Towards Few-Body QCD on a Quantum Computer

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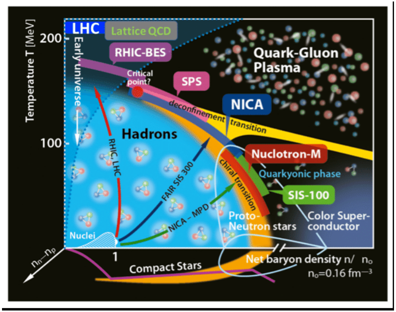
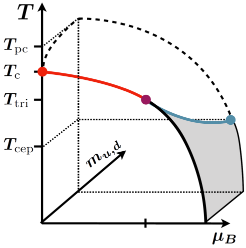
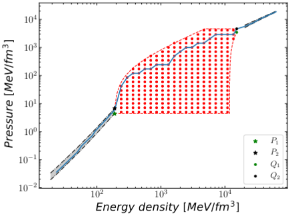
Outline

Phase transition in QCD? EoS at finite μ_B?







Lattice cannot tell:

Reaching the region $\mu_B/T > 3$ is a major challenge for any of the currently used approaches in lattice QCD calculations as well as for collider based heavy ion experiments that search for the CEP.

From arxiv:2212.11107: "50 years of QCD", pág. 85 and M. Evangelina Lope Oter thesis

Sign problem

Limitation due to fermions. In the **grand-canonical** ensemble

$$PV = k_B T \ln \left\{ \mathrm{T_r} exp \left(-\beta(\hat{H} - \mu \hat{N}) \right) \right\} = k_B T \ln Z$$

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Partition function sampled on the lattice:

$$Z = \int \prod_{x_0=1}^{N_\tau} \prod_{x_i=1}^{N_\sigma} \prod_{\hat{\nu}=0}^{3} \mathcal{D}U_{x,\hat{\nu}} e^{-S_G} \times \prod_{f=u,d,s,\ldots} \det M_f(m_f, \mu_f)$$

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If $\mu_f \in \mathbb{R}$, $\det M_f(m_f, \mu_f) = \pm \rightarrow$ convergence problem

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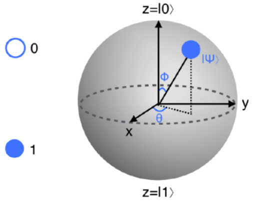
Not on QC: Codification of fermion states and unitary evolution

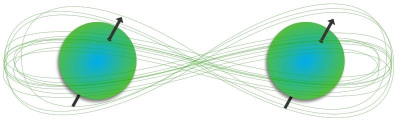
Bits & qubits

Quantum memory: Composition of many highly-controllable systems, **qubits if 2-level**, e.g. superconducting circuits.

- Superpositions: $\cos\Phi|0\rangle + \sin\Phi e^{i\theta}|1\rangle$
- Entanglement: $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$



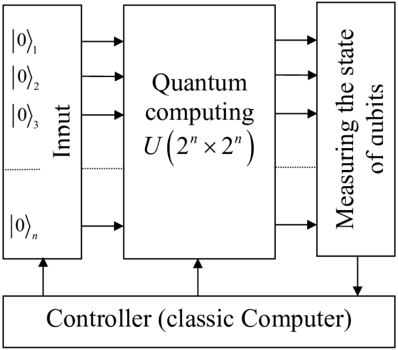
bit *qubit*

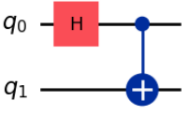


$\mathbf{n}_q$ qubits $\rightarrow$ $\mathbf{N} = 2^{\mathbf{n}_q}$, exponential grown (curse of dimensionality):

- 1 qbit: $\{|0\rangle, |1\rangle\} \rightarrow \alpha|0\rangle + \beta|1\rangle$
- 2 qbits:
  $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} \rightarrow \alpha|00\rangle + \beta|10\rangle + \gamma|10\rangle + \delta|11\rangle$

