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Quantum Computation for the Understanding of Mass

Simulating Quantum Field Theories

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Introduction

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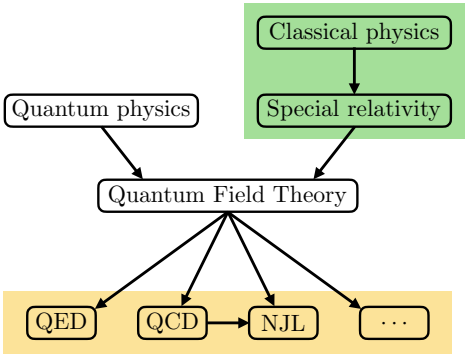
Nature is described through the mathematical framework provided by **Quantum Field Theory**.

- The different implementations of Quantum Field Theory are referred to as quantum field theories themselves.
- Quantum Chromodynamics (QCD) is the theory of the strong nuclear force.
- QCD holds many mysteries (e.g. **mass generation** phenomena).
- Many aspects of quantum field theories cannot be studied using classical computers.
- Physicists seek alternative tractable models to study interesting aspects of QCD.



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The Nambu–Jona-Lasino model (NJL) I

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An important path forward is to develop methods to simulate these models on quantum computers. This effort is only just beginning, however, it has only been achieved for relatively simple problems.

- **Nambu–Jona-Lasino model** (NJL) in $1+1$ dimensions: an effective field theory, regarded as a low-energy approximation to QCD.
- Originally developed pre-QCD to describe nucleons via an effective two-body point interaction. Nowadays gets reinterpreted as a theory of quarks.
- Inspired by the **BCS theory of superconductivity**.
- It retains certain key features of QCD, such as the so called Goldstone modes and **dynamical chiral symmetry breaking**; which in turn is responsible for the creation of dressed mass.
- This model can be solved nonperturbatively through the standard leading order truncation; an important characteristic since verifying the solutions returned by any quantum computation is currently a major challenge.

The Nambu–Jona-Lasino model (NJL) II

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The NJL **Lagrangian density** that we will make use of looks like:

$$\mathcal{L}(x) = \bar{\psi}_\alpha(x)\left(\delta_{\alpha\beta} i\partial\!\!\!/ - \hat{m}_{\alpha\beta}\right)\psi_\beta(x) + \mathcal{L}_I(x)$$

$$\mathcal{L}_I(x) = \frac{1}{2} G_\pi \left[\bar{\psi}_\alpha(x)\psi_\alpha(x)\right]^2$$

From this expression for the Lagrangian density we can obtain the corresponding **Hamiltonian density** through the Legendre transform. In special, for $1+1$ dimensions:

$$\mathcal{H} = -\frac{i}{2}\bar{\psi}_\alpha\gamma^1(\partial_1\psi_\alpha) + \frac{i}{2}\left(\partial_1\bar{\psi}_\alpha\right)\gamma^1\psi_\alpha + \bar{\psi}_\alpha\hat{m}_{\alpha\beta}\psi_\beta - \frac{1}{2}G_\pi\left(\bar{\psi}_\alpha\psi_\alpha\right)^2$$

Dressed mass and the gap equation I

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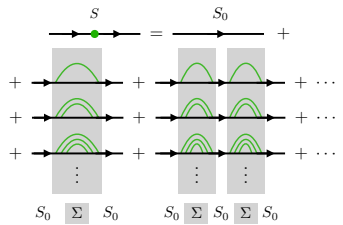
The **bare and dressed masses** appear on the bare quark propagator S_0, and the NJL dressed quark propagator S respectively:

$$S_0^{-1} \triangleq \not{p} - m + i\varepsilon$$

$$S^{-1} \equiv S_{\text{NJL}}^{-1} \triangleq \not{p} - M + i\varepsilon$$



We can find a relationship between these two by solving the **gap equation**:

$$S^{-1} = S_0^{-1} - 2iG_\pi \int \frac{\mathrm{d}^2 p}{(2\pi)^2} N_{\text{color}} N_{\text{flavor}} \mathrm{Tr}_{\mathrm{D}}[S]$$

$$M \simeq m + 4iG_\pi N_{\text{color}} N_{\text{flavor}} \int \frac{\mathrm{d}^2 p}{(2\pi)^2} \frac{M}{p^2 - M^2}$$

Dressed mass and the gap equation II

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To solve this last expression we first perform a **Wick rotation** $p_0 \to ip_2 \quad \Rightarrow \quad (p_0)^2 \to -(p_2)^2$, followed by a transformation to **polar coordinates**:

$$M \simeq m + N_{\text{color}} N_{\text{flavor}} \frac{G_\pi}{\pi} \int_0^\infty \frac{M}{p_E^2 + M^2} \mathrm{d}p_E^2$$

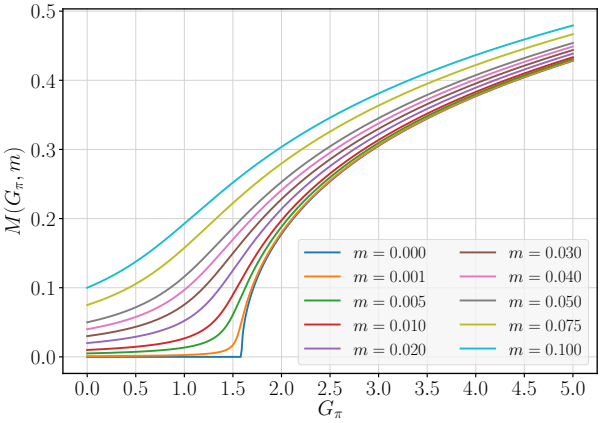
Finally, to make the integral converge, we introduce **proper time regularization**:

$$\frac{1}{x^n} = \frac{1}{(n-1)!} \int_0^\infty \mathrm{d}\tau\, \tau^{n-1} \exp[-\tau x] \to \frac{1}{(n-1)!} \int_{1/\Lambda_{UV}^2}^{1/\Lambda_{IR}^2} \mathrm{d}\tau\, \tau^{n-1} \exp[-\tau x]$$

$$M \simeq m + M N_{\text{color}} N_{\text{flavor}} \frac{G_\pi}{\pi} \int_{1/\Lambda_{UV}^2}^{1/\Lambda_{IR}^2} \frac{\mathrm{d}\tau}{\tau} \exp\left[-\tau M^2\right]$$

Where Λ_{IR} and Λ_{UV} are the **infrared and ultraviolet cutoffs** respectively.

