Variable particle number on a quantum computer

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Outline

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Concept

Quantum Simulation Algorithm

1. Choose a codification for the states of the system
2. Initiate the quantum computer memory to $|\psi(0)\rangle$
3. Decompose the unitary $U(t) = \exp(-itH/\hbar)$ into elementary gates and evolve $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
4. Measure expectation value $\langle\psi(t)|\hat{O}|\psi(t)\rangle$

In this talk

Particles in the QC (instead of fields, so no Kogut-Süsskind today)

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Particles in the QC (instead of fields, so no Kogut-Süsskind today)

Simple calculations at hand

Example: Triply heavy baryons
with QCD Cornell potential

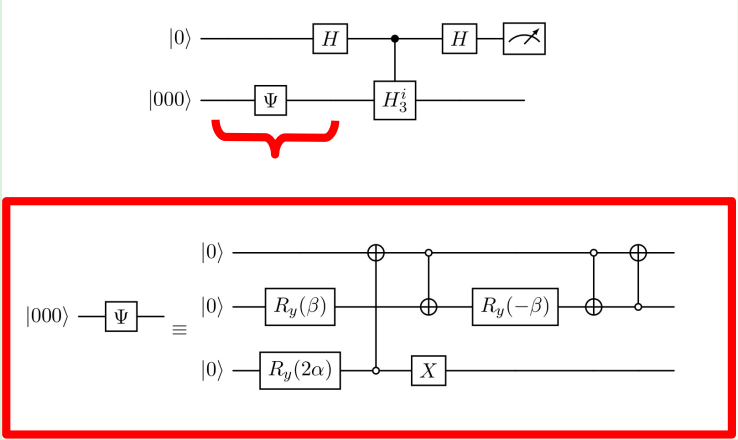
$$V(r) = \frac{\alpha_s}{r} + \sigma r$$

Computed by
Nicolás Martínez de Arenaza,
2024 graduating cohort

Baryon (composition)	$\Omega(bbb)$	$\Omega(bbc)$	$\Omega(bcc)$	$\Omega(ccc)$
This work	14270 ± 340	11210 ± 350	8100 ± 350	4940 ± 340
Variational pNRQCD	14700 ± 300	11400 ± 300	8150 ± 300	4900 ± 250
Coulomb variational	14370 ± 80	11190 ± 80	7980 ± 70	4760 ± 60
QCD sum rules	13280 ± 100	10460 ± 110	7443 ± 150	4670 ± 150
Quark counting	14760 ± 180	11480 ± 120	8200 ± 90	4925 ± 90
MIT bag model	14300	11200	8030	4790

With very few qubits (quantum computer = small diagonalizer)

State preparation & measurement of Hamiltonian



These may be simple calculations but already working...

Outline

Particle into a “register” of several qubits

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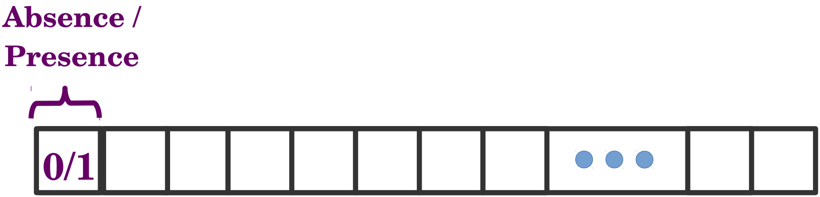

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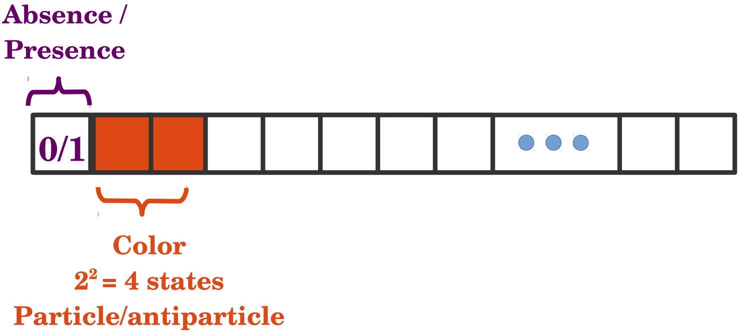

