Quantum Simulation of Fermionic Systems

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This work is part of a project involving quantum computation of fermionic Hamiltonians

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Outline

Quantum Simulation of Fermionic Systems: towards a QCD-inspired method for existing and near-term quantum computer devices.

A meson is a "quantum circuit"

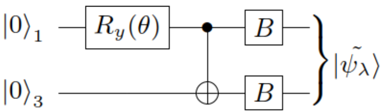


Figure: Ry rotation by θ on qubit 1, followed by CNOT gate, and possibly a B gate, corresponding to a basis change, which is necessary for some Pauli terms in the Hamiltonian

It is important to emphasise that whatever model/approximation to QCD one favours, it should obey to three conditions:

- It has to "contain" confinement,
- It has to be chiral symmetric and, despite that,
- possess a mechanism for spontaneous breaking of chiral symmetry (SχSB).

Introduction

There is a class of models which can address, at one stroke, all the three above conditions: they are chiral symmetric, they display SχSB, and, on top, they allow for chiral restoration. This class of models can be thought as to solve QCD in the Gaussian approximation for gluonic cummulants. This approximation becomes exact in the limit of heavy quarks.

This talk is divided into three section.

1. A brief description of qubits and quantum gates;
2. an introduction to the Jordan-Wigner and Bravyi-Kitaev transformations;
3. a summary of the physics of quark quartic interactions and its relation with SχSB;
4. a brief presentation of the actual quantum computation.

Qubits and quantum gates

1. The state space for a single qubit is given by $\{a|0\rangle + b|1\rangle\}\,,\ |a|^2 + |b|^2 = 1.$
2. $a|0\rangle + b|1\rangle \leftrightarrow c\,\{a|0\rangle + b|1\rangle\}\,,\ |c|^2 = 1$ describe the same qubit; $\{a|0\rangle + b|1\rangle, a'|0\rangle + b'|1\rangle\}$ with $a/b = e^{i\varphi}|a|/|b|$ represent two different qubits;
3. the standard basis for n qubits is a 2^n basis: $\{|0,0...0\rangle, |0...,0,1\rangle, |0,...,1,0\rangle, |1,...,1\rangle\} \Leftrightarrow |0\rangle, |1\rangle, ...|2^n - 1\rangle$;
4. to a single qubit corresponds one complex number. To a n-qubit we have $2^n - 1$ complex numbers. Since $2^n - 1 \gg n$, most of n-qubits cannot be described as a tensor product of separated n qubits

Definition

States that cannot be described by tensor products of n single qubit states are called *entangled states*.

For instance the entangled Bell state $|\Phi^+\rangle$,

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\{|00\rangle + |11\rangle\} \neq \{a1|0\rangle + a2|1\rangle\} \otimes \{b1|0\rangle + b2|1\rangle\}$$

cannot be described by the tensor product of two separate single qubits. The notion of entanglement is not absolute: a system of n-qubits can be entangled in terms of some sub-registers and not in relation to others. Example: $|\Psi\rangle =$

$$\frac{1}{2}\left(|0\rangle_1|0\rangle_2|0\rangle_3|0\rangle_4 + |0\rangle_1|1\rangle_2|0\rangle_3|1\rangle_4 + |1\rangle_1|0\rangle_2|1\rangle_3|0\rangle_4 + |1\rangle_1|1\rangle_2|1\rangle_3|\rangle_4\right)$$
$$= \frac{1}{\sqrt{2}}\left(|0\rangle_1|0\rangle_3 + |1\rangle_1|1\rangle_3\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle_2|0\rangle_4 + |1\rangle_2|1\rangle_4\right),$$

is separable in relation of sub-registers {1,3} and {2,4}but entangled in relation to sub-registers {1,2} and {3,4}.

