Work Summary

Thoughts on variational method under symmetric spin configurations.

Main Work

1. Variational method under symmetric spin configurations
2. Addition of the penalty Hamiltonian
3. Possible new encodings
4. Variational method results

1 Variational method under symmetric spin configurations

As shown in the previous report, when simulating the dynamics, symmetry properties of the Hamiltonian in its spin up and spin down components can be used to reduce the controls to the ones with the same symmetry. For example, see the following table for a list of controls that exhibit the symmetry. In simulating dynamics, it is often observed that the performance of GRAPE with these controls applied is normally better than the ones with independent controls.

Controls		
Control terms	Names	Nicknames
$\left\{\hat{a}_1 + \hat{a}_1^\dagger, i\left(\hat{a}_1 - \hat{a}_1^\dagger\right), \sigma_{1,x}, \sigma_{1,y}\right\}$ and $\left\{\hat{a}_2 + \hat{a}_2^\dagger, i\left(\hat{a}_2 - \hat{a}_2^\dagger\right), \sigma_{2,x}, \sigma_{2,y}\right\}$	Independent controls	independent
$\left\{\hat{a}_1 + \hat{a}_1^\dagger + \hat{a}_2 + \hat{a}_2^\dagger, i\left(\hat{a}_2 - \hat{a}_2^\dagger\right) + i\left(\hat{a}_1 - \hat{a}_1^\dagger\right), \sigma_{1,x} + \sigma_{2,x}, \sigma_{1,y} + \sigma_{2,y}\right\}$	Identical controls	identical
$\left\{\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1 \hat{a}_2^\dagger, i\left(\hat{a}_1^\dagger \hat{a}_2 - \hat{a}_1 \hat{a}_2^\dagger\right)\right\}$	Beam splitter	bs
$\left\{\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1 \hat{a}_2^\dagger\right\}$	Beam splitter with symmtry	symbs
$\left\{\hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_1 \hat{a}_2, i\left(\hat{a}_1^\dagger \hat{a}_2^\dagger - \hat{a}_1 \hat{a}_2\right)\right\}$	Mode squeezer	sq
$\left\{\hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_1 \hat{a}_2, i\left(\hat{a}_1^\dagger \hat{a}_2^\dagger - \hat{a}_1 \hat{a}_2\right)\right\}$	Mode squeezer with symmtry	symsq

Therefore, it is desirable to used these properties in variational method as well. However, for variational method, the ground state's symmetry properties can not be determined beforehand.

Let the Hilbert space be expressed as $\hat{H}_\uparrow \otimes \hat{H}_\downarrow$. The Hamiltonian is exchange symmetric, i.e.

$$\hat{H} = \sum_{i,j} \hat{H}_i \otimes \hat{H}_j = \hat{P}\hat{H}\hat{P} = \sum_{i,j} \hat{H}_j \otimes \hat{H}_i.$$

Then, applying the conventional derivation, if $|v\rangle$ is an eigenstate of Hamiltonian $\hat{H}$,

$$\hat{P}\left(\hat{H}|v\rangle\right) = \hat{P}\left(\lambda|v\rangle\right) = \lambda\hat{P}|v\rangle$$

and

$$\hat{P}\left(\hat{H}|v\rangle\right) = \left(\hat{P}\hat{H}\hat{P}\right)\hat{P}|v\rangle = \hat{H}\left(\hat{P}|v\rangle\right).$$

Thus, any eigenstate of $\hat{H}$ should also be an eigenstate of the exchange operator $\hat{P}$, which only has eigenvalues of ± 1. Therefore, the ground state should either be symmetric or anti-symmetric under exchange of spin-up and spin-down states.

If using the symmtric version of the controls, then the unitary

$$U = e^{-i\left(\sum_i \epsilon_i \hat{A}_i\right)\tau}$$

is also exchange symmetric. The final states evolved from the initial state through the unitary has the same symmetry as the initial state. Thus, for example, I can try the symmetric initial state

$$|\uparrow\downarrow, \uparrow\downarrow, -, -\rangle$$

and the anti-symmetric initial state

$$\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow, \downarrow\downarrow, -, -\rangle - |\downarrow\downarrow, \uparrow\uparrow, -, -\rangle\right)$$

to cover both possible cases, and use the lower energy one as the ground state.

