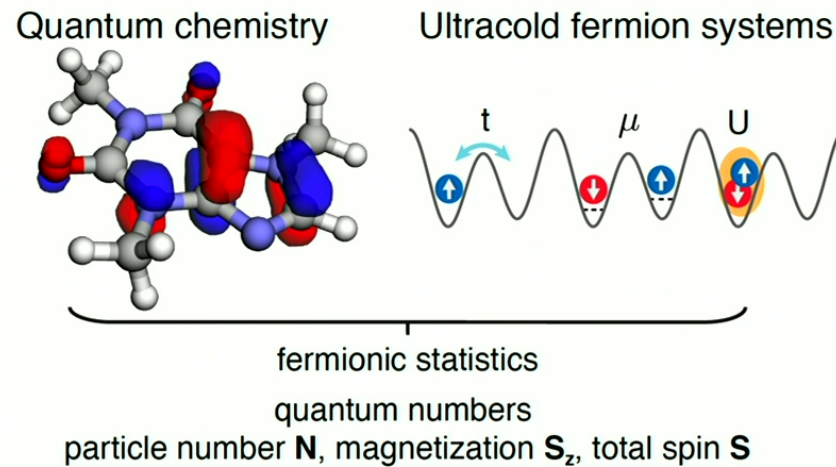
$$\begin{aligned} H^{\text{BK}} = & f_0 \mathcal{I} + f_1 \sigma_0^z + f_2 \sigma_1^z + f_3 \sigma_2^z + f_4 \sigma_1^z \sigma_0^z + f_5 \sigma_2^z \sigma_0^z \\ & + f_6 \sigma_3^z \sigma_1^z + f_7 \sigma_2^x \sigma_1^x \sigma_0^x + f_8 \sigma_2^y \sigma_1^y \sigma_0^y + f_9 \sigma_2^z \sigma_1^z \sigma_0^z \\ & + f_{10} \sigma_3^z \sigma_2^z \sigma_0^z + f_{11} \sigma_3^z \sigma_2^z \sigma_1^z + f_{12} \sigma_3^z \sigma_2^x \sigma_1^x \sigma_0^x \\ & + f_{13} \sigma_3^z \sigma_2^y \sigma_1^y \sigma_0^y + f_{14} \sigma_3^z \sigma_2^z \sigma_1^z \sigma_0^z, \end{aligned} \quad (\text{B1})$$

Difficult to solve fermionic problems with spins

D. Gonzalez-Cuadra ... P. Zoller, arXiv: 2303.06985 (2023)



Quantum chemistry and cold fermions

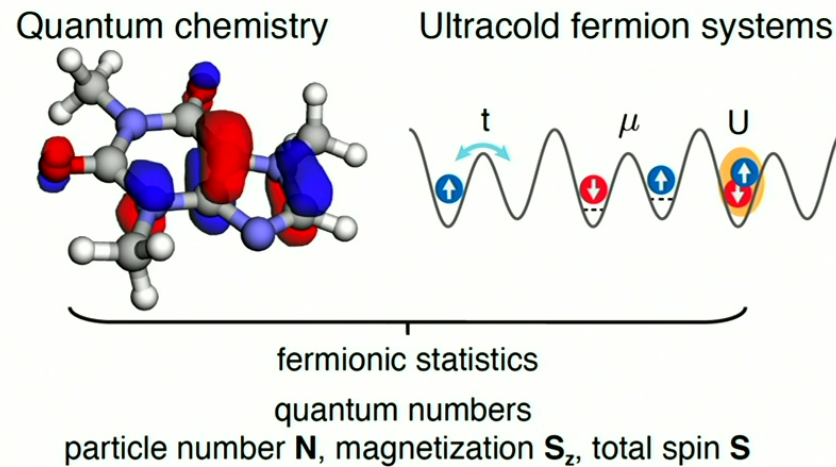


Ultracold fermions

- Conserved quantum numbers
- Targeted preparation of total spin \mathbf{S}



Quantum chemistry and cold fermions



Ultracold fermions

- Conserved quantum numbers
- Targeted preparation of total spin \mathbf{S}

But

- Translationally invariant Hamiltonians
- Short-range interactions

Analogue Quantum Chemistry Simulation
J. Argüello-Luengo... I. Cirac., Nature **574**, 215 (2019)



Quantum Chemistry with Superlattices



Daniel Dux

Jin Zhang

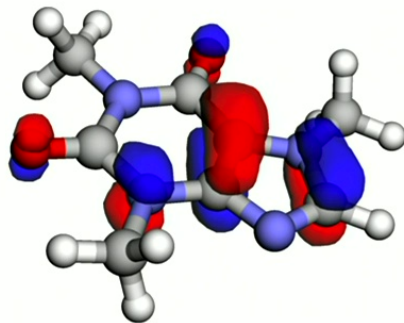
Naman Jain



Christian Gogolin



Bundesministerium
für Bildung
und Forschung



- Chemicals/polymers company
- Exploring quantum methods for computational chemistry
- Optimization problems for molecules

G.-L. Anselmetti *et al.*, *New J. Phys.* **23** (2021) 113010
O. Oumaruet *et al.*, *arxiv:2212.07957* (2022)
T. O'Brien *et al.*, *Nature Physics.* **19** 1787 (2023)

Can quantum chemistry problems be mapped to ultracold fermions in lattices?

Our work: F. Gkritsis, ..., P.Preiss, *arXiv* 2409.05663 (2024)

30.9.2024

Philipp Preiss - Max Planck Institute of Quantum Optics



Variational Quantum Eigensolvers

- Trial wavefunction with few parameters

$$|\Psi_{\text{trial}}\rangle = U(\vec{\varphi}, \vec{\theta})|\Psi_0\rangle$$

- Evaluate energy functional

$$\mathcal{H} = \sum_{ij} h_{ij}^{(1)} c_i^\dagger c_j + \sum_{ijkl} h_{ijkl}^{(2)} c_i^\dagger c_j^\dagger c_k c_l$$

$$E_{\text{var}}(\vec{\varphi}, \vec{\theta}) = \langle \Psi_{\text{trial}} | H | \Psi_{\text{trial}} \rangle$$

- Minimize $E_{\text{var}}(\vec{\varphi}, \vec{\theta})$ to approximate ground state

G-L Anselmetti et al., New J. Phys. **23** (2021) 113010



Variational Quantum Eigensolvers

- Trial wavefunction with few parameters

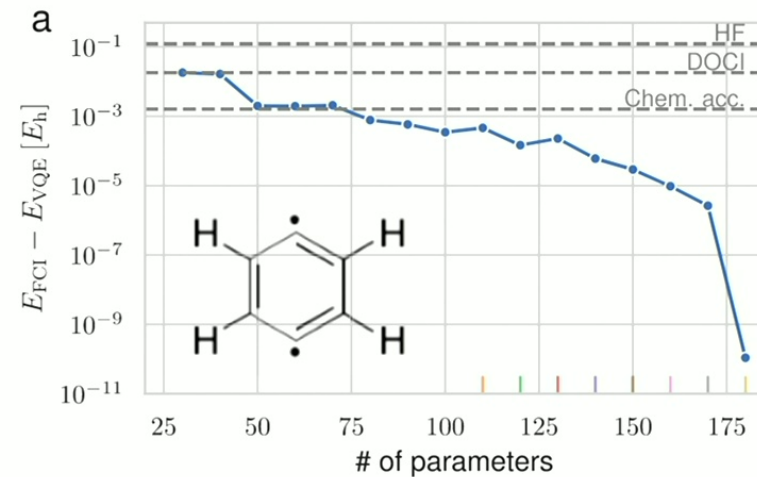
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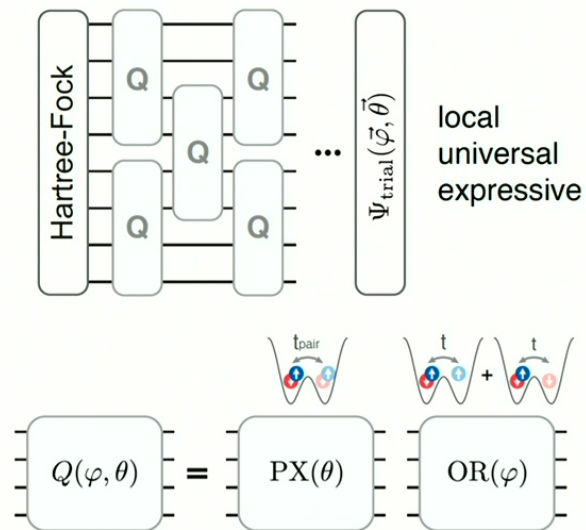