- In the standard basis, the operator $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is given by, $a|0\rangle\langle 0| + b|0\rangle\langle 1| + c|1\rangle\langle 0| + d|1\rangle\langle 1|$.
- Pauli operations: The Pauli transformations are the most commonly used single-qubit transformations

$$I = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad X = |1\rangle\langle 0| + |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};$$

$$Y = -|1\rangle\langle 0| + |0\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \; Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- The Hadamard Transformation

$$H = |0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- The standard basis is $|0\rangle \Rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|1\rangle \Rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

- The C-NOT Gate (controlled not gate). If the first qubit is 0 leaves the second qubit unchanged, if not flips the second qubit:

$$
\begin{aligned}
C_{NOT} &= |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X \\
&= |0\rangle\langle 0| \otimes (|0\rangle\langle 0| + |1\rangle\langle 1|) + |1\rangle\langle 1| \otimes (|1\rangle\langle 0| + |0\rangle\langle 1|) \\
&= |00\rangle\langle 00| + |01\rangle\langle 01| + |11\rangle\langle 10| + |10\rangle\langle 11|
\end{aligned}
$$

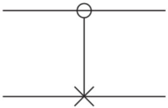


Figure: Gate C-NOT

- C-NOT entangles a system that was separable

$$
C_{NOT} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle = \\
= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),
$$

- and because it is its own inverse it can also disentangle an entangled state

General single qubits transformations

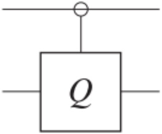


Figure: Gate C-Q

- In general we may have a C-Q gate: $\Lambda Q = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes Q$, so that $C_{NOT} = \Lambda X$

- All the single-qubit transformations can be written as combinations of phase shifts $e^{i\delta} I$ and,

$$R(\beta) = \begin{pmatrix} \cos(\beta) & \sin(\beta) \\ -\sin(\beta) & \cos(\beta) \end{pmatrix}, \quad T(\alpha) = \begin{pmatrix} e^{I\alpha} & 0 \\ 0 & e^{-I\alpha} \end{pmatrix}$$

- Any Operator $Q = e^{i\delta} I T(\alpha) R(\beta) T(\gamma)$

Mapping fermion occupation numbers and qubits

Local fermion modes

- the fermion creation and annihilation operators act on local fermion modes (LFM $\in$ the fock space $\mathcal{F}$) as follows:

$$\hat{a}|n_0, \cdots, n_{j-1}, \mathbf{1}, n_{j+1}, \cdots, n_{m-1}\rangle =$$
$$= (-1)^{\sum_{s=0}^{j-1}} |n_0, \cdots, n_{j-1}, \mathbf{0}, n_{j+1}, \cdots, n_{m-1}\rangle$$
$$\hat{a}|n_0, \cdots, n_{j-1}, \mathbf{0}, n_{j+1}, \cdots, n_{m-1}\rangle = 0$$

- With the usual commutation rules $\left\{\hat{a}_j^\dagger, \hat{a}_k\right\} = \delta_{jk}, \ \{\hat{a}_j, \hat{a}_k\} = 0$
- We can identify the LFM with a qubit Hilbert space $\mathcal{H}$:

$$|n_0, n_1, \cdots, n_{m-1}\rangle \Rightarrow |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{m-1}\rangle, \ \ n_i = \{0, 1\}$$

- But it is different to operate on the qubit Hilbert space and on the LFM Fock space: *the order matters!*

- Using $\hat{a}^\dagger \hat{a} = (1 - \sigma_z)/2$, we can build the following transcriptions of qubit operations into Fock space operators: $\Lambda e^{i\varphi}$, $\Lambda \sigma_z$:
- It is a simple question of calculations to see that,

$$\Lambda e^{i\varphi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \Rightarrow exp\left\{ i\varphi \hat{a}_0^\dagger \hat{a}_0 \right\},$$

$$\Lambda \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \Rightarrow exp\left\{ i\pi \hat{a}_0^\dagger \hat{a}_0 \hat{a}_1^\dagger \hat{a}_1 \right\}$$