Quantum memory advanced by **unitary gates: H, X,Y,Z, CNOT**



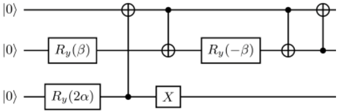


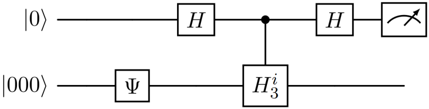
Preparation of state
$\Phi_{00} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

Can be used to solve variational problems:

$$H = T + V = \frac{\nabla^2}{2\mu} + \sigma r - \frac{\alpha_s}{r}.$$

H decomposed in unitary gates $H_3^i \to \langle H \rangle$



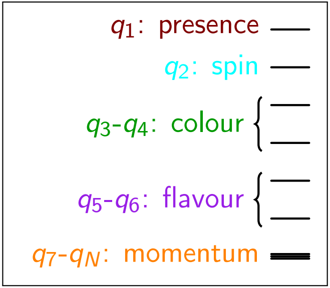


Baryon (composition)	$\Omega(bbb)$	$\Omega(bbc)$	$\Omega(bcc)$	$\Omega(ccc)$
This work	14270 ± 340	11210 ± 350	8100 ± 350	4940 ± 340
Variational pNRQCD	14700 ± 300	11400 ± 300	8150 ± 300	4900 ± 250
Coulomb variational	14370 ± 80	11190 ± 80	7980 ± 70	4760 ± 60
QCD sum rules	13280 ± 100	10460 ± 110	7443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

arXiv:2407.07232 & arXiv:2202.03333

One-particle codification

Each quantum # a set of qubits, each particle a register:



Quark register

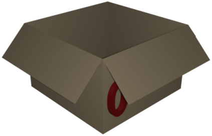
Empty register

$$|\Omega\rangle = |0\rangle \otimes |0\rangle \otimes |00\rangle \otimes |00\rangle \otimes |0\dots0\rangle$$

Pack/unpack with operators

$$a^\dagger_{s,c,f,p}|\Omega\rangle = |1\rangle \otimes |s\rangle \otimes |c\rangle \otimes |f\rangle \otimes |p\rangle$$

$$a_{s,c,f,p}|1\rangle \otimes |s\rangle \otimes |c\rangle \otimes |f\rangle \otimes |p\rangle = |\Omega\rangle$$

$a^\dagger_{s,c,f,p}$  $=$ 

Add more registers for multi-particle states

$|\Omega\rangle = |\Omega\rangle_3 \otimes |\Omega\rangle_2 \otimes |\Omega\rangle_1$:

We would like

$$a^\dagger_{p_1} |\Omega\rangle = |p_1\rangle \,, \quad a^\dagger_{p_2} |p_1\rangle = |p_2\rangle \, |p_1\rangle \,, \text{ etc}$$

How to define $|p_2\rangle \, |p_1\rangle$? Use **presence** qubits to control:

$$\mathfrak{C}_{00}|0\rangle = |0\rangle \,, \quad \mathfrak{C}_{11}|0\rangle = 0, \text{ etc}$$

and divide $a^\dagger_{p_1}$:

$$a^\dagger_{p_1} = a^\dagger_{p_1,1} + a^\dagger_{p_1,2} + a^\dagger_{p_1,3}$$

so that memory is filled **in order**.

Three particles: $(|\Omega\rangle_1 = |0\rangle_1 |0\ldots 0\rangle_1)$

$|\Omega\rangle = |\Omega\rangle_3 \otimes |\Omega\rangle_2 \otimes |\Omega\rangle_1$:

$a^\dagger_{p_1,1}|\Omega\rangle = |\Omega\rangle_3 \otimes |\Omega\rangle_2 \otimes |1 p_1\rangle_1$:

$$a^\dagger_{p_1,1} = \mathbb{P}^{(2)}_0 \otimes \left(\mathfrak{C}_{10} \otimes \mathfrak{s}^\dagger_{p_1}\right)_1$$

$a_{p_2,2}|1 p_2\rangle|1 p_1\rangle = |\Omega\rangle_3 \otimes |\Omega\rangle_2 \otimes |1 p_1\rangle_1$:

$$a_{p_2,2} = \mathbb{P}^{(1)}_0 \otimes (\mathfrak{C}_{01} \otimes \mathfrak{s}_{p_2})_2 \otimes \mathbb{P}^{(1)}_1$$

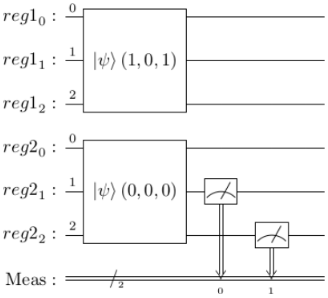
$\mathbb{P}^{(n)}_i$: projector over i-occupied registers for n total registers.