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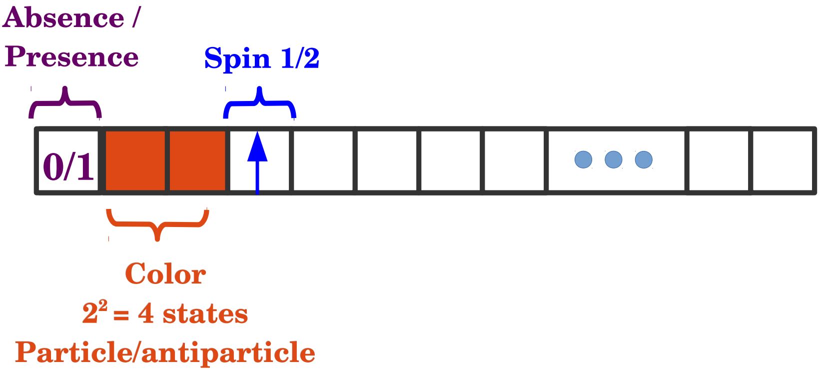

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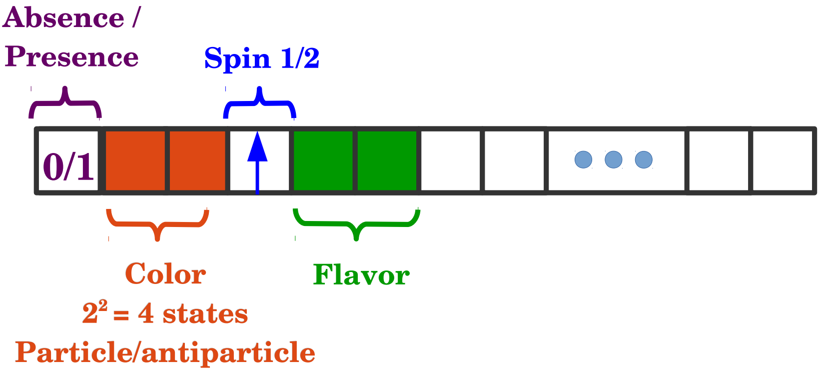
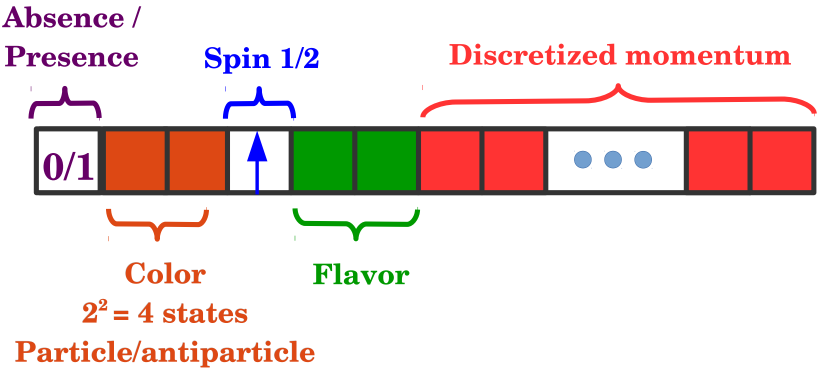
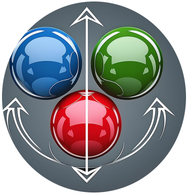


Momenta: N_p values $\rightarrow \log_2 N_p$ qubits



Particle into a "register" of several qubits

- 8^3 momentum grid $\Longrightarrow$ 9 momentum qubits $\Longrightarrow$ 15 qubits/quark
- Currently: IBM Eagle Chips with 127 qubits
- Already in business for quark model-size computations



Outline

Fermion anticommuting creator/destructor operators

$$\left\{b_p^\dagger, b_q\right\} = \delta_{p,q}\,\mathbb{I} \quad \left\{b_p^\dagger, b_q^\dagger\right\} = \left\{b_p, b_q\right\} = 0$$

- Generate Fock space $\{|\Omega\rangle, |p\rangle, |q\rangle, \ldots, |pq\rangle, \ldots\}$

$$b_p^\dagger b_q^\dagger |\Omega\rangle = |pq\rangle, \quad b_k |pq\rangle = \delta_{pk}|q\rangle - \delta_{qk}|p\rangle$$

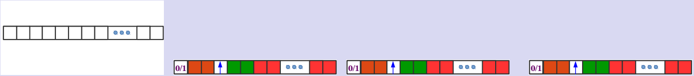
- Creation of two-equal excitations forbidden

$$b_p^\dagger b_p^\dagger |\Omega\rangle = -b_p^\dagger b_p^\dagger |\Omega\rangle \to b_p^\dagger b_p^\dagger |\Omega\rangle = 0$$