- $\Lambda \sigma_z : \; |00\rangle \to |00\rangle, \; |10\rangle \to |10\rangle, \; |10\rangle \to |10\rangle, \; |11\rangle \to (-1)|11\rangle$
- So a two LFM operator $\hat{X}\{j,k\}$ corresponds to a two qubit operator $\mathcal{X}[j,k]$ as follows ($D[l,m] = \Lambda\sigma_z[l,m]$):
  $\hat{X}\{j,k\} = D[k-1,k]\cdots D[j+1,k]\mathcal{X}[j,k]D[j+1,k]\cdots D[k-1,k]$

Jordan-Wigner and Bravyi-Kitaev operators

Jordan-Wigner operators

- Qubit creation and annihilation operators can be described as, $\hat{Q}^\dagger = |1\rangle\langle 0| = \frac{1}{2}(\sigma_x - i\sigma_y), |; \hat{Q}^- = |0\rangle\langle 1| = \frac{1}{2}(\sigma_x + i\sigma_y)$ These operators act on local qubits and do not know about the Pauli statistics. This information for a given $\hat{Q}_i$ is stored in al qubits $i < j$. This set is known as the Parity (I dislike this name) set $\mathcal{P}(i)$. the set of qubits that determines the global commutation number $p_i = \sum_{j<i} n_j$, with n_j the LFM in site i: $\{0, 1\}$. Then we have:
- $\hat{a}_i^\dagger = \sigma^- \otimes_{j<i} \sigma_{z\,i} = \sigma^- \otimes \sigma_{z\,\mathcal{P}(i)}$; $\hat{a}_i = \sigma^+ \otimes_{j<i} \sigma_{z\,i} = \sigma^+ \otimes \sigma_{z\,\mathcal{P}(i)}$
- $\{\sigma^+, \sigma^-\} = I$.

Bravyi-Kitaev operators

- We look for a transformation $\beta_{2m} = \left(\begin{array}{c|c} \beta_{2m-1} & 0 \\ \hline 0 & \\ \leftarrow 1 \rightarrow & \beta_{2m-1} \end{array}\right)$; $\beta_1 = 1$
- Example (4 qubits): $2^m = 4 \rightarrow m = 2 \Rightarrow \beta_2 = \left(\begin{array}{c|c} 1 & 0 \\ \hline 1 & 1 \end{array}\right)$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} q_1 = f_1 \\ q_2 = f_1 + f_2 \\ q_3 = f_3 \\ q_4 = f_1 + f_2 + f_3 + f_4 \end{bmatrix}.$$

- The update set $U(j) = \{q_n\}$, $n > j$ to be updated when we change LFM f_j. Ex: $U(1) = \{2, 4\} \Rightarrow \hat{a}_1 = \sigma_1^+ \sigma_{x2} \sigma_{x4}$. $U(3) = \{4\} \Rightarrow \hat{a}_3 \simeq \sigma_3^+ \sigma_{x4} \Rightarrow \sigma_{z2} \sigma_3^+ \sigma_{x4} \Rightarrow$ *Parity Set*
- even q_j : $\hat{a}_2 = \frac{1}{2}(\sigma_{z1}\sigma_{x2} + I\sigma_{y_2})\sigma_{x4}$, $\hat{a}_4 = \frac{1}{2}(\sigma_{z2}\sigma_{z3}\sigma_{x4} + i\sigma_{y_4})$
- odd q_j Needs another set the Flip Set, the Flip Set $\subset$ Parity Set.

II – Microscopic quark description of Hadrons

It is important to emphasise that whatever model/approximation to QCD one favours to address hadronic states, it should obey to three conditions:

- It has to "contain" confinement,
- It has to be chiral symmetric and, despite that,
- possess a mechanism for spontaneous breaking of chiral symmetry ($S\chi SB$). There is a class of models which can address, at one stroke, all the three above conditions: they are chiral symmetric, they display $S\chi SB$, and, on top, they allow for chiral restoration. This class of models can be thought as to address QCD in the Gaussian approximation for gluonic cummulants.

