Towards Digital-Analog Simulations using Superconducting Qubits and Resonators

R. Roma[1,2], **F. Wilhelm-Mauch**[1,2], **D. Bagrets**[2,3]

1. Theoretical Physics, Universität des Saarlandes, 66123 Saarbrücken, Germany
2. Forschungszentrum Jülich GmbH, Germany
3. Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

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Abstract

The digital simulation of an electron-phonon system, and more in general of fermion-boson systems, on quanutm computers in the NISQ era is an hardous task, since it's not clear how to generalize current state of the art methods, i.e. VQE, for such systems. To circumvent this problem, we aim to develop a scheme capable of performing digital-analog simulations of similar models . We propose an hybrid architecture based on superconducting qubits and resonators with the purpose of employing the Variation Cluster Approximation, which requires the measurement of Green's functions. The proposed method will be tested on the Hubbard-Holstein model, so as to obtain its phase graph.

Test Model

The test model is the **Hubbard-Holstein model**[1]:

$$H = -\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow} t_j(c^*_{j+1\sigma}c_{j\sigma} + c^*_{j\sigma}c_{j+1\sigma}) + \sum_{j=1}^{L} U_j n_{j\uparrow}n_{j\downarrow} + - g\sum_{J,j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow} n_{j,\sigma}(b_J + b_J^\dagger) + \sum_{J=1}^{L}\omega_J b_J b_J^\dagger$$

The model describes the following phenomena:

- **electron hopping**
- **electron on-site repulsion**
- **electron-phonon Holstein interaction**
- **energy of the vibrational modes**

The model is a generalization of the Fermi-Hubbard model which accounts for the interaction between the electrons in the Fermi-Hubbard lattice and the vibrations of said lattice.
The minimal problem that can be considered is the two-site model, which allows for two electrons each, each coupled to a single boson, at half filling.

Simplified problem

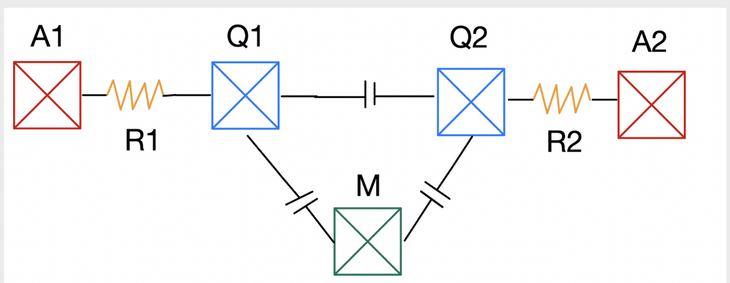
To further simplify the problem, we first introduce a *spinless-fermions* version of the Fermi-Hubbard model, which is the following:

$$H = -\sum_{j=1}^{L-1} t_j(c^*_{j+1}c_j + c^*_j c_{j+1}) - g\sum_{J,j=1}^{L-1} n_j(b_J + b_J^\dagger) + \sum_{J=1}^{L}\omega_J b_J b_J^\dagger$$

In this model we keep the Holstein interaction as is, while we consider the electrons spinless fermions which conserve their anti-commutation relation. The minimal problem for this version is the two-site version, which allows for a fermion per site, each couple to a boson, at half filling.

The device

Here we present the device for the simplified model we consider:



The shown elements are as follows:

- $Q1$, $Q2$: qubits identifying the two sites. Since in the model at half filling there is a single fermion, so $|1>$ shows the presence of the fermion.
- M: qubit used for the measurement of the correlators of Q1 and Q2, so as to calculate their Green's function
- $R1$, $R2$: resonators coupled respectively to $Q1$ and $Q2$, they are used to store the phonon coupled to each fermion
- $A1$, $A2$: ancillary qubits used to measure the state of the $R1$ and $R2$

$Q1$, $Q2$ and R are coupled via 2-Qubit gates. We allow for two possible choices:

- C-phase gate, realized via a resonator coupling
- iSWAP, realized via a direct capacitive coupling, as shown in figure

Particle Mapping

- We encode phonons in the resonators $R1$ and $R2$ using NOON states[2]:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|N,0\rangle + e^{i\phi}|0,N\rangle) \qquad (1)$$

  allowing by the $Q_i - R_i - A_i$ structures.
- We encode the fermions using the following procedure:
  1. introduce the Majorana fermions:
     $$x_i = c_i + c_i^\dagger \qquad y_i = i(c_i - c_i^\dagger)$$
  2. encode the Majorana fermions using Jordan-Wigner encoding

Ground State Preparation

We propose the following procedure to get to the ground state:

1. we prepare a **decoupled** initial state:
   - we use the Variational Hamiltonian Ansatz to prepare the ground state of the electronic part of the model
   - we prepare the resonators in their ground state
2. we turn the electron-phonon interaction on
3. we evolve the system for a single Trotter step
4. we obtain a **quenched state**
5. perform the correlator measurements
6. run the variational algorithm for the inter-cluster interaction
7. we evaluate the grand-canonical potential

This procedure would provide a first approximation of the behaviour of the model. Further precision can be achieved by adding further Trotter steps in the time evolution of the model, obtaining an **equilibrium state**.

Variation Cluster Approximation [3]

We choose the **Variational Cluster Approximation** for the simulation. It consists in the following steps:

1. identify the minimal cluster as a subset of the full model lattice
2. evaluate the Green's function of the minimal cluster
3. add the inter-cluster interaction and some symmetry-breaking terms if needed
4. use the Green's function of the cluster to evaluate the grand-canonical potential of the full lattice

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