Example: Initializing

Most basic particle: scalar with three momenta

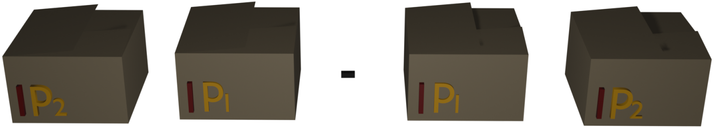
$$|00\rangle \rightarrow None, \ |01\rangle \rightarrow |p_0\rangle, \ |10\rangle \rightarrow |p_1\rangle, \ |11\rangle \rightarrow |p_2\rangle$$

```python
# Register definition
reg1 = QuantumRegister(3,name = "reg1") # two p-qubits
reg2 = QuantumRegister(3,name = "reg2")
# Classical register to measure
meas = ClassicalRegister(2, name = "Measurement")
circuit = QuantumCircuit()
circuit.add_register(reg1)
circuit.add_register(reg2)
circuit.add_register(meas)

# Register initialization
circuit.initialize(IndexTobinary(0,2)+"1", reg1)
circuit.initialize("00"+"0", reg2)

# Measurement
circuit.measure(reg2[1:],[0,1])

circuit.draw(output = "latex",idle_wires = False)
```



Particle-statistics & unitarity

$$\left\{ b^\dagger_{p_1}, b_{p_2} \right\} = \delta_{p_1 p_2} \mathbb{I} \rightarrow \text{Add antisymmetrizer } \mathcal{A}:$$



Problems with unitarity:

- $\mathbb{P}_i^{(n)}$, $\mathfrak{C}_{10}$, etc. are not unitary $\rightarrow$ **exponentiate**
- $\mathcal{A}$ is not unitary $\rightarrow$ scrap qubits

With $\mathcal{A}_{j \leftarrow j-1}$ define

$$b^\dagger_{p_1, j} = \mathcal{A}_{j \leftarrow j-1} \cdot \left(\mathbb{C}_{10} \otimes \mathfrak{s}^\dagger_{p_1} \right)_2 \otimes \mathbb{P}_1^{(1)}$$

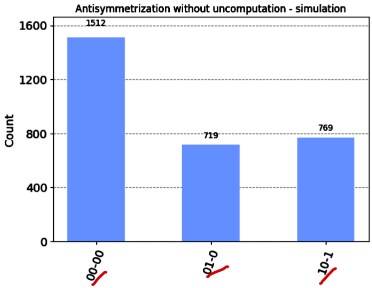
Example: Antisymmetrizing

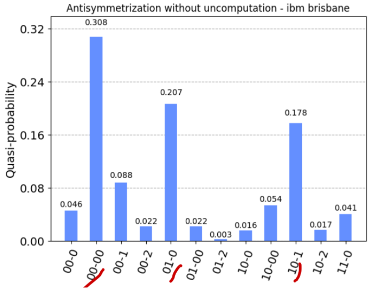
$$|\phi_0\rangle = \frac{1}{\sqrt{2}}\left(|\Omega\rangle_2|1p_0\rangle_1 + |1p_1\rangle_2|1p_0\rangle_1\right)$$

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle_{ax}|\Omega\rangle_2|1p_0\rangle + \frac{1}{\sqrt{2}}\left(|10\rangle_{ax} - |01\rangle_{ax}\right)|1p_1\rangle_2|1p_0\rangle\right)$$

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}|00\rangle_{ax}|\Omega\rangle_2|1p_0\rangle + \frac{1}{2}\left(|10\rangle_{ax}|1p_1\rangle_2|1p_0\rangle_1 - |01\rangle_{ax}|1p_0\rangle_2|1p_1\rangle_1\right)$$

Measuring 2nd register...