Think of constructor/destructor methods in object programming

jth-Register implementation

$$b_{q,j}^{(n)\dagger} = \mathcal{A}_{j\leftarrow j-1} \cdot \mathbb{P}_0^{(n-j)} \otimes \left(\mathfrak{C}_{10} \otimes \mathfrak{s}_q^{\dagger}\right)_j \otimes \mathbb{P}_{j-1}^{(j-1)}$$



jth-Register implementation

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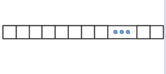

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Set / scrap operators

$$\mathfrak{s}_q^\dagger \quad / \quad \mathfrak{s}_q$$

set / scrap the quantum numbers

Apply them to

the first unoccupied / last occupied particle register

Control operators on the presence qubit

$$
\begin{aligned}
\mathfrak{C}_{00}|0\rangle &= |0\rangle \quad \text{Empty} \to \text{Empty}\\
\mathfrak{C}_{11}|1\rangle &= |1\rangle \quad \text{Full} \to \text{Full}\\
\mathfrak{C}_{10}|0\rangle &= |1\rangle \quad \text{Empty} \to \text{Full}\\
\mathfrak{C}_{01}|1\rangle &= |0\rangle \quad \text{Full} \to \text{Empty}
\end{aligned}
$$

With usual computer

`if ... then ...`

`else ... endif`

`switch ... case`

Others zero

Wait... zero on a quantum computer?

Everything exponentiated later, $\mathbb{I}$ to the rescue!

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Projector over j occupied registers

$\mathbb{P}_j^{(n)}$ constructible from those control operators

$$\mathbb{P}_j^{(n)} = \left[(\ldots)_n \otimes \ldots \otimes (\mathfrak{C}_{00} \otimes \mathfrak{i})_{j+1}\right] \otimes \left[(\mathfrak{C}_{11} \otimes \mathfrak{i})_j \otimes \ldots \otimes (\ldots)_1\right] \ ,$$

(Anti)symmetrize only the last added particle

jth-Register implementation

$$b^{(n)\dagger}_{q,j} = \underbrace{\mathcal{A}_{j\leftarrow j-1}}_{\text{Step antisymmetrizer}} \cdot \mathbb{P}_0^{(n-j)} \otimes \left(\mathfrak{C}_{10} \otimes \mathfrak{s}^\dagger_q\right)_j \otimes \mathbb{P}_{j-1}^{(j-1)}$$

Step (anti)symmetrizer

Example: add 1 particle to a memory already containing 1 particle:

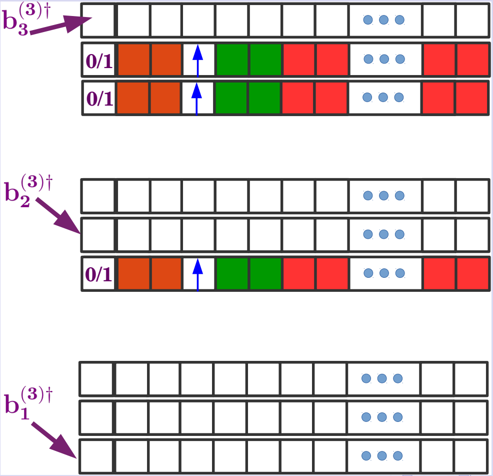
$$b_{q_1}^{(2)\dagger} = b_{q_1,1}^{(2)\dagger} + \underbrace{\frac{1}{\sqrt{2}}\left(\mathbb{I}\otimes\mathbb{I} - \mathcal{P}_{21}\right)}_{\equiv \mathcal{A}_2} b_{q_1,2}^{(2)\dagger} \, .$$

More generally

$$\mathcal{A}_{n\leftarrow n-1} = \frac{1}{\sqrt{n}}\left(\mathbb{I}^{\otimes n} - \mathcal{P}_{n(n-1)} - \mathcal{P}_{n(n-2)} - \ldots - \mathcal{P}_{n2} - \mathcal{P}_{n1}\right)$$

All-register implementation

$$b_q^{(n)\dagger} = \sum_j b_{q,j}^{(n)\dagger}$$



We would like $\left\{ b^{(n)}_{q_1}, b^{(n)\dagger}_{q_2} \right\} = \delta_{q_1,q_2}$