- the Hamiltonian we will be using, reads,

$$
\begin{aligned}
H_{\text{eff.}} &= \int d\mathbf{x}\bar{\psi}(\mathbf{x},t)\overbrace{(-i\alpha\cdot\nabla+\beta m)}^{\mathcal{K}}\psi(\mathbf{x},t) - \\
&- \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\rho^a_\mu(\mathbf{x},t)\mathcal{V}^{ab}_{\mu\nu}(\mathbf{x}-\mathbf{y})\rho^b_\nu(\mathbf{y},t), \qquad (1)
\end{aligned}
$$

- with,

$\rho^a_\mu(\mathbf{x},t) = \bar{\psi}(\mathbf{x},t)\gamma_\mu\frac{\lambda^a}{2}\psi(\mathbf{x},t),\ \mathcal{V}^{ab}_{\mu\nu}(\mathbf{x}-\mathbf{y}) = g_{\mu 0}g_{\nu 0}\delta^{ab}V_0(|\mathbf{x}-\mathbf{y}|)$

and,

$$
\psi_{fc}(\mathbf{x},t) = \sum_s\int\frac{d\mathbf{k}}{(2\pi)^3}[u_s(\mathbf{k})b_{fcs}(\mathbf{k})e^{-ik_0t}+v_s(\mathbf{k})d^\dagger_{fcs}(-\mathbf{k})e^{ik_0t}]e^{i\mathbf{k}\cdot\mathbf{x}},
$$

Bogolioubov Transformations

- ψ_{fc} can be thought as an inner product between a Fock space $\mathcal{F} = \left\{\hat{b}, \hat{d}\right\}$ and an Hilbert space $\mathcal{H} = \{u, v\}$:

$$\psi_{fc} = \{u(k), v(k)\} \cdot \left\{\hat{b}, \hat{d}^{\dagger}\right\} = \{u(k), v(k)\}\, \mathcal{R}(\phi)^T \mathcal{R}(\phi) \left\{\hat{b}, \hat{d}^{\dagger}\right\}$$

$$\mathcal{R}(\phi) = \begin{bmatrix} \widehat{B} \\ \widehat{D}^{+} \end{bmatrix}_s = \begin{bmatrix} \cos\phi & -\sin\phi M_{ss'} \\ \sin\phi M^{\star}_{ss'} & \cos\phi \end{bmatrix} \begin{bmatrix} \widehat{b} \\ \widehat{d}^{+} \end{bmatrix}_{s'}$$

- With, the $^3P_0$ Coupling (Parity $+$):

$$M_{ss'} = -\sqrt{8\pi} \sum_{m_l m_s} \begin{bmatrix} 1 & 1 & |0 \\ m_l & m_s & |0 \end{bmatrix} \times \begin{bmatrix} 1/2 & 1/2 & |1 \\ s & s' & |m_s \end{bmatrix} \hat{k}_{1m_l} \left|\frac{1}{2}, s\right\rangle\left\langle\frac{1}{2}, s'\right|$$

- The new Vacuum is:

$$|\widetilde{0}>= Exp\left\{\widehat{Q}_0^+ - \widehat{Q}_0\right\}|0>$$

$$\widehat{Q}_0^+(\Phi) = \sum_{cf}\int d^3p\,\phi(p)\,M_{ss'}(\hat{p})\widehat{b}_{fcs}^+(\mathbf{p})\,\widehat{d}_{fcs'}^+(-\mathbf{p})$$

- So the new spinors associated with the new Fock space must read

$$\left[\begin{array}{c} U \\ V \end{array}\right]_{p,s} = \left[\begin{array}{cc} \cos\phi(p) & -\sin\phi(p)\; M^*_{ss'}(\hat{p}) \\ \sin\phi(p)\; M_{ss'}(\hat{p}) & \cos\phi(p) \end{array}\right]\left[\begin{array}{c} u \\ v \end{array}\right]_{p,s}$$

.