Fermionic operators

Field-theory like $b_q^{(n)\dagger} = \sum_j b_{q,j}^{(n)\dagger}$:

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

Adjoint to find annihilator. With those we find:

Anticommutation relations

$$\left\{b_{q_1}^{(n)}, b_{q_2}^{(n)\dagger}\right\} = \overbrace{\delta_{q_1,q_2} \left(\mathfrak{C}_{00} \otimes \mathbb{I}\right)_n \otimes \mathbb{I}^{(n-1)}}^{\text{canonical}} + \underbrace{\mathcal{A}_{n\leftarrow n-1} \cdot \left(\mathfrak{C}_{11} \otimes \mathfrak{s}_{q_1}^\dagger \mathfrak{s}_{q_2}\right)_n \otimes \mathbb{P}_{n-1}^{(n-1)} \cdot \mathcal{A}_{n\leftarrow n-1}}_{\text{boundary term}}$$

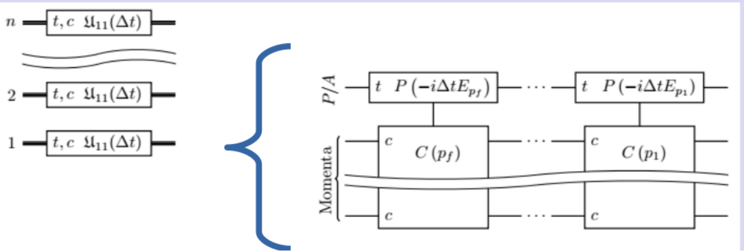
Free evolution

From $\hat{H}_{11}^{(n)} = \sum_p E_p\, a_p^{(n)\dagger} a_p^{(n)}$, using properties of $\mathbb{P}_i^{(j)}$ and $\mathfrak{C}_{11}$:

Free evolution

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

$$\mathfrak{U}_{11}(\Delta t) \equiv \exp\left[-i\Delta t \sum_p E_p \mathfrak{s}_p^{\dagger} \mathfrak{s}_p\right]$$



Example: Free evolution

Implementing $\mathfrak{U}_{11}(\Delta t) = \exp\left[-i\Delta t \sum_p E_p \mathfrak{s}_p^\dagger \mathfrak{s}_p\right]$ is easy:

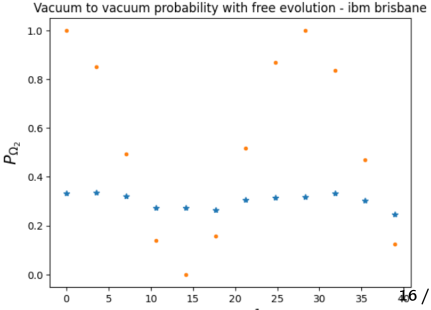
$$\mathfrak{s}_{p_0}^\dagger \mathfrak{s}_{p_0} = |01\rangle\langle 01| = \frac{1}{4}(I+Z)(I-Z)$$

exponentials of **I,X,Y,Z** built-in.

$$U_{11}(\Delta t)|\phi_0\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_0\Delta t}|\Omega\rangle_2|1p_0\rangle_1 + e^{-i(E_1+E_0)\Delta t}(|1p\rangle_2|1p_0\rangle_1)_A\right)$$

return to $|\Omega\rangle_2|1p_0\rangle_1$ to see oscillation in amplitude ($E_1 = 223$ MeV):

```
# "Create" particle on 2nd register
circuit.append(Mode_rot("00",1,np.pi/4,2), re
# Antisymmetrize
SA.Step_Adg(circuit,2, uncompute = False)
# U_11(i)
circuit.append(free_evol(i,[0,1,2]),reg1[1:])
circuit.append(free_evol(i,[0,1,2]),reg2[1:])
# Return 2nd register to vacuum
SA.Step_A(circuit,2, uncompute = False)
circuit.append(Mode_rot("00",1,-np.pi/4,2), r
# Measure
circuit.measure(reg2[1:],[0,1])
```