G-L Anselmetti et al., New J. Phys. **23** (2021) 113010



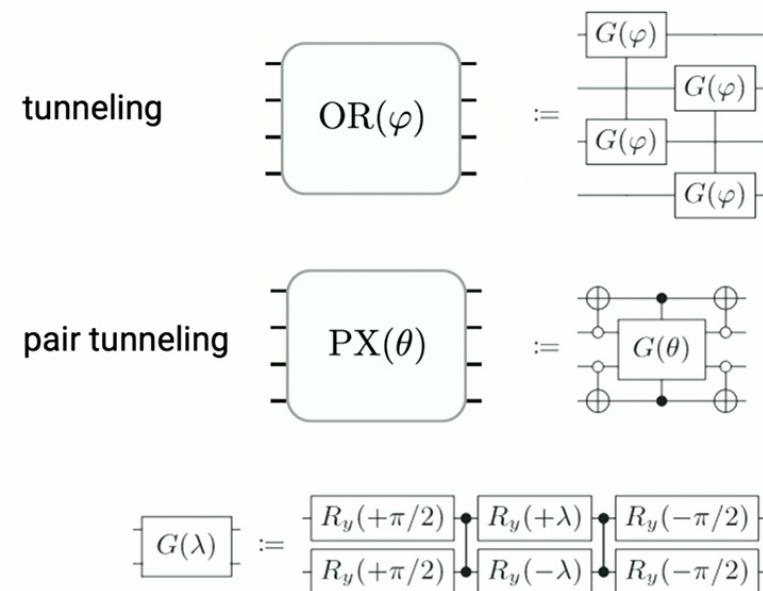
Fermionic algorithms

Quantum number preserving (QNP) fabrics



- Good quantum numbers N, S_z, S
- Universal parametrization of the wavefunction

Spin representation:



G-L Anselmetti *et al.*, New J. Phys. **23** (2021) 113010



Fermion mapping

RESEARCH ARTICLE | PHYSICS | 6



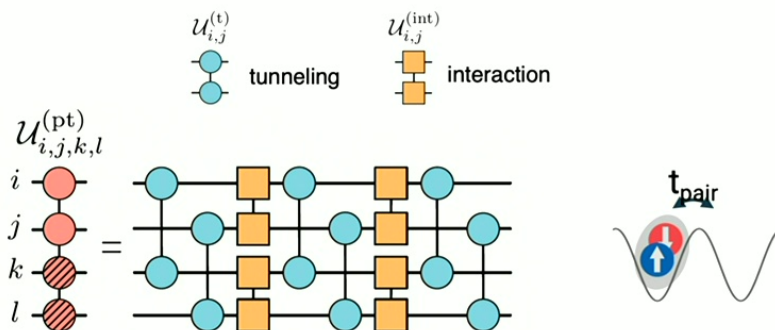
Fermionic quantum processing with programmable neutral atom arrays

D. González-Cuadra , D. Bluvstein, M. Kalinowski, R. Kaubruegger, N. Maskara, P. Naldesi, T. V. Zache , A. M. Kaufman, M. D. Lukin, H. Pichler, B. Vermersch, Jun Ye , and P. Zoller  [Authors Info & Affiliations](#)

Edited by Jean Dalibard, College de France, Paris, France; received March 15, 2023; accepted July 26, 2023

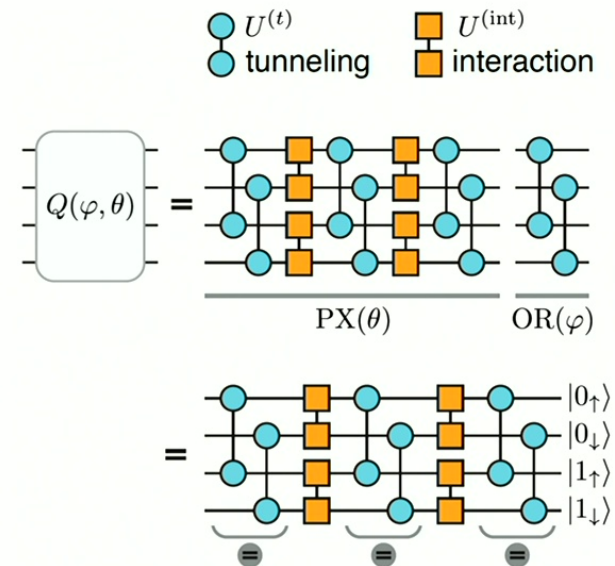
August 22, 2023 | 120 (35) e2304294120 | <https://doi.org/10.1073/pnas.2304294120>

Arbitrary fermionic terms from tunneling and interaction



D. Gonzalez-Cuadra *et al.*, PNAS 120, e2304294120 (2023)

QNP fabric with fermion terms

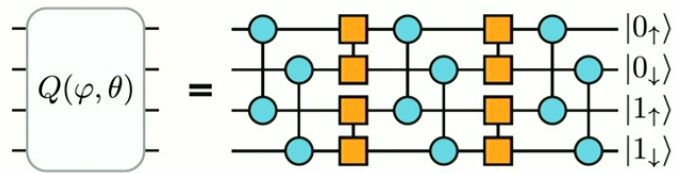


- Tunneling operations with 'locked' parameters
- Depth 5 (c.f. spin scheme: 17 CNOTs + rotations)