Dressed mass and the gap equation III



N_{Dirac}	N_{color}	N_{flavor}	Λ_{IR}	Λ_{UV}
$1+1 \to 2$	1	1	0.240 GeV	0.645 GeV

Lattice formulation I

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We can define the Hamiltonian of the system as the integral over space of the Hamiltonian density:

$$H = \int \mathcal{H}(x)\mathrm{d}x = \int \left\{ \bar{\psi}_\alpha(x)\left(\hat{m}_{\alpha\beta} - \delta_{\alpha\beta} i\gamma^1\partial_1\right)\psi_\beta(x) - \frac{1}{2}G_\pi\left[\bar{\psi}_\alpha(x)\psi_\alpha(x)\right]^2 \right\}\mathrm{d}x$$

For a basis where:

$$\psi_\alpha = \begin{bmatrix}\psi_{\alpha,+}\\ \psi_{\alpha,-}\end{bmatrix}, \quad \bar{\psi}_\alpha \triangleq \psi_\alpha^\dagger\gamma^0, \quad \gamma^0 = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \quad \gamma^1 = \begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}$$

Dropping the flavor indices to avoid clutter we can then write the kinetic term as:

$$\bar{\psi}\left(-i\gamma^1\partial_1\right)\psi = \frac{i}{2}\left\{\left[\psi_+^\dagger(\partial_1\psi_-) - \left(\partial_1\psi_+^\dagger\right)\psi_-\right] + \left[\psi_-^\dagger(\partial_1\psi_+) - \left(\partial_1\psi_-^\dagger\right)\psi_+\right]\right\}$$

Lattice formulation II

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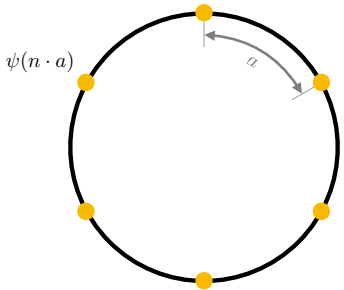
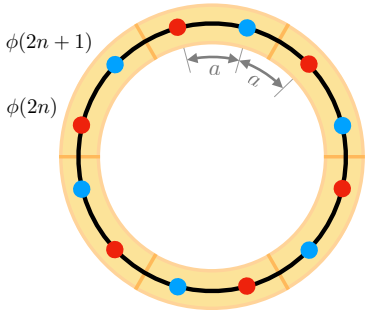
The two groups in brackets are essentially equivalent to one another by virtue of exchanging positive and negative energy components. This is the motivation behind **staggered fermion lattices**, which use two computational lattice sites for each theoretical value of ψ.





Lattice formulation III

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Sites in the staggered computational lattice are labeled using a parameter $n \in \mathbb{Z}$ such that all evaluations of ψ are made at integer multiples of the distance a:

$$\phi(n) \triangleq \sqrt{a} \begin{cases} \psi_+\left(\frac{n}{2}a\right), & 2 \mid n \\ \psi_-\left(\frac{n-1}{2}a\right), & 2 \nmid n \end{cases}$$

These newly defined operators obey the **canonical commutation relations for fermions**:

$$\left[\phi^\dagger(p), \phi(q)\right]_+ = \delta_{pq}\,, \quad \left[\phi(p), \phi(q)\right]_+ = 0$$

Finally, thanks to the periodic boundary conditions, we can write:

$$H_N^{(K)} = \frac{i}{2a} \sum_{n=0}^{2N-1} \left[\phi^\dagger(n)\phi(n+1) - \phi^\dagger(n+1)\phi(n)\right]$$

Lattice formulation IV

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From this Hamiltonian, we can now recover the **masless Dirac equation** in the continuum limit; which serves as proof of correctness:

$$\dot{\phi}(n) = i\left[H_N^{(K)}, \phi(n)\right]_- = \frac{\phi(n+1) - \phi(n-1)}{2a}$$

In terms of the original fields, this is:

$$\dot{\psi_+} = \frac{\Delta\psi_-}{\Delta x}, \quad \dot{\psi_-} = \frac{\Delta\psi_+}{\Delta x}$$

Lastly, taking the limit when $a \to 0$:

$$\frac{\partial}{\partial t}\psi = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial x}\psi \equiv \hat{\alpha}_1 \frac{\partial}{\partial x}\psi$$

Multi-flavor lattice I

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To obtain the other components of the Hamiltonian from the expressions in the Hamiltonian density, which are written in terms of **Dirac bilinears**, we need to restore the flavor indices and deal with them in the computational lattice.

Assuming that each flavor is independent, we could simply repeat the same procedure over different computational lattices and sum the results for all flavors. For instance, assuming that the **mass matrix is diagonal** (i.e. $\hat{m}_{\alpha\beta} = \text{diag}[m_0, m_1, \ldots]$):

$$\int \bar{\psi}_\alpha \psi_\alpha \mathrm{d}x \quad \rightarrow \quad \sum_{n=0}^{N-1} \left[\phi_\alpha^\dagger(2n)\phi_\alpha(2n) - \phi_\alpha^\dagger(2n+1)\phi_\alpha(2n+1) \right] = \sum_{n=0}^{2N-1} (-1)^n \phi_\alpha^\dagger(n)\phi_\alpha(n)$$

Multi-flavor lattice II

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However the interaction will always introduce **cross-flavor terms** rendering this invalid:

$$\int \left(\sum_{\alpha} \bar{\psi}_{\alpha} \psi_{\alpha} \right)^2 \mathrm{d}x \;=\; \int \left[\sum_{\alpha} \left(\bar{\psi}_{\alpha} \psi_{\alpha} \right)^2 + 2 \sum_{\alpha < \beta} \left(\bar{\psi}_{\alpha} \psi_{\alpha} \right) \left(\bar{\psi}_{\beta} \psi_{\beta} \right) \right] \mathrm{d}x$$

To solve this, we will build a single computational lattice with all the components of the field associated to different flavors stitched together back-to-back. The resulting operators are:

$$\phi_{\alpha}(n) \equiv \phi(n + 2N\alpha) \triangleq \sqrt{a} \begin{cases} \psi_{\alpha,+}\left(\frac{n}{2} a\right), & 2 \mid n \\ \psi_{\alpha,-}\left(\frac{n-1}{2} a\right), & 2 \nmid n \end{cases}$$

$$\left[\phi_{\alpha}^{\dagger}(p), \phi_{\beta}(q) \right]_{+} = \delta_{\alpha\beta} \delta_{pq}\,, \quad \left[\phi_{\alpha}(p), \phi_{\beta}(q) \right]_{+} = 0$$

Multi-flavor lattice III

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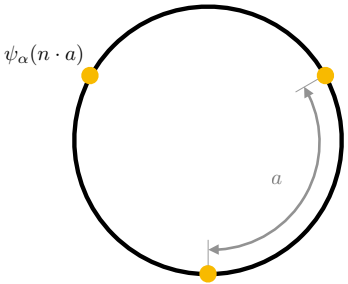
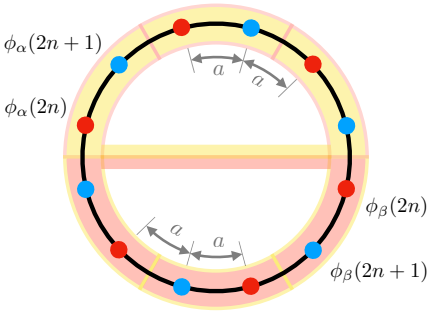
With **periodic boundary conditions** applied on each flavor separately (i.e. not crossing over to other flavors $\phi_\alpha(2N) = \phi_\alpha(0) \neq \phi_{\alpha+1}(0)$).