Exponentiation with changing # of particles

Simplest particle-number changing term

$$U_{10}(\Delta t) = e^{-i\Delta t \sum_p \lambda_p \sum_j \left(b^{(n)\dagger}_{p,j} + b^{(n)}_{p,j}\right)}$$

Arbitrary number created on each step, use $e^{A+B+\frac{1}{2}[A,B]} + ... = e^A e^B$ (Baker-Campbell-Hausdorff formula), one at a time:

$$\mathcal{U}_{10}(\Delta t) = \prod_j \exp\left[-i\Delta t \sum_p \lambda_p (b^{(n)\dagger}_{p,j} + b^{(n)}_{p,j})\right] + O((\Delta t)^2)$$

just systematically improveable errors. We expect this to do

$$e^{-i\Delta t\left(b^{(n)\dagger}_{p,2} + b^{(n)}_{p,2}\right)} |\Omega\rangle_2 |1p_0\rangle_1 = \alpha |\Omega\rangle_2 |1p_1\rangle_1 + \beta \left(|1p\rangle_2 |1p_1\rangle_1\right)_A$$

how to avoid scrap qubits and fullfil **Pauli exclusion principle**?

To avoid scrap qubits, introduce new operators

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

if P **largest** on memory

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

if register j empty

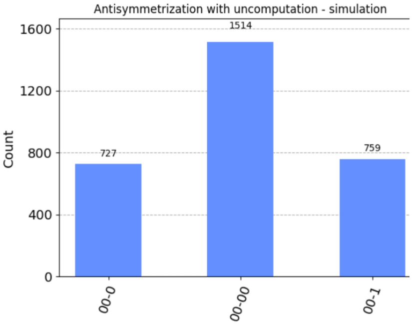
key: "Locate the Largest" algorithm to disentangle auxiliary:

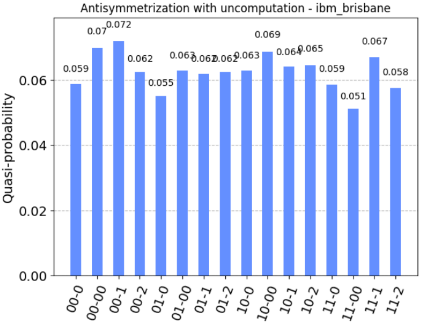
$$|\phi\rangle = \frac{1}{\sqrt{2}} \left(|10\rangle_{ax} |1P\rangle_2 |1p\rangle_1 - |01\rangle_{ax} |1p\rangle_2 |1P\rangle_1\right)$$

goes to

$$LL|\phi\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle_{ax} |P\rangle |p\rangle - |00\rangle_{ax} |p\rangle |P\rangle\right) = |00\rangle_{ax} \left(|P\rangle |p\rangle\right)_A$$

Disentangling qubits is expensive, depth ≈ 2300, currently maximum ≈ 600:





For Pauli exlusion principle, define fermion interchanger:

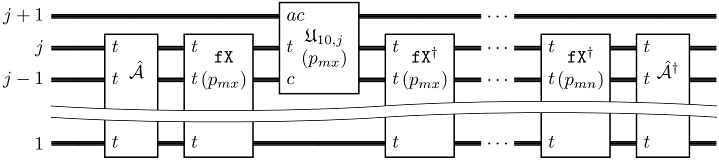
$$\mathtt{fX}_j\,(p) = (\mathfrak{C}_{00})_j \otimes \mathtt{fS}_j\,(0, p) + (\mathfrak{C}_{11})_j \otimes \mathtt{fS}_j\,(L, p)$$

Tadpole evolution

$$\mathcal{U}^f_{10} \;=\; \prod_j \left(\sum_{\substack{l=0 \\ l \neq j, j-1}} \mathbb{P}_l^{(n)} + \hat{\mathcal{A}}^\dagger_{j \leftarrow j-1} \cdot \prod_p \hat{\mathfrak{U}}_{10}(p) \cdot \hat{\mathcal{A}}_{j \leftarrow j-1} \right) \;+\; \mathcal{O}\left(\Delta t^2\right)$$

$$\hat{\mathfrak{U}}_{10}(p) = \mathtt{fX}_j^\dagger\,(p) \cdot \mathbb{P}_0^{(n-j)} \otimes \mathfrak{U}_{10,j}\,(\Delta t, \lambda_p) \otimes \mathbb{P}_{j-1}^{(j-1)} \cdot \mathtt{fX}_j\,(p)$$

$$\mathfrak{U}_{10,j}(\Delta t, \lambda_p) = \exp\left(-i \Delta t \lambda_p \left(\mathfrak{C}_{10} \otimes \mathfrak{s}_p^\dagger + \mathfrak{C}_{01} \otimes \mathfrak{s}_p\right)_j\right).$$