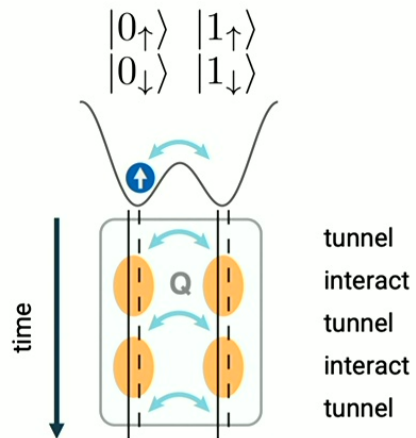


Lattice realization

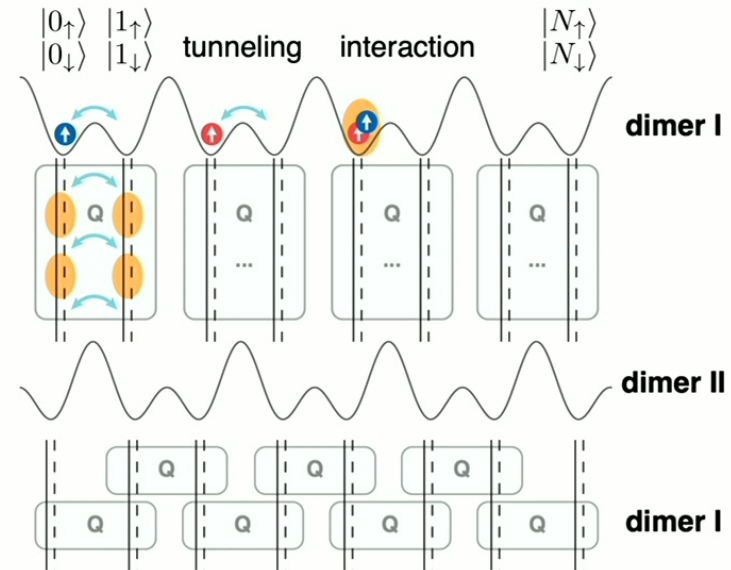
Q-gate representation



Double-well



Superlattice

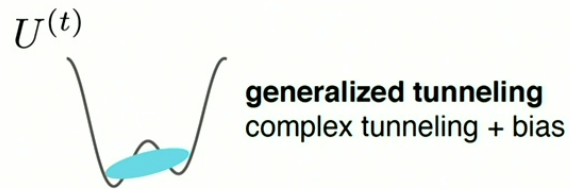


Hubbard superlattice naturally realizes the full QNP fabric

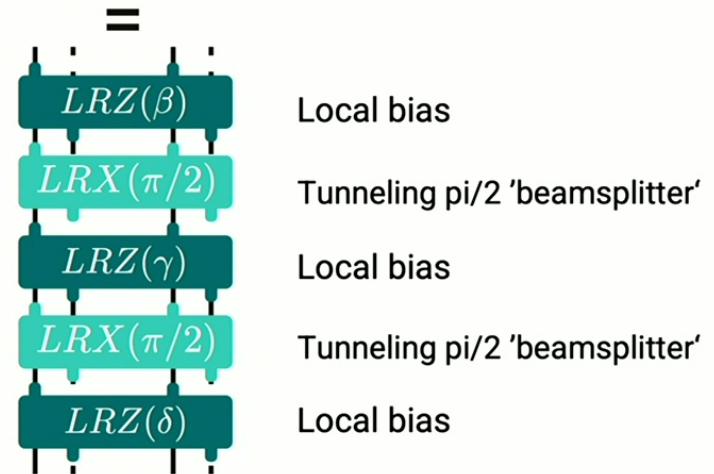
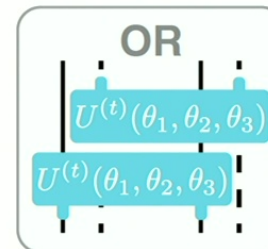


Experimentally friendly $U(t)$

$$U_{i,j}^{(t)}(\vec{\theta}) \equiv e^{-i\left[\frac{\theta_1}{2}(e^{-i\theta_2}c_i^\dagger c_j + \text{H.c.}) + \frac{\theta_3}{2}(n_i - n_j)\right]}$$



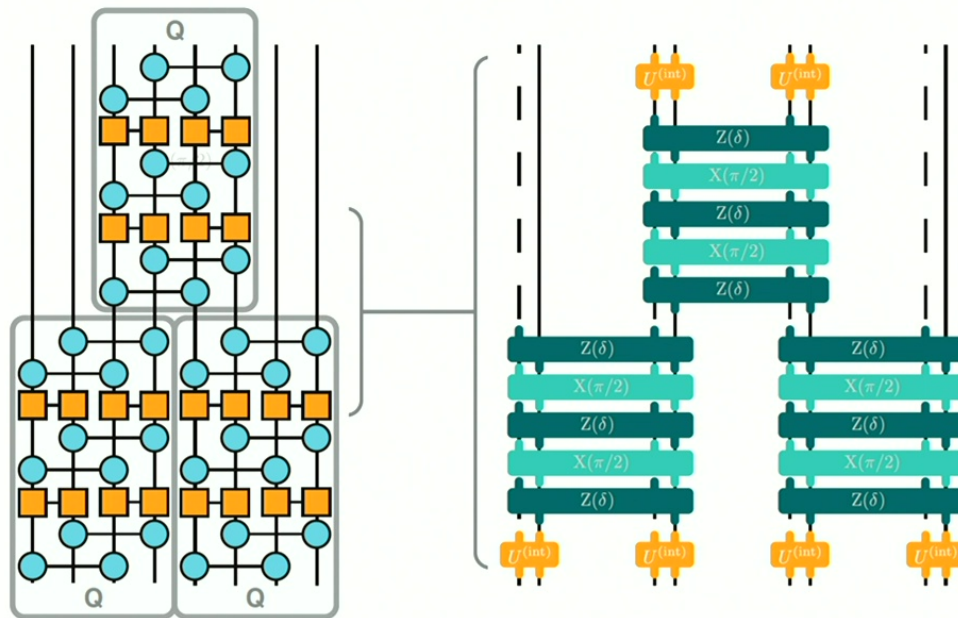
Freedom to choose experimental realization



Z3X2: Three bias and two tunneling pulses



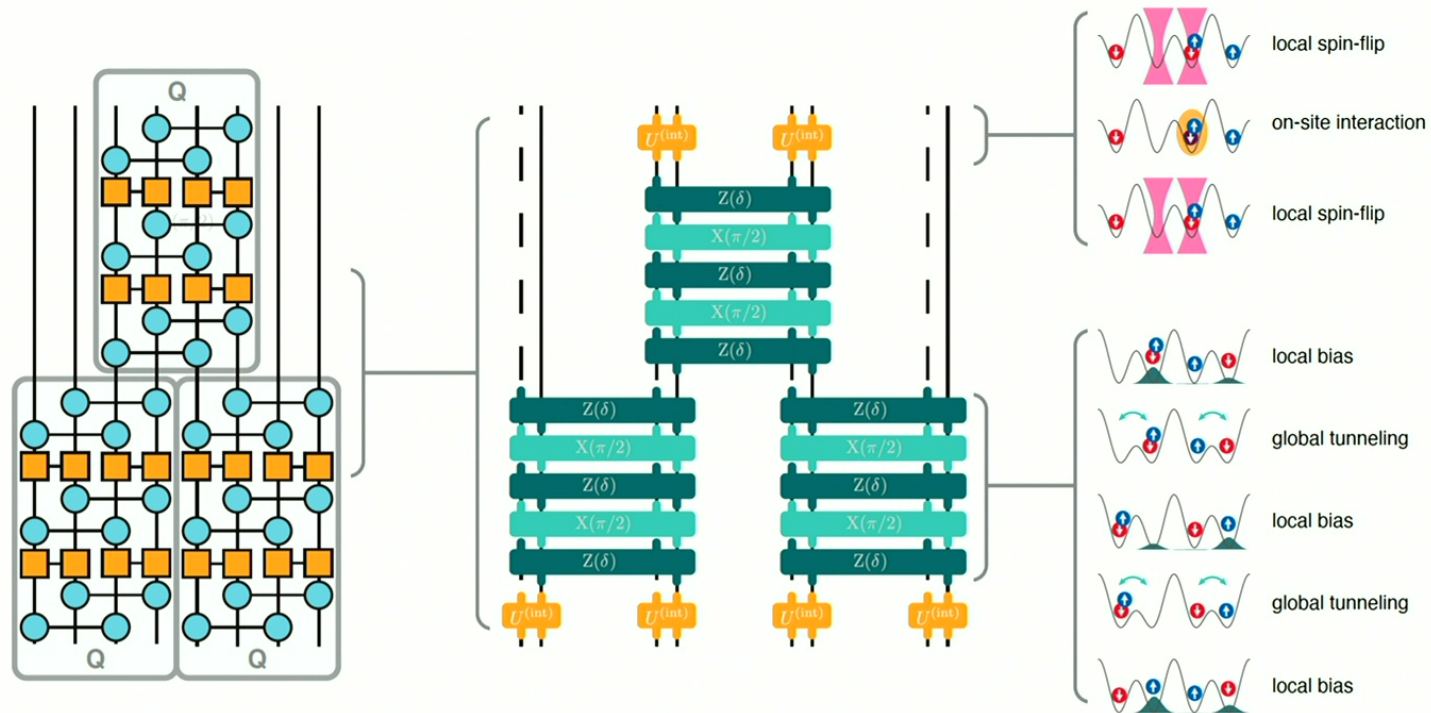
Fermionic circuits



- **Local** bias and interaction
- **Global** tunneling/beamsplitter pulses



Fermionic circuits



- **Local** bias and interaction
- **Global** tunneling/beamsplitter pulses



Measurements in VQE

- Trial wavefunction with few parameters

$$|\Psi_{\text{trial}}\rangle = U(\vec{\varphi}, \vec{\theta})|\Psi_0\rangle$$

- Evaluate energy functional

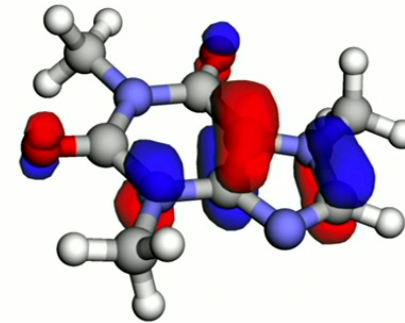
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- Minimize $E_{\text{var}}(\vec{\varphi}, \vec{\theta})$ to approximate ground state