Instead we get, with boundary condition $b^\dagger|n\rangle = 0$,

Boundary term @ full memory

$$\left\{ b^{(n)}_{q_1}, b^{(n)\dagger}_{q_2} \right\} = \overbrace{\delta_{q_1,q_2} \left(\mathfrak{C}_{00} \otimes \mathfrak{i}\right)_n \otimes \mathbb{I}^{(n-1)}}^{canonical\ up\ to\ n-1\ particles} + \underbrace{A_{n\leftarrow n-1} \cdot \left(\mathfrak{C}_{11} \otimes \mathfrak{s}^\dagger_{q_1} \mathfrak{s}_{q_2}\right)_n \otimes \mathbb{P}^{(n-1)}_{n-1} \cdot A_{n\leftarrow n-1}}_{\text{finite, full memory with n}}$$

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Example: Number operator for bosons

$$N^{(n)} = \sum_p \sum_{j,j'} a^{(n)\dagger}_{p,j} a^{(n)}_{p,j'}$$

$$= \sum_j \mathcal{S}_{j\leftarrow j-1} \cdot \mathbb{P}_0^{(n-j)} \otimes \left(\mathfrak{C}_{11} \otimes \sum_p \mathfrak{s}^\dagger_p \mathfrak{s}_p \right)_j \otimes \mathbb{P}^{(j-1)}_{j-1} \cdot \mathcal{S}_{j\leftarrow j-1}$$

Aply to symmetric j-particle state:

$$N^{(n)}|\Omega\rangle_n \dots |\Omega\rangle_{j+1}(\underbrace{|1p_j\rangle_j} \dots |1p_1\rangle_1)_S = \underbrace{j}\, |\Omega\rangle_n \dots \left(|1p_j\rangle_j \dots |1p_1\rangle_1\right)_S$$

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Back to step (anti)symmetrizers: not invertible

- Want unitary operations on a Quantum Computer

- But $\mathcal{A}_{n \leftarrow n-1}$ not invertible

where did this symmetric state come from?

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Step (anti)symmetrizers are projectors

Which gnomon cast the shadow?

Solution: ordered memory

Wanted: invertible $\hat{\mathcal{A}}_{j\leftarrow j-1}$,

$$\begin{aligned} b^{(n)\dagger}_{p,j} &= \mathcal{A}_{j\leftarrow j-1}\cdot \mathbb{P}_0^{(n-j)}\otimes\left(\mathfrak{C}_{10}\otimes\mathfrak{s}^\dagger_p\right)_j\otimes\mathbb{P}^{(j-1)}_{j-1} \\ &\equiv \hat{\mathcal{A}}^\dagger_{j\leftarrow j-1}\cdot \mathbb{P}_0^{(n-j)}\otimes\left(\left(\mathfrak{C}_{10}\otimes\mathfrak{s}^\dagger_p\right)_j\otimes\mathbb{P}^{(j-1)}_{j-1}\right)_{f,ord}\cdot\hat{\mathcal{A}}_{j\leftarrow j-1}, \end{aligned}$$

$$|\Omega\rangle_j\left(|1p_{j-1}\rangle_{j-1}\cdots|1p_1\rangle_1\right)_{\mathcal{A}} \xrightarrow{\hat{\mathcal{A}}^\dagger_{j\leftarrow j-1}} |\Omega\rangle_j\left(|1p_{j-1}\rangle_{j-1}\cdots|1p_1\rangle_1\right)_{\mathcal{A}}$$

(do nothing)

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(antisymmetrize from "last is largest").

(Similar to Abrams & Lloyd, PRL 79 2586, 1997)

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Solution: ordered memory

From (anti)symmetric to ordered *Locate the Largest* algorithm

Outline

1. Foreword
2. Onto field theory: encoding particles
3. Encoding canonical operators
   - Creation (destruction) operators
   - (Anti)commutation rules
4. Evolution operators
   - Free evolution
   - Exponentiating interaction terms
5. Outlook

Evolution from free Hamiltonian part

- $\mathcal{U}_{11}^{b}\left(\Delta t\right) = \exp\left(-i\Delta t \sum_{q} E_q a_q^{(n)\dagger} a_q^{(n)}\right)$
- Exponent similar to number operator
- Conserved particle number(no $\mathfrak{C}_{10}$ or $\mathfrak{C}_{01}$)
- Chemical potential enters here $E \to E \pm \mu$ (embarrassingly trivial)