- Therefore,

$$\psi_{fc}(\mathbf{x},t) = \sum_s \int \frac{d\mathbf{k}}{(2\pi)^3}[U_s(\mathbf{k})B_{fcs}(\mathbf{k})e^{-ik_0t}+V_s(\mathbf{k})D^\dagger_{fcs}(-\mathbf{k})e^{ik_0t}]e^{i\mathbf{k}\cdot\mathbf{x}},$$

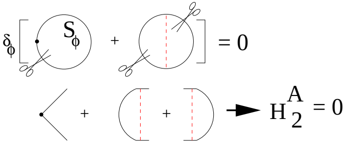
Mass Gap equation

- In general, after Wick contractions, any quartic Hamiltonian $H = \widehat{H}_{normal}[\phi] + \widehat{H}_{anomalous}[\phi]$ with $\widehat{H}|0>= \widehat{H}_{anomalous}[\phi]|0> \neq 0$.
- $\widehat{H}_{2\ [normal]} = \int d^3p\, E(p) \left[\widehat{b}^+_{fsc}\mathbf{p})\widehat{b}_{fsc}(\mathbf{p}) + \widehat{d}^+_{fsc}(-\mathbf{p})\widehat{d}_{fsc}(-\mathbf{p})\right]$,
- with $E(p) = A(p)\sin\varphi + B(p)\cos(\varphi(p))$
- $\widehat{H}_{2\ [anomalous]} =$
  $\int d^3p\, [A[p]S_\varphi) - B[p]C_\varphi] \times \left[M_{ss'}\,\widehat{b}^+_{fsc}(\mathbf{p})\widehat{d}^+_{fsc}(-\mathbf{p}) + h.c.\right]$
- Find function $[\varphi(p)]$, such that $[A[p]\sin(\varphi) - B[p]\cos(\varphi)] = 0$
- $A(p) = E(p)\sin(\varphi(p)); B(p) = E(p)\cos(\varphi(p))$
- $S_f = \dfrac{i}{\not p - m \underbrace{-(A(p) - m) - (p - B(p)\hat{\not p}}_{\Sigma(p)}}$

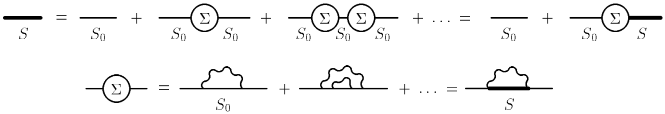
We have several ways of obtaining the mass Gap

1. Variation in φ:,

It is the same as to cut the fermion propagators S_ϕ,



2. The full propagator $S(p)$ is given by the Dyson series



3. Ward identity $i(p-p')^\mu \Gamma_\mu(p,p') = S_f^{-1}(p') - S_f^{-1}(p)$, with,

$$\Gamma_\mu(p,p') = \gamma_\mu + i\int \frac{d^4q}{(2\pi)^4} K(q)\Omega\, S(p'+q)\times\Gamma_\mu(p'+q,p+q)\Omega S(p'+q)$$

Bethe-Salpeter Equations

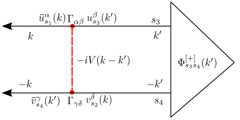
Using the diagrammatic blocks we can also construct Bethe-Salpeter equations (BS) for the mesonic states, namely

$$\Phi^{[+]}_{s_1 s_2}(\mathbf{k},0)=$$

$$=\int \frac{d^4k'}{(2\pi)^4} \mathcal{S}_q(\vec{k}',\tfrac{M}{2}+w)\, \mathcal{S}_{\bar{q}}(-\vec{k}',\tfrac{M}{2}-w)\times$$

$$\times\left[\bar{u}^{\alpha}_{s_1}(\vec{k})\Gamma_{\alpha\beta}\, u^{\beta}_{s_1}(\vec{k}')\right]\left[\bar{v}^{\gamma}_{s_4}(\vec{k}')\Gamma_{\gamma\delta}\, v^{\delta}_{s_2}(\vec{k})\right]\times$$