Measuring the energy is extremely challenging

G-L Anselmetti et al., New J. Phys. **23** (2021) 113010



m active spin orbitals

1. Types of terms

- Long-range off-diagonal coherences $\langle c_{\sigma,i}^\dagger c_{\sigma',j}^\dagger c_{\sigma',k} c_{\sigma,l} \rangle$
- Measurements can only access densities $\langle n_{\sigma,i} n_{\sigma',j} \rangle$

2. Number of terms

- Hamiltonian with m^4 correlator terms
- E.g. for $m=100$ need to measure 10^8 (small) quantities



Double Factorization: Coherences

- Approximate H by basis rotations into n_l 'leaves'
- Each leaf is **diagonal in $n_i n_j$**

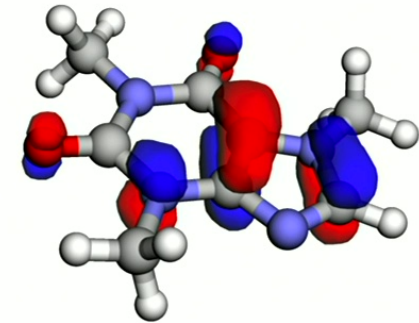
$$\hat{H} \approx \hat{H}_{\text{DF}} = U_0 \hat{p}^{(1)} U_0^\dagger + \sum_{l=1}^{n_l} U_l \hat{p}_l^{(2)} U_l^\dagger$$

$$n_l \leq m(m+1)/2$$

$$\hat{p}^{(1)} = \sum_{i=1}^m h_i \hat{n}_i \quad \hat{p}_l^{(2)} = \sum_{i,j=1}^m h_{i,j}^l \hat{n}_i \hat{n}_j$$

- Only density-density measurements required $\langle n_{\sigma,i} n_{\sigma',j} \rangle$

O. Oumarou, ..., C. Gogolin, arXiv:2212.07957(2022)
E. Hohenstein, ..., R. Parrish, J. Chem. Phys. 158, 114119 (2023)





Double Factorization: Coherences

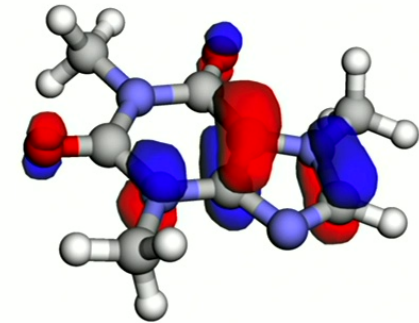
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- Only density-density measurements required $\langle n_{\sigma,i} n_{\sigma',j} \rangle$



Basis rotations U_l from Double Factorization:

- U_l can be implemented by orbital rotations
- Brick-wall structure with linear depth
- Subset of state preparation!

Simple access to off-diagonal coherences

O. Oumarou, ..., C. Gogolin, arXiv:2212.07957(2022)
E. Hohenstein, ..., R. Parrish, J. Chem. Phys. 158, 114119 (2023)



Number of terms

Dealing m^4 terms

- In principle need m^2 different bases

$$\hat{H} \approx \hat{H}_{\text{DF}} = U_0 \hat{p}^{(1)} U_0^\dagger + \sum_{l=1}^{n_l} U_l \hat{p}_l^{(2)} U_l^\dagger$$

$$n_l \leq m(m+1)/2$$

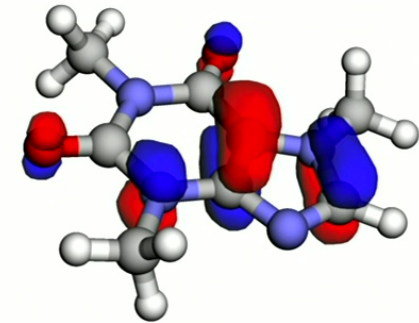
$$\hat{p}_l^{(2)} = \sum_{i,j=1}^m h_{i,j}^l \hat{n}_i \hat{n}_j$$

Double Factorization:

- Minimize n_l for target accuracy
- Conditions U_l for minimal variance
- Automatically assigns shot counts

Shot count reduction

- In practice need $n_l \ll m^2/2$ different bases
- E.g. for HF with $m=16$ orbitals: 16 bases instead of 136
- Reduces shot counts by 1-2 orders of magnitude



O. Oumarou, ..., C. Gogolin, arXiv:2212.07957(2022)
E. Hohenstein, ..., R. Parrish, J. Chem. Phys. 158, 114119 (2023)



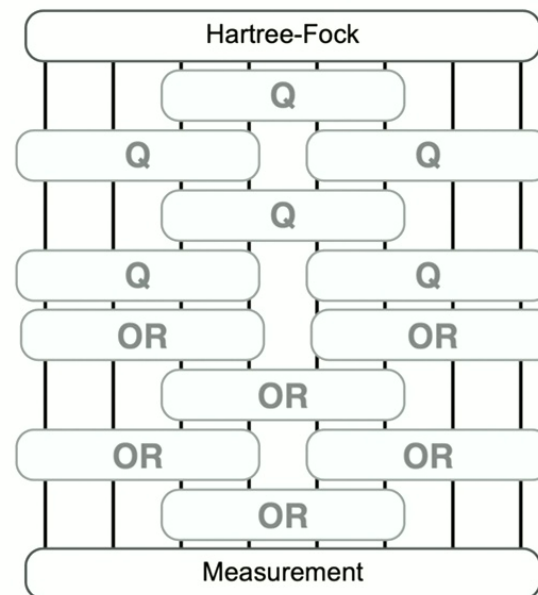
Double factorization

Gate fabric

VQE preparation
QNP fabric
4 layers of Q-gates
alternating dimerization

$\Psi_{\text{trial}}(\vec{\varphi}, \vec{\theta})$ →

Basis rotation
Orbital rotation for l^{th} leaf
Repeat for m_l leaves



- Measure different 'leaves'
- State prep is identical
- Only the final basis rotation changes



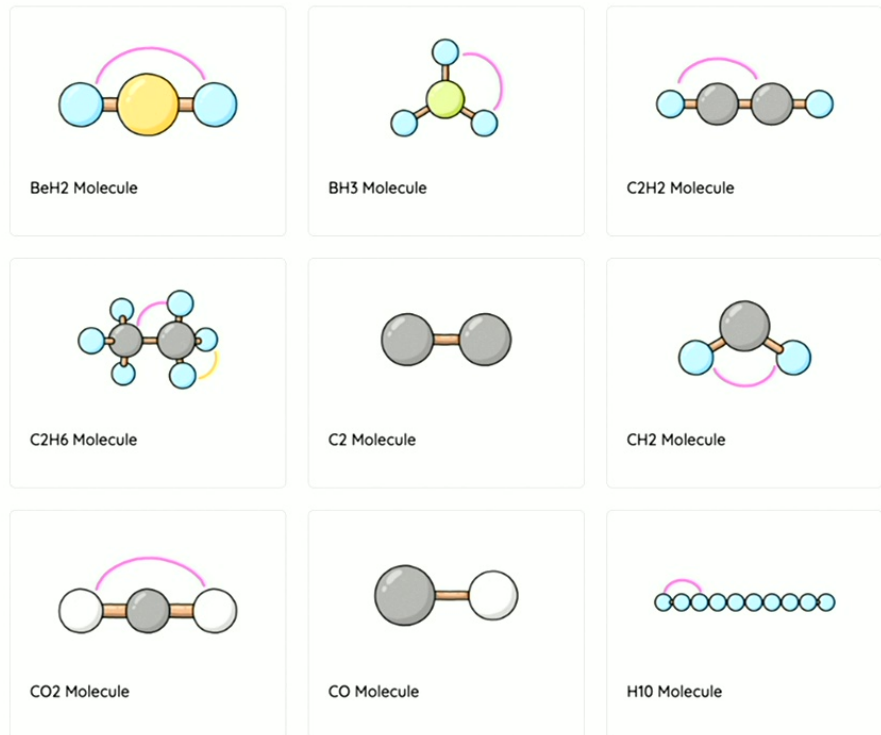
Code integration

```
import pennylane as qml

H, qubits = qml.qchem.molecular_hamiltonian(symbols, coordinates)
print("Number of qubits = ", qubits)
print("The Hamiltonian is ", H)

Number of qubits = 4
The Hamiltonian is (-0.2427450126094144) [Z2]
+ (-0.2427450126094144) [Z3]
+ (-0.042072551947439224) [I0]
+ (0.1777135822909176) [Z0]
+ (0.1777135822909176) [Z1]
+ (0.12293330449299361) [Z0 Z2]
+ (0.12293330449299361) [Z1 Z3]
+ (0.16768338855601356) [Z0 Z3]
```