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Evolution from free Hamiltonian part

Exponentiate $a^{(n)\dagger}_{q,j'} a^{(n)}_{q,j}$ using idempotency of projectors & commuting symmetrizers

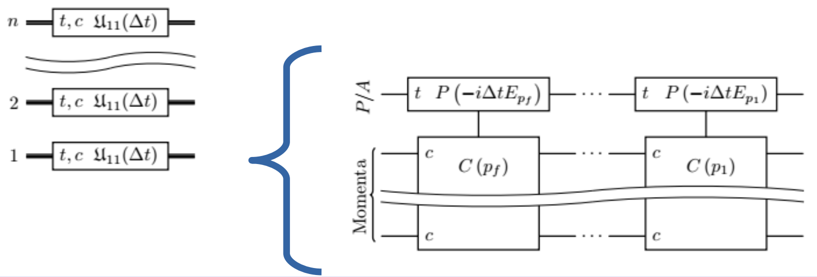
Free evolution

$$\mathcal{U}^{f}_{11}\left(\Delta t\right) = \mathbb{P}^{(n)}_0 + \sum_{i=1}^{n} \mathbb{P}^{(n-i)}_0 \prod_{k=i}^{1} \otimes \left(\mathfrak{C}_{11} \otimes \mathfrak{U}_{11}\left(\Delta t\right)\right)_k$$

with $\mathfrak{U}_{11}(\Delta t) \equiv \exp\left[-i\Delta t \sum_q E_q \mathfrak{s}^{\dagger}_q \mathfrak{s}_q\right]$ directly implementable

Individual particle propagation

Schematic circuit



- Left: Each particle register evolves separately
- Right: Within a register, the phase rotating with the energy is controlled by the momentum qubits

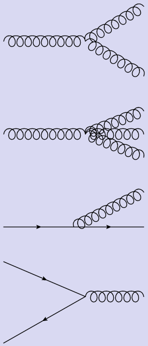
Full Hamiltonian $H = H_2 + H_3 + H_4 \dots$

Would like to factorize: $U = U_2 \times U_3 \times U_4$ but. . .

Baker-Campbell-Hausdorff rule for noncommuting exponents

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\dots}$$

$$\prod_I e^{-itH_I} \neq e^{-it\sum_I H_I}$$



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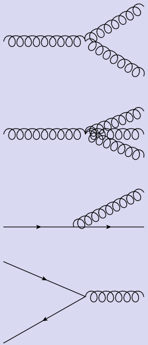


$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\ldots}$$

$$\prod_l e^{-itH_l} \neq e^{-it\sum_l H_l}$$

Expansion with a controllable error

Trotter decomposition

$$\lim_{r\to\infty}\left(\prod_l e^{-iH_l t/r}\right)^r = e^{-it\sum_l H_l}$$

- BCH formula to 1st order $\implies$

$$e^{-iHt/r} - \prod_l e^{-iH_l t/r} = \frac{1}{2}\underbrace{\left(\frac{t}{r}\right)^2}_{small\ \ param.}\sum_{l<l'}[H_l, H_{l'}] + h.o.$$

Expansion with a controllable error

- With $\max_l ||H_l|| = h$, accuracy ϵ requires

$$r = \mathcal{O}\left(\frac{{n_q}^{2k} h^2 t^2}{\epsilon}\right)$$

Trotter steps

- n_q^k Hamiltonian terms give a gate complexity

$$L = \mathcal{O}\left(\frac{{n_q}^{3k} h^2 t^2}{\epsilon}\right)$$

A complexity polinomial in $n_{\text{qubits}} \rightarrow$ efficient!