$$\times[+i\mathcal{V}(\vec{k}-\vec{k}')]\ \Phi^{[+]}_{s_3 s_4}(\vec{k}')$$



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$$-$$

$$\int \frac{d^4k'}{(2\pi)^4} \mathcal{S}_q(\vec{k}',-\tfrac{M}{2}+w)\, \mathcal{S}_{\bar{q}}(-\vec{k}',-\tfrac{M}{2}-w)\times$$

$$\times\left[\bar{u}^{\alpha}_{s_1}(\vec{k})\Gamma_{\alpha\beta}\, v^{\beta}_{s_1}(\vec{k}')\right]\left[\bar{u}^{\gamma}_{s_4}(\vec{k}')\Gamma_{\gamma\delta}\, v^{\delta}_{s_2}(\vec{k})\right]\times$$

$$\times[-i\mathcal{V}(\vec{k}-\vec{k}')]\ \Phi^{[-]}_{s_3 s_4}(\vec{k}'),$$

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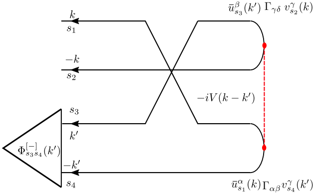


- If we integrate out the quark energies and then proceed to integrate it, from the left, with $\int \frac{d^3k}{(2\pi)^3} {\Phi^{[+]}}^{\dagger}_{s_1 s_2}(\mathbf{k}, 0)$ we get,

$$\int \frac{d^3k}{(2\pi)^3} \Big[{\Phi^{[+]}}^{\dagger}_{s_1 s_2}(k)(E_q(k) + E_{\bar{q}}(k)){\Phi^{[+]}}_{s_1 s_2}(k) + \\ + \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} {\Phi^{[+]}}^{\dagger}_{s_1 s_2}(k) \mathcal{V}_{s_1 s_2; s_3 s_4}(k, k') {\Phi^{[+]}}_{s_3 s_4}(k') \Big] = M.$$

- Sums in the spin indices are understood and $\mathcal{V}_{s_1 s_2; s_3 s_4}(k, k\prime)$ stands for $\left[\bar{u}^{\alpha}_{s_1}(\vec{k})\Gamma_{\alpha\beta} u^{\beta}_{s_1}(\vec{k}')\right] \left[-i\mathcal{V}(\vec{k} - \vec{k}')\right] \left[\bar{v}^{\gamma}_{s_4}(\vec{k}')\Gamma_{\gamma\delta} v^{\delta}_{s_2}(\vec{k})\right]$
- Then, provided we define the constants,

$$U = \int \frac{d^3k}{(2\pi)^3} \left[{\Phi^{[+]}}^{\dagger}_{s_1 s_2}(k)(E_q(k) + E_{\bar{q}}(k)){\Phi^{[+]}}_{s_1 s_2}(k) \right]$$

$$V = \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} {\Phi^{[+]}}^{\dagger}_{s_1 s_2}(k) \mathcal{V}_{s_1 s_2; s_3 s_4}(k, k') {\Phi^{[+]}}_{s_3 s_4}(k'),$$

An effective qubit equivalent Hamiltonian

- we can build, in an abstract space of qubits $|q_1 q_2 ...\rangle$, an Hamiltonian that for the sub-sector $|q_1, q_2\rangle$ has the same eigenvalues than the Hamiltonian:

$$\hat{H} = \frac{1}{2} U(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2) + V(\hat{a}_1^\dagger \hat{a}_1 \hat{a}_2^\dagger \hat{a}_2),$$

  where $\hat{a}_1^\dagger |0, q_2\rangle = |1, q_2\rangle$ and $\hat{a}_1 |1, q_2\rangle = |0, q_2\rangle$. A similar expression for $\hat{a}_2$, with $\hat{a}_1$ acting as a representative for the quark and $\hat{a}_1$ for the antiquark.
- We can substitute the integrals by a grid of sums which will be tantamount to introduce a "grid pair of qubit operators"
- Once this is done we can replace the qubit operators by, either Jordan-Wigner operators or Bravyi-Kitaev operators and use, if needed be, quantum computing to evaluate them.