Multi-flavor lattice IV

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All in all, we obtain the following discretized NJL Hamiltonian for $1+1$ dimensions, any number of flavors N_{flavor}, N physical lattice sites, and $2N \cdot N_{\text{flavor}}$ computational lattice sites:

$$H_N = H_N^{(M)} + H_N^{(K)} + H_N^{(G)}$$

$$H_N^{(M)} = \sum_{\alpha} \sum_{n=0}^{2N-1} (-1)^n \, m_\alpha \phi_\alpha^\dagger(n) \phi_\alpha(n)$$

$$H_N^{(K)} = \frac{i}{2a} \sum_{\alpha} \sum_{n=0}^{2N-1} \left[\phi_\alpha^\dagger(n) \phi_\alpha(n+1) - \phi_\alpha^\dagger(n+1) \phi_\alpha(n) \right]$$

$$H_N^{(G)} = -\frac{G_\pi}{2a} \sum_{n=0}^{N-1} \left[\sum_{\alpha} \tilde{H}_N^{\alpha\alpha}(n) + 2 \sum_{\alpha<\beta} \tilde{H}_N^{\alpha\beta}(n) \right]$$

$$\tilde{H}_N^{\alpha\beta}(n) \triangleq \left[\phi_\alpha^\dagger(2n) \phi_\alpha(2n) - \phi_\alpha^\dagger(2n+1) \phi_\alpha(2n+1) \right] \times \left[\phi_\beta^\dagger(2n) \phi_\beta(2n) - \phi_\beta^\dagger(2n+1) \phi_\beta(2n+1) \right]$$

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Fermion-qubit mappings

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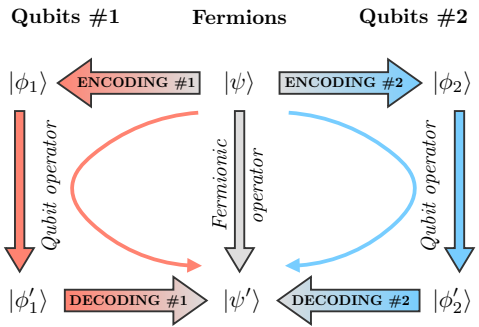
Generally speaking, quantum computers cannot work with any given operator directly. Therefore, in order to simulate this or any other Hamiltonian in a quantum processor, one needs to efficiently map its component operators onto ones suitable for operating in such machines. The most commonly used of these is the **Pauli set**.



Jordan-Wigner mapping I

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The Pauli exclusion principle introduces a powerful liaison between fermions in the same quantum state. For this reason, even a non-interacting gas of fermions is still highly correlated. However, it turns out that in one spatial dimension spin-$\frac{1}{2}$ particles (i.e. qubits) behave much like fermions. Particularly, we choose:

$$|\uparrow\rangle \equiv |0\rangle\,, \quad |\downarrow\rangle \equiv |1\rangle$$
$$|\downarrow\rangle \equiv \phi^\dagger\,|0\rangle\,, \quad |\uparrow\rangle \equiv \phi\,|1\rangle$$
$$\phi \to \sigma^+\,, \quad \phi^\dagger \to \sigma^-$$

The mapping that the Jordan–Wigner transform introduces is designed on the **occupation number basis**, which associates spin “down” and “up” with occupied and unoccupied fermion states respectively (or vice versa).

Jordan-Wigner mapping II

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To prove that this is valid, we can define the following equivalences by drawing inspiration from raising and lowering operators in angular momentum theory:

$$\sigma^1 \equiv \phi^\dagger + \phi$$
$$\sigma^2 \equiv i\left(\phi^\dagger - \phi\right)$$
$$\sigma^3 \equiv 1 - 2\phi^\dagger\phi$$

Making use of the properties of fermion creation and annihilation operators, comprised within their canonical commutation relations, these can be shown to behave algebraically like **Pauli matrices**:

$$\left[\sigma^p, \sigma^q\right]_- = 2i\epsilon_{pqr}\sigma^r$$
$$\left[\sigma^p, \sigma^q\right]_+ = 2\delta_{pq}$$

Jordan-Wigner mapping III

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We can recover the usual spin raising and lowering hermitian conjugate operators:

$$\sigma^{\pm} \triangleq \frac{1}{2}\left(\sigma^1 \pm i\sigma^2\right)$$

All this allows us to use these spins as a basic model for fermions:

$$\left[\phi, \phi^\dagger\right]_+ = 1 \quad \rightarrow \quad \left[\sigma^+, \sigma^-\right]_+ = 1$$

Unfortunately, this only works for single-fermion representations; since independent spins commute, while independent fermions anticommute.

$$\left[\sigma^+(p), \sigma^-(q)\right]_- = \delta_{pq}\,, \quad \left[\sigma^+(p), \sigma^-(q)\right]_+ \neq \delta_{pq}$$
$$\left[\phi(p), \phi^\dagger(q)\right]_- \neq \delta_{pq}\,, \quad \left[\phi(p), \phi^\dagger(q)\right]_+ = \delta_{pq}$$

Jordan-Wigner mapping IV

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A way to fix this issue is by defining $N(l) = \phi^\dagger(l)\phi(l)$ as the hermitian number operator for state l, and attaching a so called unitary **string operator** $S(n)$ to the fermion operators:

$$S(n)\phi(n) \to \sigma^+(n)$$
$$\phi^\dagger(n)S^\dagger(n) \to \sigma^-(n)$$
$$S(n) = \exp\Big[-i\pi\textstyle\sum_{l<n}\big[N(l) + s(l)\big]\Big]$$

The $s(l)$ terms in the string operator are scalars associated to **gauge transformations** and do not add much to the transform. With this new mapping, Pauli matrices get redefined to:

$$\sigma^1(n) \equiv \phi^\dagger(n)S^\dagger(n) + S(n)\phi(n)$$
$$\sigma^2(n) \equiv i\Big[\phi^\dagger(n)S^\dagger(n) - S(n)\phi(n)\Big]$$
$$\sigma^3(n) \equiv 1 - 2\phi^\dagger(n)\phi(n)$$