Qchem (35)





Code integration

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+ (0.1777135822909176) [Z1]
+ (0.12293330449299361) [Z0 Z2]
+ (0.12293330449299361) [Z1 Z3]
+ (0.16768338855601356) [Z0 Z3]

```
Circuit for leaf 6 to be run 41219 times:
0: - HartreeFock(2.00,2.00)
1: - HartreeFock(2.00,2.00)
2: - HartreeFock(2.00,2.00)
3: - HartreeFock(2.00,2.00)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(1.57)-LatticeRX(1.57)
4: - HartreeFock(2.00,2.00)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(1.57)-LatticeRX(1.57)
5: - HartreeFock(2.00,2.00)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(1.57)-LatticeRX(1.57)
6: - HartreeFock(2.00,2.00)
7: - HartreeFock(2.00,2.00)

-LatticeRZ(10.21)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(1.57)-LatticeRX(1.57)
-LatticeRZ(10.21)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(1.57)-LatticeRX(1.57)

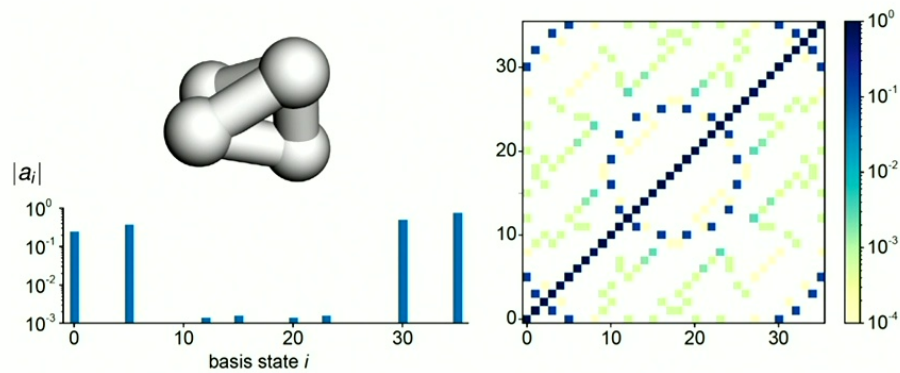
-LatticeRZ(10.21)-Uint(1.10)
-LatticeRZ(10.21)-Uint(1.10)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(4.71)-LatticeRX(1.57)
-LatticeRZ(10.21)-Uint(1.10)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(4.71)-LatticeRX(1.57)

-LatticeRZ(-0.79)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(4.71)-LatticeRX(1.57)
-LatticeRZ(-0.79)-LatticeRZ(-2.36)-LatticeRX(1.57)-LatticeRZ(4.71)-LatticeRX(1.57)
```



Example: Tetrahedral H_4

- Paradigmatic 'strongly correlated' molecule

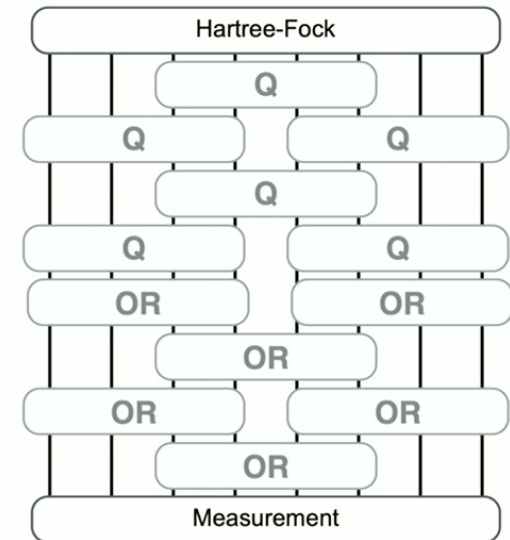


Gate fabric

VQE preparation
QNP fabric
4 layers of Q-gates
alternating dimerization

$$\Psi_{\text{trial}}(\vec{\varphi}, \vec{\theta}) \longrightarrow$$

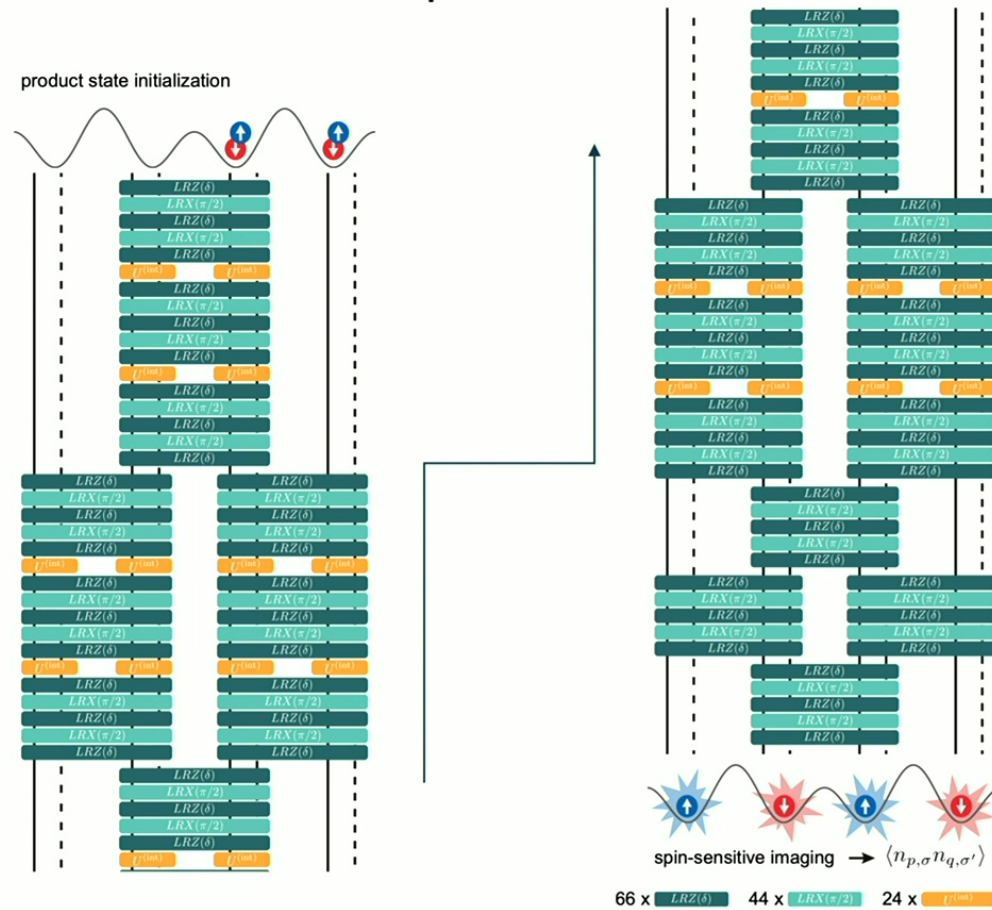
Basis rotation
Orbital rotation for l^{th} leaf
Repeat for m_l leaves