Example of a calculation

- As a generic example let's consider

$$H_{\text{eff.}}^{q_1\bar{q}_2} = H_{\text{const.}} + \frac{1}{2}V_{q_1}\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{1}{2}V_{\bar{q}_2}\left(a_4^\dagger a_4 + a_3^\dagger a_3\right) + $$
$$+\frac{1}{2}U\left(a_1^\dagger a_1 a_3^\dagger a_3 + a_2^\dagger a_2 a_4^\dagger a_4\right) + V_{cross}\left(a_1 a_4 a_3 a_2\right) + V_{cross}\left(a_1^\dagger a_4^\dagger a_3^\dagger a_2^\dagger\right).$$

- After a B-K transformation we get,

$$H_{BK} = H_{\text{const.}} + \frac{1}{8}(2(U + 2(V_{q_1} + V_{q_2}))-$$
$$-(U + 2V_{q_1})(\sigma_{z1} + \sigma_{z1}\sigma_{z2}) - (U + 2V_{q_2})(\sigma_{z3} + \sigma_{z2}\sigma_{z3}\sigma_{z4})+$$
$$+U(\sigma_{z1}\sigma_{z3} + \sigma_{z1}\sigma_{z3}\sigma_{z4})-$$
$$-V_{\text{cross}}\{(\sigma_{x1}\sigma_{z2}\sigma_{x3} + \sigma_{x1}\sigma_{x3}\sigma_{z4} + \sigma_{x1}\sigma_{z2}\sigma_{x3}\sigma_{z4} + \sigma_{x1}\sigma_{x3})-$$
$$-(\sigma_{y_1}\sigma_{z2}\sigma_{y_3} + \sigma_{y_1}\sigma_{y_3}\sigma_{z4} + \sigma_{y_1}\sigma_{z2}\sigma_{y_3}\sigma_{z4} + \sigma_{y_1}\sigma_{y_3})\})$$

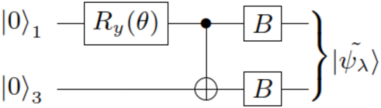
- qubits 2 and 4 are only acted upon by σ_z. Therefore these two qubits can be removed and the Hamiltonian and eigenstate can be simplified to:

$$\begin{aligned}\tilde{H}_{BK} = H_{\text{const.}} + \frac{1}{4}(U + 2(V_{q_1} + V_{q_2}) \\ - (U + 2V_{q_1})\,\sigma_{z1} - (U + 2V_{q_2})\,\sigma_{z3} + U\,\sigma_{z1}\sigma_{z3} \\ + 2V_{\text{cross}}\,\left(\sigma_{y1}\sigma_{y3} - \sigma_{x1}\sigma_{x3}\right))\end{aligned}$$

with, $|\tilde{\psi}_\lambda\rangle = a|00\rangle + b|11\rangle,\ |a|^2 + |b|^2 = 1$

Qiskit Explanation

- Let us choose a given θ, say,$\pi/6$. Then $|\tilde{\psi}_\lambda\rangle = \frac{\sqrt{3}}{2}|00\rangle + \frac{1}{2}|11\rangle$



$\langle 00|\sigma_{z1}\ \sigma_{z3}|00\rangle = \langle 0|\sigma_{z1}|0\rangle\langle 0|\sigma_{z3}|0\rangle) =$
$1 \times\ 1 = 1$
$\langle 11|\sigma_{z1}\ \sigma_{z3}|11\rangle = -1 \times\ -1 = 1$

So in this case the average of the 8192 times will

be 1 no matter what.