Jordan-Wigner mapping V

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We now retrieve the correct statistics. Of course, we would like to express the string operator in terms of the Pauli set so that we can move it to the other side of the transformation. Fortunately, we can do so by expanding the number operators:

$$\exp\left[\pm i\pi \sum_{l<n} N(l)\right] = \prod_{l<n} \exp\left[\pm i\pi \phi^\dagger(l)\phi(l)\right] = \prod_{l<n}\left[1 - 2\phi^\dagger(l)\phi(l)\right] = \prod_{l<n} \sigma^3(l)$$

$$S(n) = \prod_{l<n} e^{-i\pi s(l)}\sigma^3(l)$$

Finally, our **choice of gauge** will be such that $s(l) = s \in (-1, 1]\ \forall l$ and the string operator is hermitian for all values of n. All in all, this can be achieved by making $s = 0$, which gives:

$$\phi(n) \to \left[\prod_{l<n} \sigma^3(l)\right]\sigma^+(n)\,, \quad \phi^\dagger(n) \to \left[\prod_{l<n} \sigma^3(l)\right]\sigma^-(n)$$

Jordan-Wigner mapping VI

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Lastly, we need to bring back flavor indices. The form of the transform will in fact be the same but, for clarity, we would like to write them down them explicitly. This will prove to be useful when dealing with the periodic boundary conditions. For this, all we need recalling is that the flavor sub-lattices had been stitched back-to-back in the final computational lattice:

$$\phi_\alpha(n) \to S_\alpha(n)\sigma_\alpha^+(n) = \left[\prod_{\beta=0}^{\alpha-1}\tilde{\sigma}_\beta^3(2N)\right]\tilde{\sigma}_\alpha^3(n)\sigma_\alpha^+(n)$$

$$\phi_\alpha^\dagger(n) \to S_\alpha^\dagger(n)\sigma_\alpha^-(n) = \left[\prod_{\beta=0}^{\alpha-1}\tilde{\sigma}_\beta^3(2N)\right]\tilde{\sigma}_\alpha^3(n)\sigma_\alpha^-(n)$$

$$S_\alpha(n) \triangleq S(n+2N\alpha)\,, \qquad \tilde{\sigma}_\alpha^3(n) \triangleq \prod_{l<n}\sigma_\alpha^3(l)$$

Refactoring the NJL Hamiltonian I

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Now that we have a way of converting from fermion to spin operators, let's apply it to the NJL Hamiltonian. To do so, we will make use of the Jordan–Wigner transform, and it is convenient to note some previous mappings first:

$$
\begin{aligned}
\phi_\alpha^\dagger(n)\phi_\alpha(n) &\rightarrow \frac{1}{2}\left[1-\sigma_\alpha^3(n)\right] \\
\phi_\alpha^\dagger(n)\phi_\alpha(n)-\phi_\alpha^\dagger(n+1)\phi_\alpha(n+1) &\rightarrow \frac{1}{2}\left[\sigma_\alpha^3(n+1)-\sigma_\alpha^3(n)\right] \\
\phi_\alpha^\dagger(n)\phi_\alpha(n+1) &\rightarrow \sigma_\alpha^-(n)\sigma_\alpha^+(n+1) \\
\phi_\alpha^\dagger(n+1)\phi_\alpha(n) &\rightarrow \sigma_\alpha^-(n+1)\sigma_\alpha^+(n) \\
\phi_\alpha^\dagger(n)\phi_\alpha(n+1)-\phi_\alpha^\dagger(n+1)\phi_\alpha(n) &\rightarrow \frac{1}{2i}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right]
\end{aligned}
$$

Refactoring the NJL Hamiltonian II

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Hence, the different parts of the Hamiltonian are:

$$
\begin{aligned}
H_N^{(M)} &\rightarrow \frac{m}{2}\sum_{\alpha}\sum_{n=0}^{2N-1}(-1)^{n+1}\sigma_\alpha^3(n) \\
H_N^{(K)} &\rightarrow \frac{1}{4a}\sum_{\alpha}\sum_{n=0}^{2N-2}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right]+ \\
&\quad \frac{1}{4a}\sum_{\alpha}\left[\prod_{l=1}^{2N-2}\sigma_\alpha^3(l)\right]\left[\sigma_\alpha^1(0)\sigma_\alpha^2(2N-1)-\sigma_\alpha^2(0)\sigma_\alpha^1(2N-1)\right] \\
H_N^{(G)} &= -\frac{G_\pi}{2a}\sum_{n=0}^{N-1}\left[\sum_{\alpha}\tilde{H}_N^{\alpha\alpha}(n)+2\sum_{\alpha<\beta}\tilde{H}_N^{\alpha\beta}(n)\right]
\end{aligned}
$$

Refactoring the NJL Hamiltonian III

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$$\tilde{H}_N^{\alpha\beta}(n) \quad \rightarrow \quad \frac{1}{4}\sum_{\substack{j=0\\k=0}}^{1}(-1)^{j+k}\,\sigma_\alpha^3(2n+j)\,\sigma_\beta^3(2n+k)\,,$$

It is important to notice that the periodic boundary conditions only enter through the kinetic term, and are responsible for the only non-local contribution. Finally, it is useful to note that:

$$\tilde{H}_N^{\alpha\alpha}(n) \quad \rightarrow \quad \frac{1}{2}\left[1-\sigma_\alpha^3(2n+1)\,\sigma_\alpha^3(2n)\right],$$

which shows an extensive **adiabatic modification** term of the form $\frac{G_\pi}{4}N_{\text{flavor}}\times\frac{N}{a}$ in the interaction Hamiltonian (i.e. coming from the unit matrix). This term gathers the two usual singularities from Quantum Field Theory: one with the size of the system as it gets larger (i.e. $\sim N$), and the other on the continuum limit (i.e. $\sim 1/a$). We drop it as a vacuum contribution.

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Space parametrization and state preparation I

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We need to find ways of exploring different quantum states — a process known as **state preparation**. In principle, with a good mapping, this can be achieved by parametrizing the Hilbert/-Fock space of states representing the system, and finding a way to prepare the corresponding quantum state in the processor. Nonetheless:

- We are significantly constrained by the type of operations allowed on the qubits.
- The dimension of the space at hand grows exponentially with the number of qubits used in the representation of the system.
- We will be interested in finding a smaller subspace containing the solution to our problem.
- Randomized, and other naive general approaches suffer from problems such as **barren-plateaus** and **suboptimal local minima**.
- Useful to have some physical intuition to constrain the amount of states that we explore; which leads to problem specific ansatezs.
- Typically divided in: (1) prepare initial state, and (2) perform a parametrized evolution.

Hamiltonian Variational Ansatz (HVA) I

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There is a family of circuits known as the Hamiltonian Variational Ansatz (HVA) — also referred to as the QAOA ansatz — which are based on **adiabatic state preparation**.