Comparison to Born series

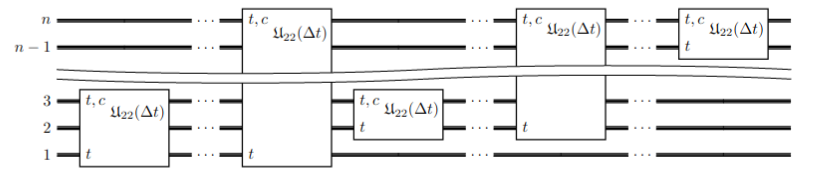
Born: $$V \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V \ldots$$

Trotter: $V \; H_0 \; V \; H_0 \ldots$

Typical term I: momentum exchange

Two particles interact and momentum, but not particle number, changes

Typical term I: momentum exchange



Typical term I: momentum exchange

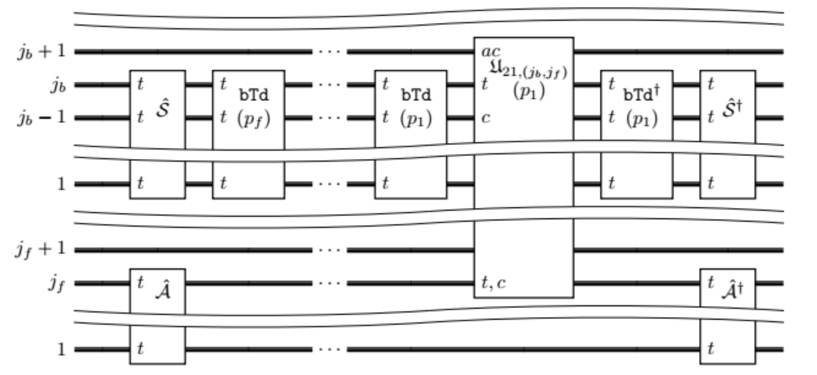
$$\mathcal{U}^{f}_{22}(\Delta t) = \mathbb{P}_0^{(n)} + \mathbb{P}_1^{(n)} + \sum_{j=2}^{n-1} \mathbb{P}_0^{(n-1-j)} \otimes \left\{ (\mathfrak{C}_{11})^{\otimes j} \right\} \left\{ \prod_{k=1}^{j} \prod_{l=1+k}^{j+1} \underbrace{\mathfrak{U}_{22,(l,k)}(\Delta t)} \right\},$$

$$\exp\left(-i2\Delta t \sum_{\xi} \lambda_{\xi} \left\{ \left(\sum_p \mathfrak{s}^{\dagger}_{p+\xi\Delta} \mathfrak{s}_p \right)_l \otimes \left(\sum_q \mathfrak{s}^{\dagger}_{q} \mathfrak{s}_{q+\xi\Delta} \right)_k + \left(\sum_q \mathfrak{s}^{\dagger}_{q} \mathfrak{s}_{q+\xi\Delta} \right)_l \otimes \left(\sum_p \mathfrak{s}^{\dagger}_{p+\xi\Delta} \mathfrak{s}_p \right)_k \right\} \right),$$

Typical term II: Particle splitting

Both particle momentum and particle number change

Typical term II: Particle splitting



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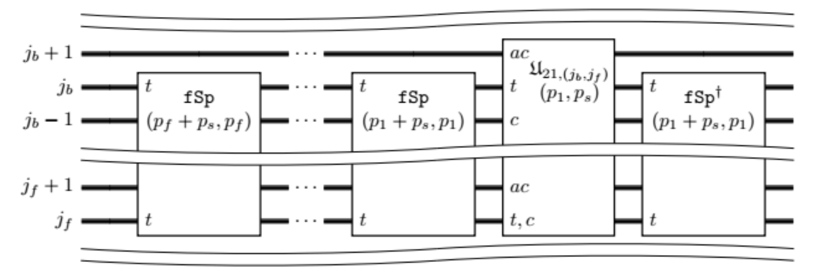

Typical term II: Particle splitting. Fermion→fermion+boson

$$\mathcal{U}_{21}(\Delta t,\lambda) = \prod_{j_b,j_f=1} \Big(\mathbb{I}^{(n)} - \mathbb{P}_0^{(n_b-j_b)} \otimes \mathbb{I} \otimes \mathbb{P}_{j_b-1}^{(j_b-1)} \otimes \mathbb{P}_{j_f}^{(n_f)} + \hat{\mathcal{S}}^\dagger_{j_b\leftarrow j_b-1}\hat{\mathcal{A}}^\dagger_{j_f\leftarrow j_f-1} \cdot \prod_s \left[\mathtt{cbX}^\dagger_{j_b}(s)\cdot \mathfrak{U}_{21,(j_b,j_f)}(s;\lambda,\Delta t)\cdot \mathtt{cbX}_{j_b}(s)\right]\cdot \hat{\mathcal{A}}_{j_f\leftarrow j_f-1}\hat{\mathcal{S}}_{j_b\leftarrow j_b-1}\Big) + \mathcal{O}\left(\Delta t^2\right)$$