- $\sigma_{x1}\ \sigma_{x3}$ case ($\sigma_{y1}\ \sigma_{y3}$ case is similar). Let $S = B^\dagger$ be the unitary operator that changes basis from Z to X, then:

$\langle\tilde{\psi}_\lambda|X|\tilde{\psi}_\lambda\rangle \Rightarrow \langle\tilde{\psi}_\lambda|(SS^\dagger)X(SS^\dagger)|\tilde{\psi}_\lambda\rangle = \langle\tilde{\psi}_\lambda|S(S^\dagger\ X\ S)S^\dagger|\tilde{\psi}_\lambda\rangle = \langle\tilde{\psi}_x|Z|\tilde{\psi}_x\rangle$

- After B gate:

$|\tilde{\psi}_\lambda\rangle = \frac{\sqrt{3}}{2}|00\rangle + \frac{1}{2}|11\rangle \to \frac{1+\sqrt{3}}{4}|00\rangle + \frac{\sqrt{3}-1}{4}|10\rangle + \frac{\sqrt{3}-1}{4}|01\rangle + \frac{1+\sqrt{3}}{4}|11\rangle \Rightarrow$

$\Rightarrow |\tilde{\psi}_\lambda\rangle = \frac{1+\sqrt{3}}{4}|00\rangle_{xx} + \frac{1+\sqrt{3}-1}{4}|10\rangle_{xx} + \frac{\sqrt{3}-1}{4}|01\rangle_{xx} + \frac{\sqrt{3}+1}{4}|11\rangle_{xx}$

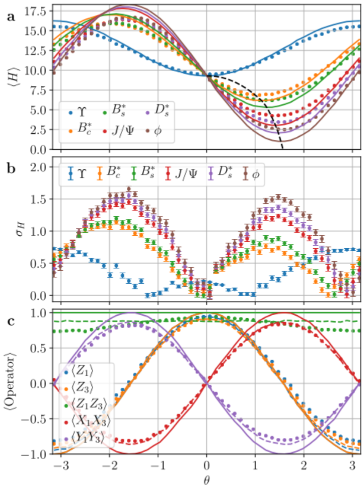
$\langle 00_{zz}|\sigma_{x1}\ \sigma_{x3}|00_{zz}\rangle = \langle 00_{xx}|\sigma_{z1}\ \sigma_{z3}|00_{xx}\rangle \ldots$

Testing Quantum Computation

	m	$H_{\text{const.}}$	V_{q_1}	$V_{\bar{q}_2}$	U	V_{cross}
Υ	9.280	9.280	2.320	2.320	2.320	0.000
B_c^*	6.155	9.280	0.759	2.320	1.540	4.919
B_s^*	5.312	9.280	0.250	2.320	1.285	5.571
J/Ψ	3.038	9.280	0.759	0.759	0.759	7.293
D_s^*	2.072	9.280	0.759	0.250	0.505	7.929
ϕ	1.000	9.280	0.250	0.250	0.250	8.647

  Table: Test parameters. They are not physical but merely used here as a demonstration set for quantum computing.

- By measuring this state in the appropriate basis several times, we can determine the expectation value of each Pauli term in the Hamiltonian, one at a time (we have the 5 terms σ_{z1}, σ_{z3}, $\sigma_{z1}\sigma_{z3}$, $\sigma_{x1}\sigma_{x3}$, and $\sigma_{y_1}\sigma_{y_3}$Y). Each expected value was calculated using 8192 measurements. In order to minimize the necessary runs in the quantum device, the same runs were used for all the particles



Testing Quantum Computation

Fig:

(a) $\langle H \rangle(\theta)$ using the exact solution (lines), and the experimental solution (points), for different particles. The black dashed line roughly indicates the position of the expected minima. (b) Deviation from exact result, with errorbars indicating the standard deviation of $\langle H \rangle(\theta)$, associated with the stochasticity of the measured results. (c) Comparison of the exact (solid lines) and experimental (points) results of the expected value of each Pauli term composing the Hamiltonian. The deviation can be mostly explained by the effect of quantum device errors (dashed lines).