Theorem (Simplified adiabatic theorem)

Under a slowly changing Hamiltonian $H(t)$ with instantaneous eigenstates $|n(t)\rangle$ and corresponding energies $E_n(t)$, a quantum system initialized in a particular eigenstate $|m(0)\rangle$, will remain in the corresponding eigenstate $|m(t)\rangle$ during the evolution.

Therefore, if we prepare an eigenstate $|\varepsilon_0(0)\rangle$ of one of the sub-Hamiltonians H_0, and slowly activate the others through activation parameters $\lambda_j(t)$, where $\lambda_j(0) = 0$, $\lambda_j(t \to \infty) = 1$, and $\dot{\lambda}_j(t) \ll 1$; we will end up with the corresponding eigenstate $|\varepsilon\rangle$ for the entire Hamiltonian:

$$|\varepsilon\rangle = \lim_{t\to\infty} \exp\left[-it\left(H_0 + \sum_{j=1} \lambda_j(t) H_j\right)\right] |\varepsilon_0(0)\rangle$$

Hamiltonian Variational Ansatz (HVA) II

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Particularly, making use of the non-commuting terms in the Hamiltonian and a simple **Trotter decomposition** we can simulate this process digitally:

$$H = \sum_j H_j\,, \quad \big[H_j, H_k\big]_- \neq 0 \quad \forall\, j \neq k$$

$$|\psi\rangle = \exp\big[-itH(t)\big]\,|\psi_0\rangle \approx \left[\prod_k^p \exp\big[-i\Delta t_k H(t_k)\big]\right]|\psi_0\rangle = \left[\prod_k^p \exp\left[-i\Delta t_k \sum_j \lambda_j(t_k) H_j\right]\right]|\psi_0\rangle$$

$$|\psi\rangle \approx \prod_k^p \left[\prod_j \exp\big[-i\Delta t_k \lambda_j(t_k) H_j\big]\right]|\psi_0\rangle$$

Hamiltonian Variational Ansatz (HVA) III

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Which, by noticing that we can control both the time steps as well as the activation parameters at will, leads to the final form of the parameterization ansatz:

$$|\psi(\theta)\rangle \triangleq \prod_{k}^{p} \left[\prod_{j} \exp\left(-i\theta_{jk} H_j\right) \right] |\psi_0\rangle$$

where p is a variable parameter that stands for the depth of the ansatz. This technique is thought to possess **favorable properties** for solving optimization problems. Specifically, these circuits have been shown to display mild or entirely absent barren plateaus, as well as almost trap-free target landscapes.

We also infer that the **initial state** $|\psi_0\rangle$ should be an eigenstate of one of the sub-Hamiltonians — according to the output eigenstate that we want to obtain. Notice that this ansatz is indeed problem specific, since it depends on the Hamiltonian of the system of interest, and physically sound as well. Finally, most of the times it is enough to have $\left[H_j, H_{j+1}\right]_- \neq 0 \ \forall j$.

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Variational algorithms I

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One of the most promising near-term applications of quantum computers is the simulation of quantum mechanics. This is because:

- Quantum phenomena are exponentially hard to recreate by classical means, whilst thought to be efficiently reproducible using quantum resources: **quantum advantage**.
- This task is believed to be achievable in the foreseeable future thanks to **hybrid quantum-classical variational algorithms**.
- Promising applicability, especially for relatively low amounts of quantum resources: **Noisy Intermediate-Scale Quantum** era (NISQ).

Variational algorithms II

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Theorem

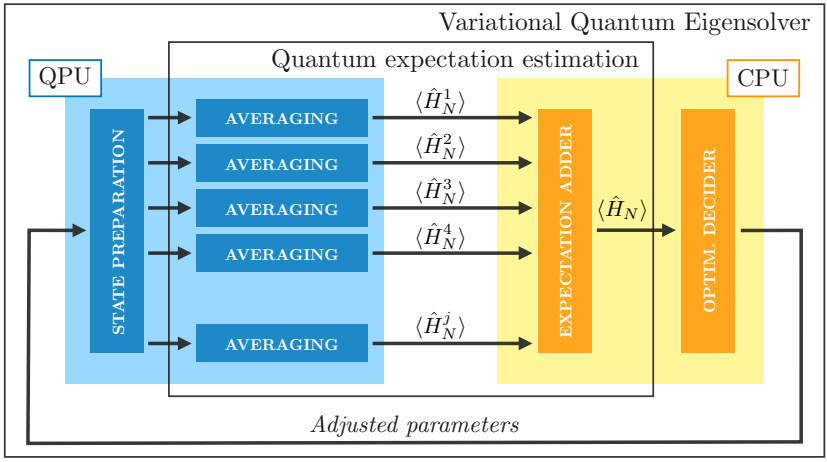
If the state $|\psi\rangle$ of a quantum system depends on some array of n parameters $\{\theta^n\}$, the optimal choice to approximate the ground state of said system (i.e. the eigenstate of its Hamiltonian $\hat{H}$ with minimum eigenvalue $\lambda_{\min}$) is the one which minimizes its Hamiltonian's expectation value $\langle\hat{H}\rangle$. Assuming $\langle\psi|\psi\rangle = 1$:

$$\langle H\rangle(\theta^n) \equiv \left\langle \psi(\theta^n) \middle| H \middle| \psi(\theta^n) \right\rangle \geq \lambda_{\min} .$$

Evaluating the expectation value of the different components making up our Hamiltonian is done through a process known as **operator averaging**:

$$H_N = \sum_{j=1}^{\text{Poly}(N)} w_j P_N^{(j)} \quad \Rightarrow \quad \langle H_N\rangle = \sum_{j=1}^{\text{Poly}(N)} w_j \left\langle P_N^{(j)} \right\rangle$$

Variational Quantum Eigensolver (VQE)



Subspace-search VQE (SSVQE) I

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Despite its success, VQE presents significant shortcomings that we would like to fix:

- Only prepare the minimum and maximum eigenstates of any given observable without having to modify it.
- Even if we were able to efficiently modify the observable to get other eigenstates, we would only be able to prepare one of those states at a time.
- Real-world problems require us to know not only the ground state, but also a number of relevant excited states.

Subspace-search VQE (SSVQE) II

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Subspace-search VQE can be summarized as:

- Construct an ansatz circuit $U(\theta)$ and choose input states $\left\{\left|\varphi_j\right\rangle\right\}_{j=0}^{k}$ which are orthogonal with each other: $\left\langle\varphi_i|\varphi_j\right\rangle = \delta_{ij}$.
- Choose arbitrary weights so that $w_i > w_j$ if $i < j$, and minimize:

$$\mathcal{L}_w(\theta) \triangleq \sum_{j=0}^{k} w_j \left\langle\varphi_j\right| U^\dagger(\theta) H U(\theta) \left|\varphi_j\right\rangle \ .$$

Defining θ^* as the set of parameters that minimizes $\mathcal{L}_w(\theta)$, the ground state $|\phi_0\rangle$, and k first excited states $\left\{\left|\phi_j\right\rangle\right\}_{j=1}^{k}$ (in order) are approximated by:

$$\left|\phi_j\right\rangle \cong U(\theta^*) \left|\varphi_j\right\rangle \ .$$

The catch with this algorithm is that it often requires a larger number of parameters and certain degree of redundancy in the way we prepare quantum states.