F. Zhang *et al.*, Phys Rev Research **3**, 013039 (2021)



Example: Tetrahedral H_4





Error analysis: H_4

Evaluate precision requirements

- Errors on fundamental LRX, LRZ, Uint gates
- Model static errors and slow fluctuations (circuit-to-circuit)

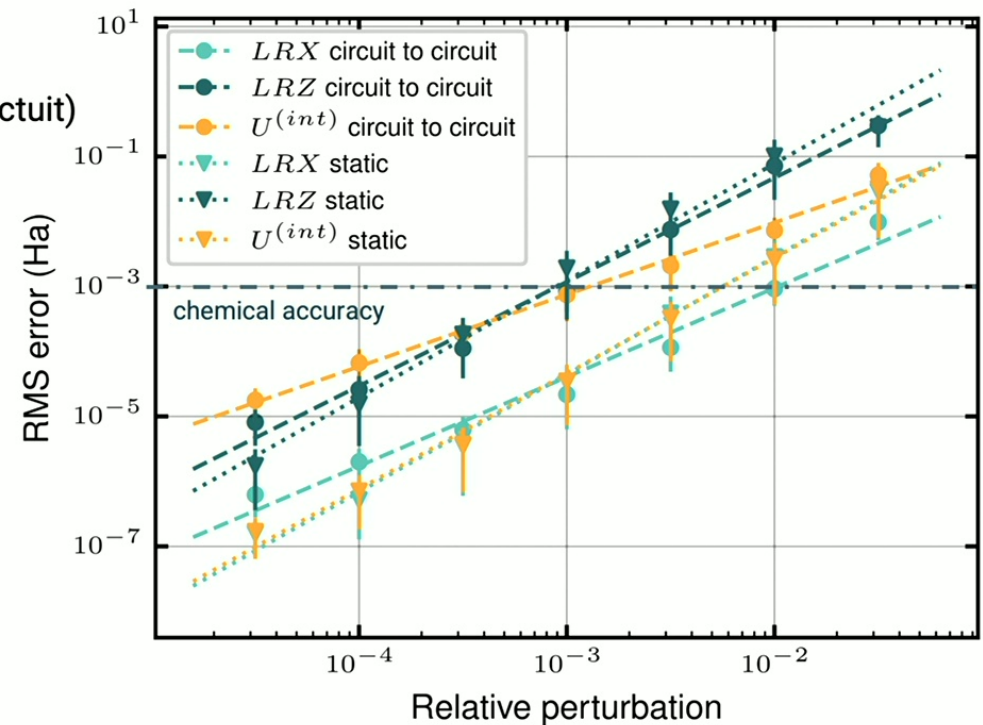
- Distorted H_4 molecule
- 8 modes = 2 double-wells
- Depth 83 in native gates

Chemical accuracy (1mHa) requires

- 150,000 measurements

- $\frac{\delta t}{t} \approx 10^{-2}$

- $\frac{\delta \mu}{\mu} \approx 10^{-3}$

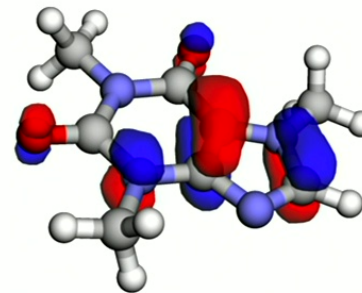




Quantum Chemistry with optical lattices

Requirements for small test molecules

- Fermionic superlattice system in 1D or 2D
- *Local* potential shifting
- *Global* tunneling operations
- *Local* spin-flip for interactions
- Gate errors 10^{-2} to 10^{-3}
- 100k -200k realizations



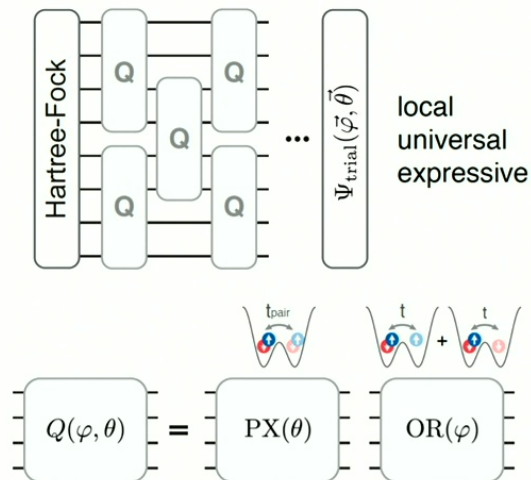
	molecule	active space	basis	RC-DF	layers	shots	depth	qubit depth
#1	H ₄ tetrahedral	(4e, 4o)	cc-pvdz	$n_l = 4$	4	1.0×10^5	83	109
#2	H ₄ tetrahedral	(4e, 4o)	sto-3g	$n_l = 3$	6	1.3×10^5	117	154
#3	H ₄ square	(4e, 4o)	sto-3g	$n_l = 7$	7	4.9×10^5	134	175
#4	H ₄ square	(4e, 4o)	sto-3g	$n_l = 7 + \text{FFF}$	7	3.0×10^5	134	175
#5	HF distance 1Å	(10e, 6o)	sto-3g	$n_l = 16 + \text{FFF}$	5	5.5×10^5	110	141

Concrete roadmap for realization of a molecular wavefunction with ultracold fermions



Open questions

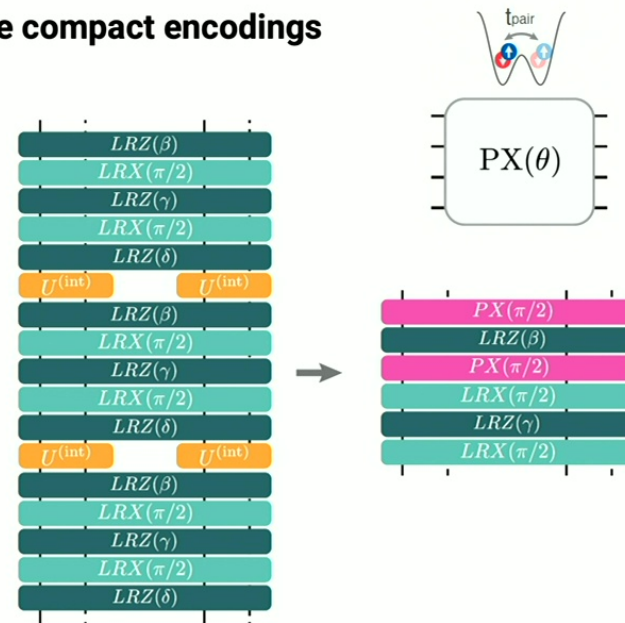
Gate counts (fermions vs. qubits)



- Here: Circuit structure *fixed* for fermions and qubits
- No scaling advantage

Alternative fermionic ansatz: Q. Li, ... A. Bayat Phys. Rev. Res. **5**, 043175 (2023)

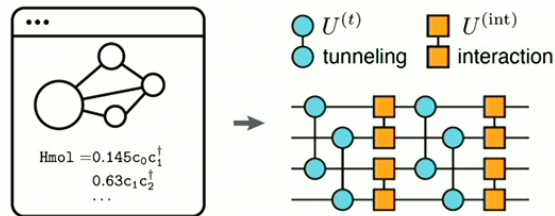
More compact encodings



Ongoing collaboration with L. Escalera, B. Schiffer, I. Cirac



Summary



1. Mapping of variational ansatz for fermions
2. End-to-end workflow from Hamiltonian to pulse sequence
3. Noise limits on gates
4. Classical pre-optimization & double factorization

Our work: F. Gkritis, ..., P. Preiss, arXiv 2409.05663 (2024)