$$\mathfrak{U}_{21,(j_b,j_f)}(s;\lambda,\Delta t) = \prod_r \Big(\mathtt{fSp}^\dagger_{(j_b,j_f)}(m,r)\cdot \mathbb{P}_0^{(n_b-j_b)} \otimes \left\{ {\mathfrak{C}_{11}}^{\otimes j_b-1} \otimes {\mathfrak{C}_{00}}^{\otimes j_f+1}\right\} \left\{\mathfrak{U}_{21,(j_b,j_f)}(r,s;\lambda,\Delta t)\right\} \otimes \mathbb{P}_{j_f-1}^{(j_f-1)} \cdot \mathtt{fSp}_{(j_b,j_f)}(m,r)\Big)$$

SWAP and eXchange

To have largest P at the front and to ensure Pauli exclusion
(before creating fermion with $|p\rangle$, try to bring p to the front)

- Fermion/Boson SWAPs (exchange entire registers)
- Fermion eXchange
  $\mathtt{fX}_j(p) = (\mathfrak{C}_{00})_j \otimes \mathtt{fS}_j(0,p) + (\mathfrak{C}_{11})_j \otimes \mathtt{fS}_j(L,p)$
  (overloads the SWAP)

Outline

1. Foreword
2. Onto field theory: encoding particles
3. Encoding canonical operators
   - Creation (destruction) operators
   - (Anti)commutation rules
4. Evolution operators
   - Free evolution
   - Exponentiating interaction terms
5. Outlook

Gate costs: polynomial in n particles and N_p momenta

Operator	Costs	
	CNOT & single-qubit	Order oracle
$\mathcal{U}_{11}$	$\mathcal{O}\left(nN_p\right)$	None
$\mathcal{U}_{22}$	$\mathcal{O}\left(n^2 N_p^3 \log_2^2 N_p\right)$	None
$\mathcal{U}_{10}$	$\mathcal{O}\left(N_p \log_2^2 N_p\right)$	$\mathcal{O}\left(n^3 N_p\right)$
$\mathcal{U}_{21}$	$\mathcal{O}\left(n_b n_f^2 N_p^2 \log_2^2 N_p\right)$	$\mathcal{O}\left(n_b^3 N_p\right)$
$\mathcal{U}'_{21}$	$\mathcal{O}\left(n_b n_f N_p^3 \log_2 N_p\right)$	$\mathcal{O}\left(n_b n_f^3 N_p^2\right)$

Outlook

- Particle encoding based on particle registers
- Useful for few-body physics: polynomial scaling with both n and N_p
- Currently working on: coding QCD in Weyl gauge, perhaps light-front gauge

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Comparison to Jordan-Wigner

Encode a momentum set $\{p_1, ..., p_{N_p}\}$:

Jordan-Wigner: Each qubit a momentum. Up to N_p particles

$$\overbrace{|\downarrow\downarrow\downarrow \dots \downarrow\rangle}^{N_p} = |\Omega\rangle \quad |\uparrow\downarrow\uparrow \dots \downarrow\rangle = |p_1 p_3\rangle \quad |\uparrow\uparrow\uparrow \dots \uparrow\rangle = |p_1 \dots p_{N_p}\rangle$$

requires $\mathcal{O}(N_p)$ qubits

Register-Particle: Each binary number a momentum. One register per particle

$$|\downarrow\rangle \overbrace{|\downarrow\downarrow \dots \downarrow\rangle}^{\log_2 N_p} = |\Omega\rangle \quad |\uparrow\rangle|\uparrow\downarrow\uparrow \dots \downarrow\rangle = |p_3\rangle \quad |\uparrow\rangle|\uparrow\uparrow\uparrow \dots \uparrow\rangle = |p_{N_p}\rangle$$

requires $\mathcal{O}(n \log_2 N_p)$ qubits if n particles

If n small $\Rightarrow$ **RP** encoding preferable

Jordan-Wigner encoding I

Fermionic algebra with Pauli operators? Consider two excitations:

$$|\downarrow\downarrow\rangle = |\Omega\rangle, \quad |\uparrow\downarrow\rangle = |p\rangle, \quad |\downarrow\uparrow\rangle = |q\rangle, \quad |\uparrow\uparrow\rangle = |pq\rangle$$