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Quantum computing the NJL model I

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- Since we would like to study both the ground state, as well as the first excited hadron state in NJL, we will be using SSVQE as our variational algorithm.
- Using HVA we can use the fact that adiabatic state preparation maps corresponding excited states, to raise our chances of getting the correct output eigenstates in SSVQE without need for redundancy.
- HVA's parametrization is based on the system's Hamiltonian, it will share its symmetries. This means that we can easily use SSVQE to get non-consecutive output eigenstates by simply using non-consecutive initial eigenstates.
- HVA requires to break up our Hamiltonian into its non-commuting components.

Quantum computing the NJL model II

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$$
\begin{aligned}
H_N^{(1)} &\triangleq \frac{1}{4a}\sum_{\alpha}\sum_{n=\text{even}}^{2N-1}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right],\\
H_N^{(2)} &\triangleq -\frac{G_\pi}{2a}\sum_{n=0}^{N-1}\left[\sum_{\alpha}\tilde{H}_N^{\alpha\alpha}(n)+2\sum_{\alpha<\beta}\tilde{H}_N^{\alpha\beta}(n)\right],\\
H_N^{(3)} &\triangleq \frac{1}{4a}\sum_{\alpha}\sum_{n=\text{odd}}^{2N-2}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right]+\\
&\quad \frac{1}{4a}\sum_{\alpha}\left[\prod_{l=1}^{2N-2}\sigma_\alpha^3(l)\right]\left[\sigma_\alpha^1(0)\sigma_\alpha^2(2N-1)-\sigma_\alpha^2(0)\sigma_\alpha^1(2N-1)\right],\\
H_N^{(4)} &\triangleq \frac{m}{2}\sum_{\alpha}\sum_{n=0}^{2N-1}(-1)^{n+1}\sigma_\alpha^3(n),
\end{aligned}
$$

Quantum computing the NJL model III

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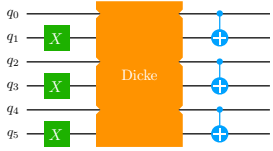
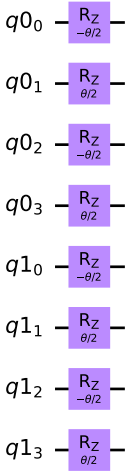
We choose the mass term for the initial states:

$$H_N^{(4)} \triangleq \frac{m}{2} \sum_{\alpha} \sum_{n=0}^{2N-1} (-1)^{n+1} \sigma_\alpha^3(n)$$

- Ground: $|\Omega_0\rangle \triangleq |\mathbb{0}\mathrm{b} \ldots 1010101010\rangle$
- Hadron: $|h_0\rangle \triangleq |\mathbb{0}\mathrm{b} \ldots 1010101001\rangle + \cdots$

Where we can build the initial hadron state by implementing **Dicke states**:





Quantum computing the NJL model IV

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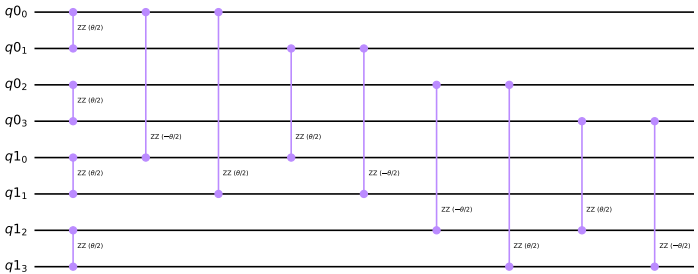
$$H_N^{(2)} \triangleq -\frac{G_\pi}{2a}\sum_{n=0}^{N-1}\left[\sum_{\alpha}\tilde{H}_N^{\alpha\alpha}(n)+2\sum_{\alpha<\beta}\tilde{H}_N^{\alpha\beta}(n)\right]$$

$$\tilde{H}_N^{\alpha\beta}(n) \quad \rightarrow \quad \frac{1}{4}\sum_{\substack{j=0\\k=0}}^{1}(-1)^{j+k}\,\sigma_\alpha^3(2n+j)\,\sigma_\beta^3(2n+k)$$



Quantum computing the NJL model V

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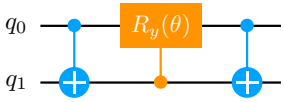
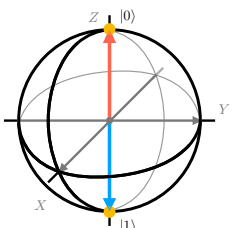
The kinetic terms of the form $XY - YX$ can be easily exponentiated by noting that:

$$\frac{1}{2}(X_1 Y_0 - Y_1 X_0) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$





- Zero eigenvalue on even parity states: single particle/antiparticle states
- Pauli Y in the subspace $\{|0\mathtt{b}\,10\rangle, |0\mathtt{b}\,01\rangle\}$: creates and annihilates particle-antiparticle pairs.

Quantum computing the NJL model VI

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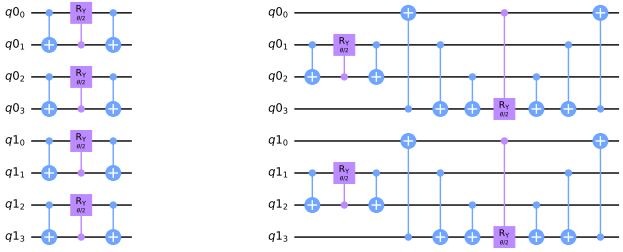
$$H_N^{(1)} \triangleq \frac{1}{4a}\sum_{\alpha}\sum_{n=\text{even}}^{2N-1}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right],$$

$$H_N^{(3)} \triangleq \frac{1}{4a}\sum_{\alpha}\sum_{n=\text{odd}}^{2N-2}\left[\sigma_\alpha^1(n+1)\sigma_\alpha^2(n)-\sigma_\alpha^2(n+1)\sigma_\alpha^1(n)\right]+$$

$$\frac{1}{4a}\sum_{\alpha}\left[\prod_{l=1}^{2N-2}\sigma_\alpha^3(l)\right]\left[\sigma_\alpha^1(0)\sigma_\alpha^2(2N-1)-\sigma_\alpha^2(0)\sigma_\alpha^1(2N-1)\right]$$



Ground and hadron states ($N = 3$, $N_{\text{flavor}} = 2$)