Next steps: Towards hardware implementations

- Precise control of motional states



- Local and global control

- Control over interactions

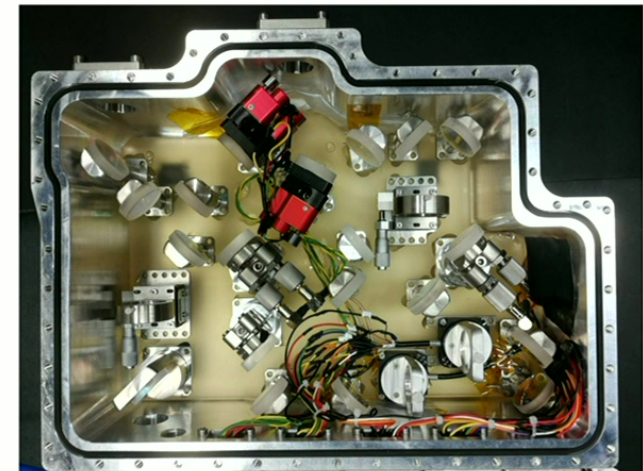
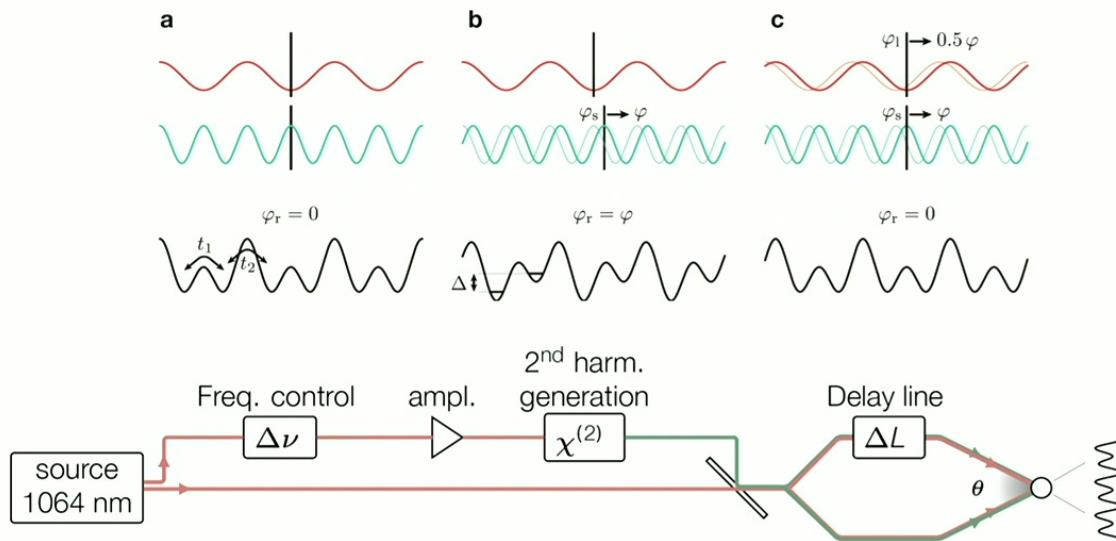




Optical Superlattices (Li 1.0)

Bichromatic xy-(super)lattices in evacuated setups with tunable relative phase

- Large homogeneous system
- High phase stability

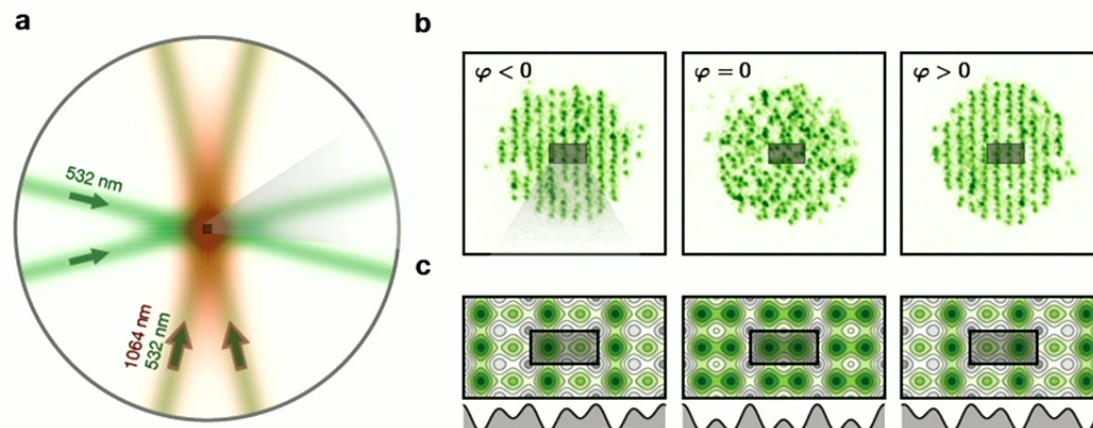


Dominik Bourgund, PhD Thesis, LMU Munich (2023)



Optical Superlattices (Li 1.0)

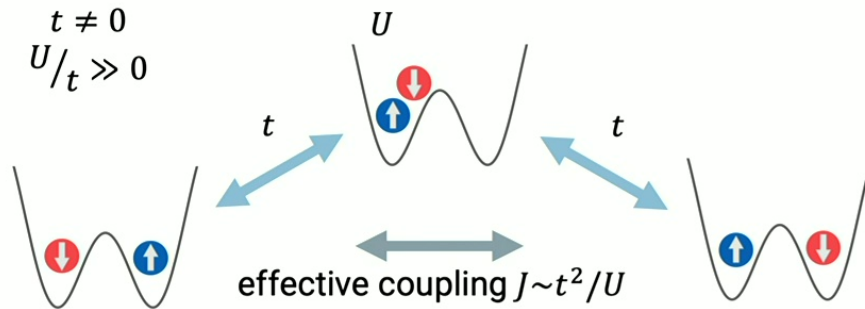
Bichromatic xy-(super)lattices in evacuated setups with tunable relative phase



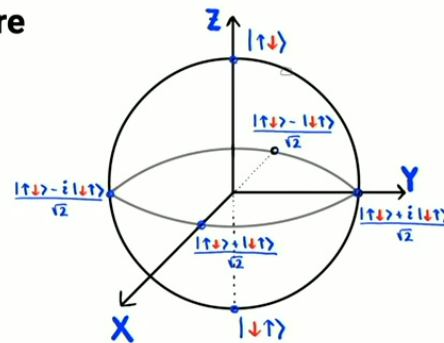


Two-qubit collisional gates

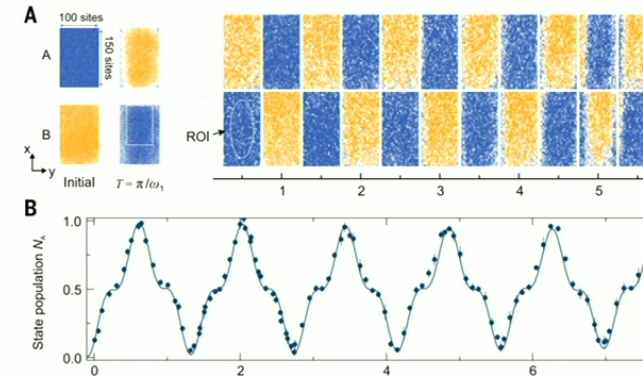
Superexchange coupling



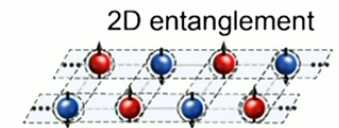
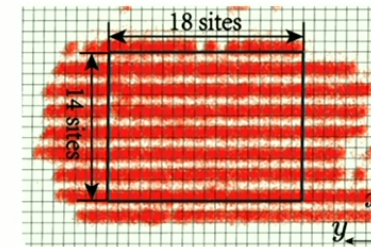
Singlet/Triplet Bloch sphere