Evolution terms asymptotics

$$\mathcal{U}^{f}_{22}(\Delta t) = \exp\left[-i\Delta t \sum_{\xi=-\Lambda}^{\Lambda}\left(\lambda_\xi \sum_{q,p} b^\dagger_{q+\xi\Delta} b^\dagger_p b_{p+\xi\Delta} b_q + h.c.\right)\right]$$

$$\mathcal{U}_{21}(\Delta t, \lambda) = \exp\left[-i\Delta t \sum_{p,k} \lambda_{k-p}\left(a^\dagger_{k-p} b^\dagger_p b_k + h.c.\right)\right]$$

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
$\mathcal{U}_{10}$	$\mathcal{O}\left(N_p \log_2^2 N_p\right)$	$\mathcal{O}\left(n^3 N_p\right)$
$\mathcal{U}_{21}$	$\mathcal{O}\left(n_b n_f^2 N_p^2 \log_2^2 N_p\right)$	$\mathcal{O}\left(n_b^3 N_p\right)$
$\mathcal{U}'_{21}$	$\mathcal{O}\left(n_b n_f N_p^3 \log_2 N_p\right)$	$\mathcal{O}\left(n_b n_f^3 N_p^2\right)$

Conclusions

- Sign problem for LQCD. Quantum Computing promising
- Register-particle codification $\rightarrow$ high-level objets & unitaries from 2nd-quantized operators

Ongoing work

- Implementation of axial gauge Hamiltonian:

$$H = \int d^3r \frac{1}{2}\left(\vec{E}^I\vec{E}^I + \vec{B}^I\vec{B}^I\right) - ig\bar{\psi}^{\dagger}\vec{\gamma}T^I\psi\vec{A}^I + \bar{\psi}\left(\vec{\gamma}\vec{\nabla} + m\right)\psi$$

- Gauss's law:

$$\mathcal{G}^a(k)\left(= J^a_Q(k) - J^{0,a}_D(k)\right)|\psi\rangle = 0$$

Unexplored territory: Renormalization? Finite memory impact and discretization errors?

Fixed particle number

We can now get unitaries by exponentiation:

$$\hat{H}_{11}^{(n)} = \sum_p E_p\, a_p^{(n)\dagger} a_p^{(n)} = \sum_p E_p \sum_{j',j} a_{p,j}^{(n)\dagger} a_{p,j'}^{(n)}$$

$$= \sum_j \mathcal{A}_{j\leftarrow j-1} \cdot \mathbb{P}_0^{(n-j)} \otimes \left(\color{blue}{\mathfrak{C}_{11}} \otimes \sum_p E_q\, \mathfrak{s}_p^\dagger \mathfrak{s}_p \right)_j \otimes \mathbb{P}_{j-1}^{(j-1)} \cdot \mathcal{A}_{j\leftarrow j-1}$$

Fixed particle # $\rightarrow$ antisymmetrizers can be conmmuted:

$$\hat{H}_{11}^{(n)} = \sum_{j,k} \mathbb{P}_0^{(n-j)} \otimes \mathbb{P}_k^{(k)} \otimes \left(\mathfrak{C}_{11} \otimes \sum_p E_p \mathfrak{s}_p^\dagger \mathfrak{s}_p \right)_{j-k} \otimes \mathbb{P}_{j-1-k}^{(j-1-k)} \cdot \frac{\mathcal{A}_{j\leftarrow j-1}}{\sqrt{j}}$$

Antisymmetrizers to the right just simplify!