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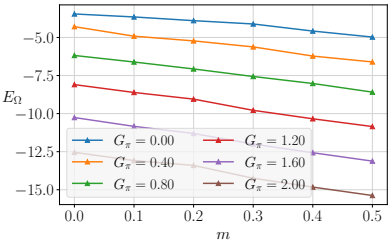

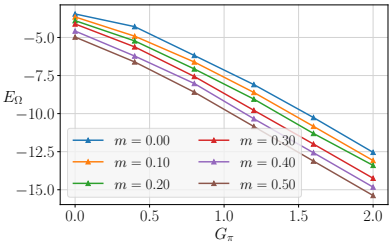

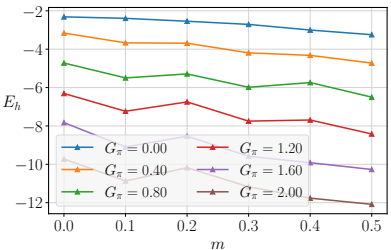

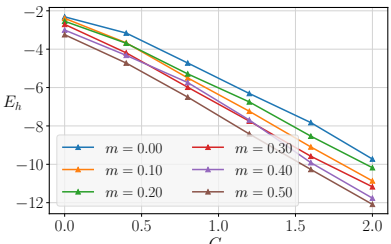

Mass generation ($N = 3$, $N_{\text{flavor}} = 2$) I

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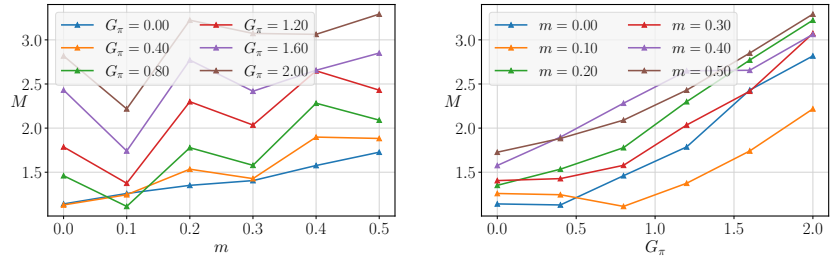
With these results, we can now obtain the hadron's mass as the difference between the hadron's energy and the computed vacuum energy:

$$M \triangleq \langle h|H_N|h\rangle - \langle \Omega|H_N|\Omega\rangle \ .$$



Mass generation ($N = 3$, $N_{\text{flavor}} = 2$) II

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Nonetheless, we can see this more clearly by introducing a new metric. To motivate its definition, let us first define the different contributions to the mass of the hadron as:

$$
\begin{aligned}
M &\triangleq M_M + M_K + M_G\,, \\
M_M &\triangleq \langle h|H_N^{(M)}|h\rangle - \langle \Omega|H_N^{(M)}|\Omega\rangle\ , \\
M_K &\triangleq \langle h|H_N^{(K)}|h\rangle - \langle \Omega|H_N^{(K)}|\Omega\rangle\ , \\
M_G &\triangleq \langle h|H_N^{(G)}|h\rangle - \langle \Omega|H_N^{(G)}|\Omega\rangle\ .
\end{aligned}
$$

Our goal here is to compare the component of mass associated with interactions M_G, and that associated with the quark masses M_M. It is then natural to define:

$$
\mathcal{M}(m, G_\pi) \triangleq \frac{M_G - M_M}{M}\,,
$$

Mass generation ($N = 3$, $N_{\text{flavor}} = 2$) III

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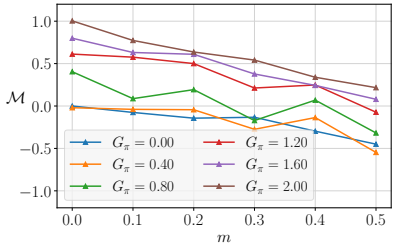
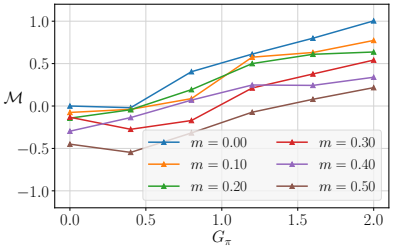
From which we can distinguish three regimes:

$$
\begin{aligned}
M &\approx M_G \quad \Rightarrow \quad \mathcal{M} \approx +1\,, \\
M &\approx M_M \quad \Rightarrow \quad \mathcal{M} \approx -1\,, \\
M_G &\approx M_M \quad \Rightarrow \quad \mathcal{M} \approx 0\,.
\end{aligned}
$$





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Algorithm outline I

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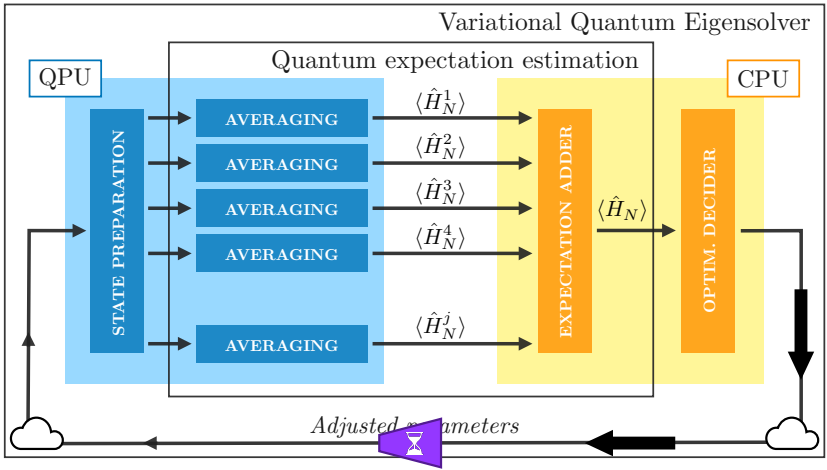
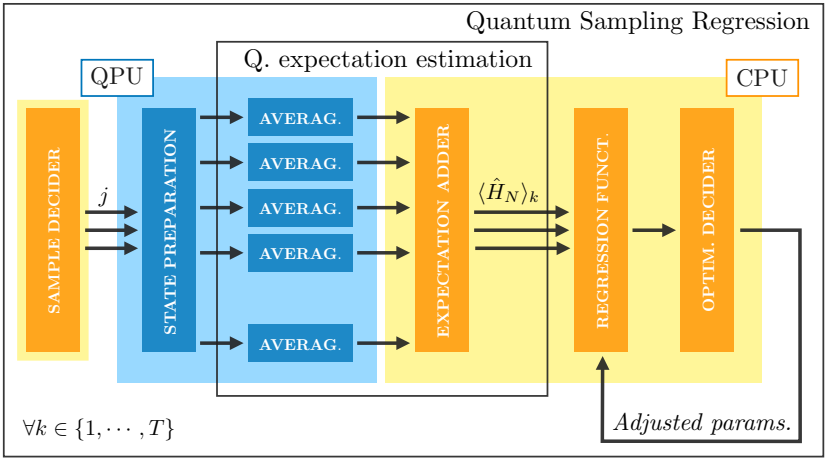


Algorithm outline II



Algorithm outline III

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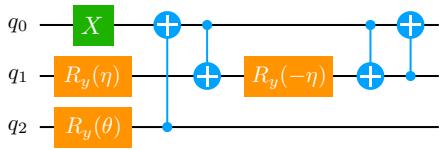
- From the **topology of the quantum circuit** in charge of state preparation, we can infer a frequency bound.
- **Fourier analysis** then allows to fully reconstruct the expectation value function.
- Through the **Nyquist-Shannon sampling theorem** we can show that our sampling technique is optimal.