Realization by Jan Wei Pan group



1250 atom pairs
99.3(1)% fidelity



B. Yang, ..., J.-W. Pan, Science **369** 550 (2020)
W.Y. Zhang...J.-W. Pan: Arxiv: 2210:02936 (2022)

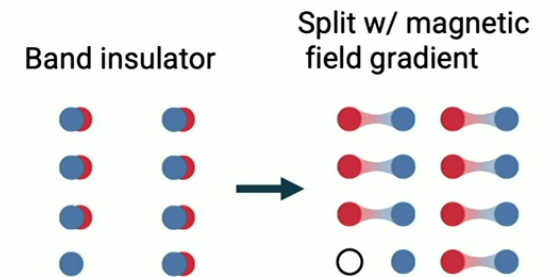
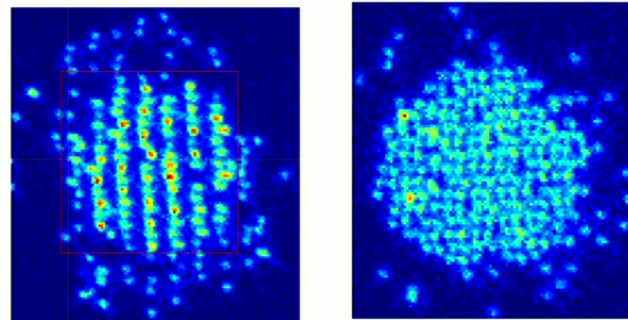


Fermionic Quantum Processing

State preparation

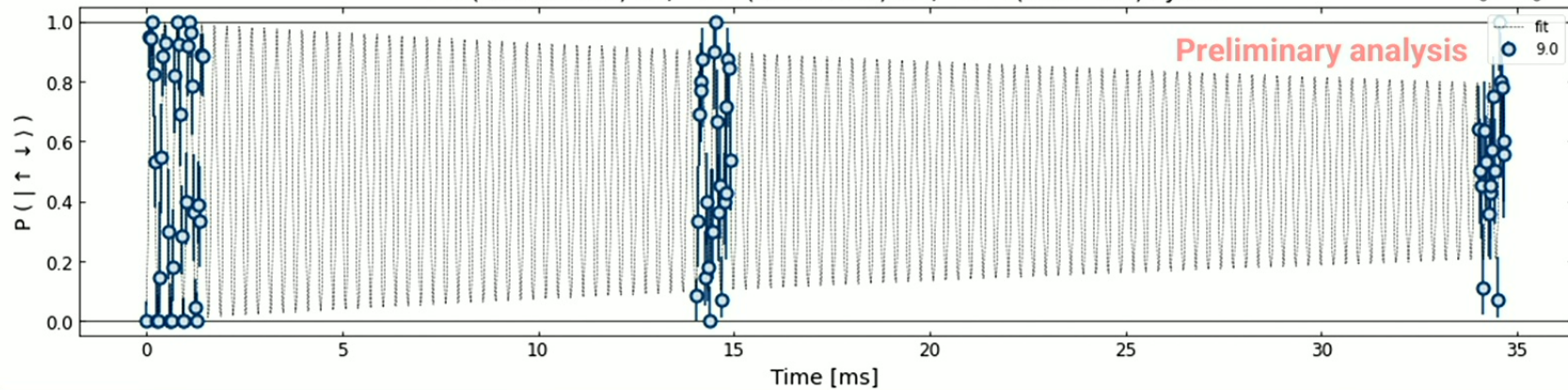
- One atom per site
- Total S_z per double-well = 0

Post-select with full spin/charge resolution



SWAP Rabi oscillations

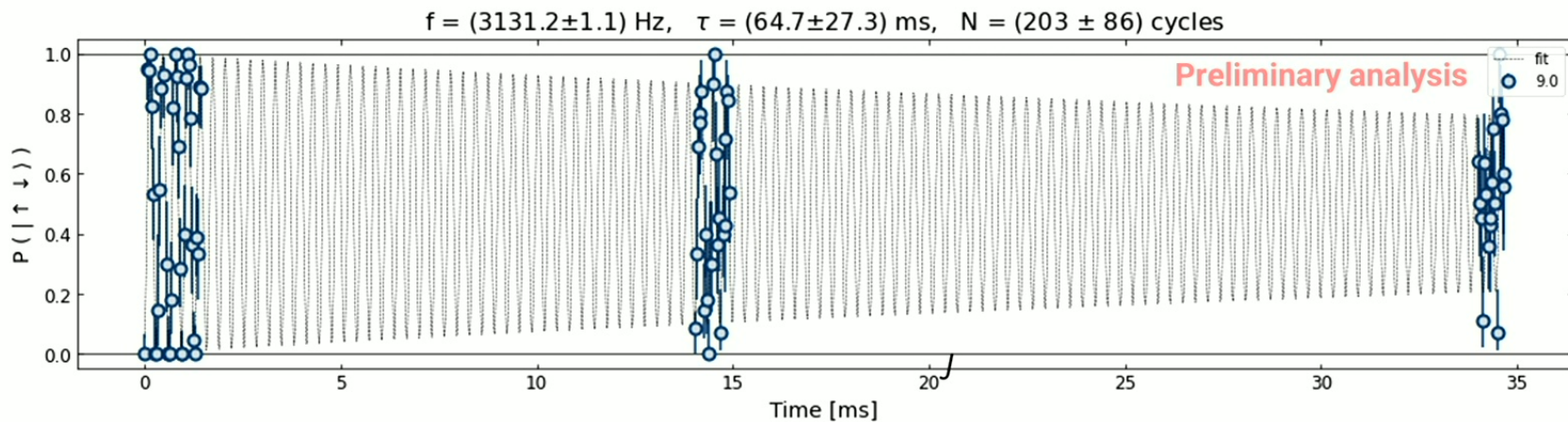
$f = (3131.2 \pm 1.1) \text{ Hz}$, $\tau = (64.7 \pm 27.3) \text{ ms}$, $N = (203 \pm 86) \text{ cycles}$



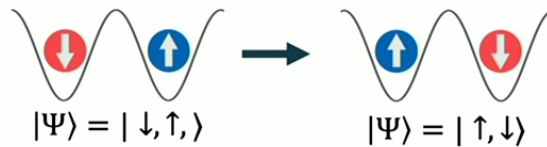


Fermionic Quantum Processing

SWAP Rabi oscillations

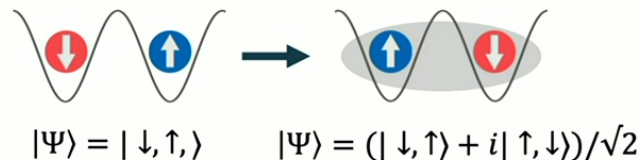


π pulse: SWAP



SWAP fidelity $F_\pi = 99.7(1)\%$ [PRELIMINARY]

$\pi/2$ pulse: $\sqrt{\text{SWAP}}$



Record entangling gate fidelities possible

Current two-qubit gate records:

Evered, ..., Lukin, *Nature* **622**, 268–272 (2023)

Bing-Shiun Tsai, ..., Endres, *arXiv:2407.20184* (2024)



Summary

Simulating quantum chemistry with ultracold fermions

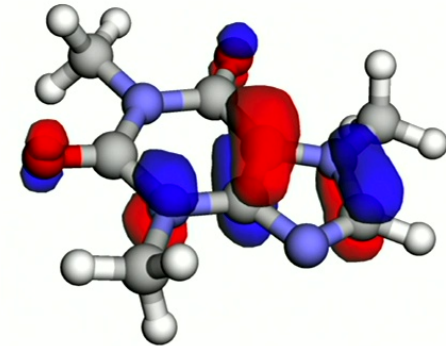
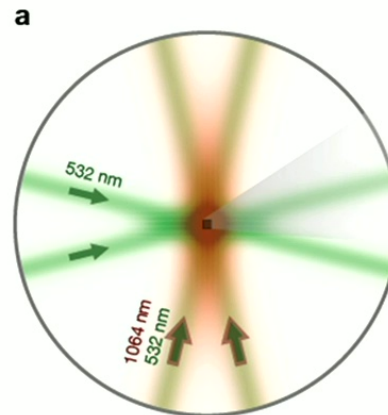
- Fermionic quantum circuits
- Preparing chemical wavefunctions in superlattices

Superlattice collisional gates

- Highly stable optical potentials
- >99% fidelity entangling gates on ~50 atoms

New machines

- UniRand: Random unitaries in optical lattices
- FermiQP: Hybrid analog-digital simulation
- Fast lattice cooling techniques



See also
Poster by **Luca Muscarella**



Thank you for your attention