For Pauli exlusion principle, define fermion interchanger:

$$\mathtt{fX}_j(p) = (\mathfrak{C}_{00})_j \otimes \mathtt{fS}_j(0,p) + (\mathfrak{C}_{11})_j \otimes \mathtt{fS}_j(L,p)$$

Empty register

$$(\mathfrak{C}_{00})_j \otimes \mathtt{fS}_j(0,p)\,|\Omega\rangle_j \underbrace{(...|1p\rangle_i...)_A}_{\text{p there}} = \underbrace{|0p\rangle_j(...|10...0\rangle_i...)_A}_{\text{creation avoided}}$$

$$(\mathfrak{C}_{00})_j \otimes \mathtt{fS}_j(0,p)\,|\Omega\rangle_j \underbrace{(...|1q\rangle_i...)_A}_{\text{no p}} = \underbrace{|\Omega\rangle_j(...|1q\rangle_i...)_A}_{\text{creation allowed}}$$

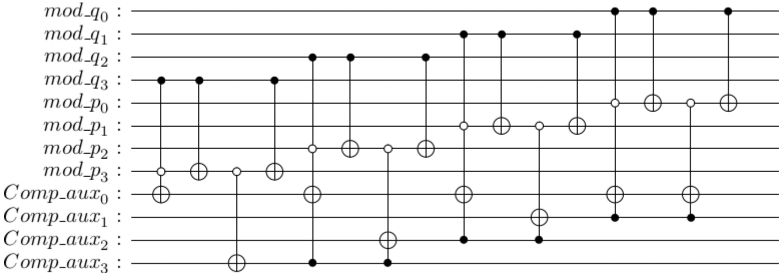
Occupied register

$$(\mathfrak{C}_{11})_j \otimes \mathtt{fS}_j(L,p)\,|1P\rangle_j \underbrace{(...|1p\rangle_i...)_A}_{\text{p there, swap}} = \underbrace{|1p\rangle_j(...|1P\rangle_i...)_A}_{\text{p on } j\text{, annihilation}}$$

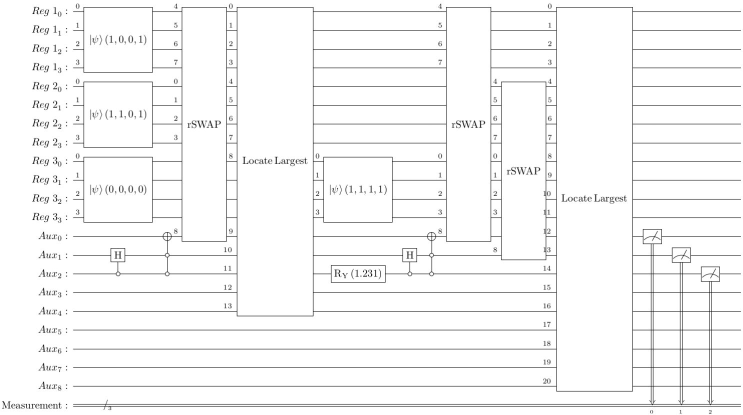
$$(\mathfrak{C}_{11})_j \otimes \mathtt{fS}_j(L,p)\,|1P\rangle_j \underbrace{(...|1q\rangle_i...)_A}_{\text{no p no swap}} = \underbrace{|1P\rangle_j(...|1q\rangle_i...)_A}_{\text{no p on } j\text{, no annihilation}}$$

Order on momenta introduced via their indices:

$$O(|x\rangle|p_i\rangle|p_j\rangle) = \begin{cases} |x \oplus 1\rangle|p_i\rangle|p_j\rangle & \text{si } i \geq j \\ |x\rangle|p_i\rangle|p_j\rangle & \text{si} i < j, \end{cases}$$



Antisymmetrizer's decomposition:



Auxiliary qubits disentangled with "Locate Largest" circuit:

$$|0,...,0\rangle|p_n,...,p_1\rangle \xrightarrow{\text{LL}} |0...,\underbrace{1}_{k_m},...,\underbrace{1}_{k_1},...,0\rangle|p_n,...,\underbrace{P}_{k_m},...,\underbrace{P}_{k_1},...,p_1\rangle,$$