Theorem (Nyquist-Shannon)

If a function $h(\theta)$ contains no angular frequencies higher than ω_S, it is completely determined by giving its ordinates at a series of points $1/2\omega_S$ apart: $\omega_{\text{sampling}} > 2\omega_S$.

Algorithm comparison I

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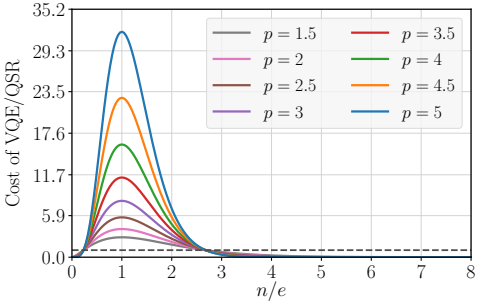
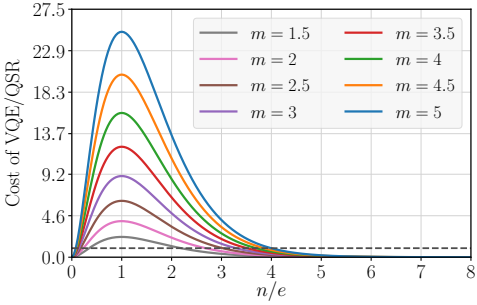
- Algorithmic complexity model: $\frac{\text{VQE}}{\text{QSR}} = \left(mn2^{-n/r}\right)^p$





Algorithm comparison II

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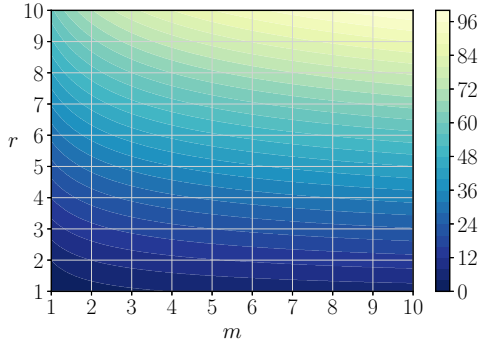
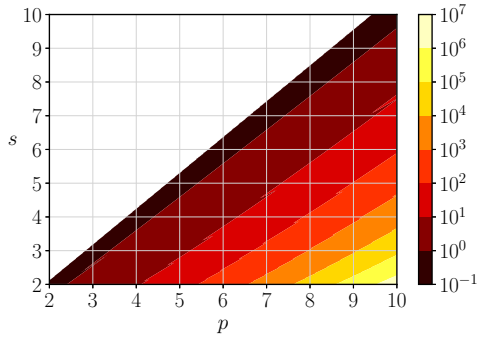
Threshold



Efficiency



$$a \triangleq \left\lceil -\frac{r}{\ln 2} W_{-1}\left(-\frac{\ln 2}{mr}\right) \right\rceil$$

$$E \approx \frac{1}{as \ln 2}\left(\frac{m}{s \ln 2}\right)^{p} \Gamma(p+1, s \ln 2, as \ln 2)$$

Benchmark

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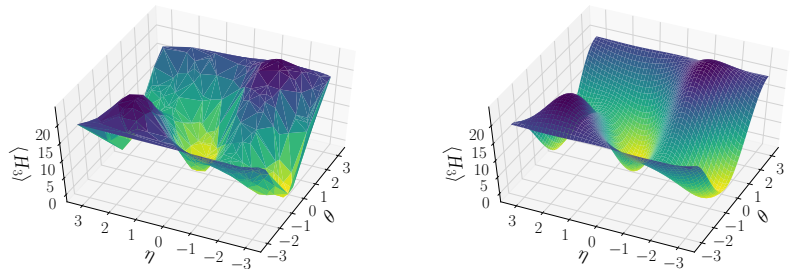

Figure: Comparison between the VQE and QSR algorithms, when reproducing an external model with two parameters. (Left) Triangulation of the expectation value function from raw samples. (Right) Approximate function obtained through the Optimal Sampling Regression method with $S_q = S_{\max} = 2\ \forall q$.

N_{params}	VQE samples	QSR samples	VQE error	QSR error
1	24	3	3.5%	1.0%
2	153	25	0.3%	0.2%

Applications of QSR

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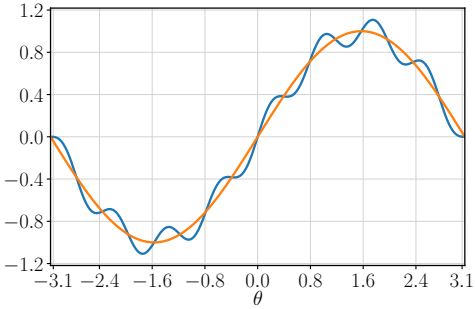
- **Oversampling** to attain higher precision.
- **Undersampling** to boost performance and get rid of small-wavelength oscillations leading to burdensome local minima.
- VQE low-resolution start-up **supplement**.
- **Proxy** to transition between simulators and real devices.
- Improve convergence by removing the stochastic nature of the quantum expectation value function.
- Avoid the exponential matrix formulation in classical computation.



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Conlcusions

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- I showcased an instance of hadron mass generation in QCD using the NJL model in $1+1$ dimensions and 2 flavors.
- I discovered a clear transition from a regime dominated by the quark masses, to a regime dominated by their interaction.
- I compiled and developed the computational techniques necessary for efficiently simulating Quantum Field Theories on a quantum computer.
- I established how revealing these kind of problems can be when addressed on quantum computers, and why Quantum Field Theory should remain a key motivation for developing QIS methods and techniques.

Future research

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- Calculation of parton distribution functions and form factors for the study of Deep inelastic scattering.
- Repeat calculations with other mappings and parametrization ansatzes.
- Increase the dimensions of our problem to $2+1$, and $3+1$.
- Explore other quantum field theories up to full QCD.
- Formalize the scalabilty of these techniques in the NISQ era and beyond.
- Develop a robust notation for these applications of QIS.

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