take

$$b_p^\dagger = \sigma^- \otimes I = \frac{X - iY}{2} \otimes I, \quad b_q^\dagger = Z \otimes \sigma^- = Z \otimes \frac{X - iY}{2}$$

then

$$\begin{aligned} \{b_p^\dagger, b_q\} &= (\sigma^- \otimes I)(Z \otimes \sigma^+) + (Z \otimes \sigma^+)(\sigma^- \otimes I) \\ &= \left(\frac{X - iY}{2} Z + Z \frac{X - iY}{2}\right) \otimes \sigma^+ = 0 \end{aligned}$$

because $\{X, Z\} = \{X, Y\} = \{Y, Z\} = 0$

Jordan-Wigner encoding II

if modes are the same, the anticommutator is

$$\{b_p^\dagger, b_p\} = (\sigma^-\sigma^+ + \sigma^+\sigma^-) \otimes I = \left(\frac{I-Z}{2} + \frac{I+Z}{2}\right) \otimes I = I \otimes I = \mathbb{I}$$

this can be generalizated to an arbitrary number of excitations

Jordan-Wigner encoding

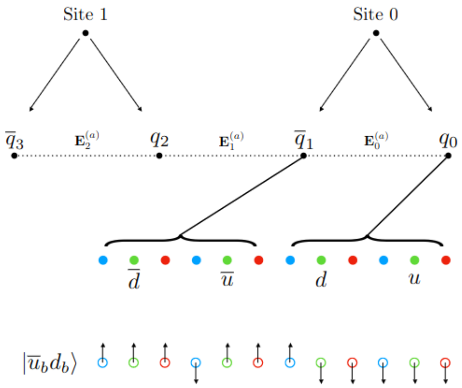
For excitations $\{p_1, ..., p_{N_p}\}$, the following operators

$$b_{p_i}^\dagger = Z^{\otimes N-i} \otimes (\sigma^-)_i \otimes I^{\otimes i-i}$$
$$b_{p_i} = Z^{\otimes N-i} \otimes (\sigma^+)_i \otimes I^{\otimes i-1}$$

satisfy the fermionic algebra

Example: quarks on the lattice

2×2×3×2=24 qubits necessary two represent two quark-antiquark pairs with two flavours, three colours and **no spin** in two positions



From **Phys Rev D** 107, 054512

- Particle excitations: $\uparrow$
- Anti-particle excitations: $\downarrow$

$$|\Omega\rangle = \overbrace{|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle}^{6\ anti-particles} \otimes \overbrace{|\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle}^{6\ particles}$$

Setting up the formalism

- One-particle vacuum is

$$|\Omega\rangle \equiv |0\rangle_{P/A} \otimes |0...0\rangle_{momentum},$$

  - Presence qubit to the left
  - Momentum qubits to the right

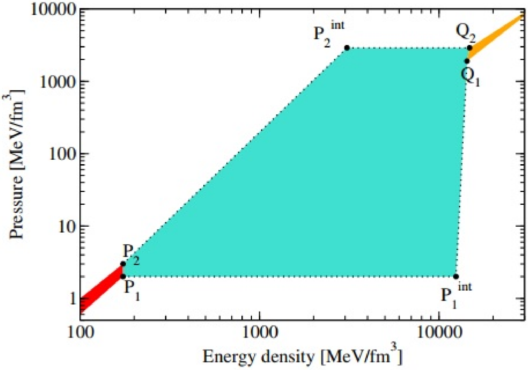
- Creation/annihilation operators are

$$a_p^\dagger \equiv \mathfrak{C}_{10} \otimes \mathfrak{s}_q^\dagger \quad \xrightarrow{h.c.} \quad a_q \equiv \mathfrak{C}_{01} \otimes \mathfrak{s}_q$$

  with $\mathfrak{C}_{ji} = |j\rangle\langle i|$, $\mathfrak{s}_q^\dagger = |q\rangle\langle 0...0|$ and
- $|q\rangle$ one of N_p binary numbers generated from $\log_2 N_p$ qubits
- To instantiate a particle:

$$a_q^\dagger|\Omega\rangle = \mathfrak{C}_{10}|0\rangle \otimes \mathfrak{s}_q^\dagger|0...0\rangle = |1\rangle \otimes |q\rangle = |1q\rangle$$

nEoS: Neutron Star Equations of State from hadron physics only



M. Alford, E. Lope-Oter, FJLE, A. Windisch, JPG 2019

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