1.1 Ground state of 2 spin-up, 2spin-down

Here provides a discussion of the exchange symmetry properties for the 2 spin-up and 2 spin-down electron case.

When $t \gg U$, as derived before, the ground state of 2 spinless fermions is degenerate and has an energy of -2J. Assume the degenerate have basis $|v_1\rangle$ and $|v_2\rangle$, then the general ground state of the spin-up and spin-down electrons is also degenerate and can be in either exchange symmetry. For example, a symmetric ground state is $|v_1\rangle \otimes |v_1\rangle$ and an antisymmetric one is $|v_1\rangle \otimes |v_2\rangle - |v_2\rangle \otimes |v_1\rangle$.

When $U \gg t$, in the rotation frame $\hat{S} = e^{-\frac{\hat{T}_+ - \hat{T}_-}{U}}$, the ground state is derived to be $|gs\rangle = \frac{1}{2\sqrt{3}}\begin{pmatrix}1\\1\\1\\1\\2\\2\end{pmatrix}$, expressed in the basis of $\begin{pmatrix}|\uparrow\uparrow\downarrow\downarrow\rangle\\|\downarrow\uparrow\uparrow\downarrow\rangle\\|\downarrow\downarrow\uparrow\uparrow\rangle\\|\uparrow\downarrow\downarrow\uparrow\rangle\\|\uparrow\downarrow\uparrow\downarrow\rangle\\|\downarrow\uparrow\downarrow\uparrow\rangle\end{pmatrix}$, with a ground state energy of $E_{ground} = -12\frac{t^2}{U}$. Here, $|gs\rangle$ and $\hat{S}$ should both be exchange symmetric. Therefore, the ground state in lab frame should be symmetric.

2 Addition of the penalty Hamiltonian

This section addresses a previously not recognized issue with the 'auxiliary' cavity levels, i.e. the levels that have no mapping to the site-occupation basis. The issue is detailed as below.

Consider the case of finding the ground state of [2,2] on 4 sites in double cavities. For each cavity, the effective dimension is $\binom{N_{site}}{N_{up}} = \binom{4}{2} = 6$. If using 10 energy levels for each cavity, there are essentially 4 'auxiliary' levels that are only accessed during the pulse sequence and, hopefully, are not occupied at the end of the pulse sequence.

Previously, the Hamiltonian is defined as

$$\hat{H} = \hat{H}_{hop} + \hat{H}_{NN},$$

where

$$\hat{H}_{hop} = \hat{H}_{cav} \otimes \hat{I} + \hat{I} \otimes \hat{H}_{cav}.$$

Here,

$$\hat{H}_{cav} = \begin{bmatrix} \hat{H}_{2e} & \\ & \hat{0} \end{bmatrix}$$

, i.e. $\hat{H}_{cav}$ has null entries except for the 6×6 matrix

$$\hat{H}_{2e} = -t \begin{pmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \end{pmatrix}.$$

Similar process can be repeated for the nearest-neighbor interaction Hamiltonian $\hat{H}_{NN}$. When finding the ground state when $U \gg t$, the theoretical solution gives the ground state as a superposition of states that are not doubly occupied and the final ground energy is in the second order of t. However, when the 'auxiliary' levels are introduced, no Hamiltonian is defined on those states including the nearest-neighbor Hamiltonian since they have no mapping on the site-occupation basis. These levels then offers new lower energy states.

For example, when the spin-up cavity is on an auxiliary level, the spin-down cavity essential does not need to worry about nearest-neighbor interaction since there is no physical mapping defined for the spin-up cavity. Therefore, the spin-down cavity acts as an independent cavity finding the ground state of 2 spin-down electrons on 4 sites, which then gives a ground state of -2t as calculated as before.

The solution can be adding penalty Hamiltonian to the 'auxiliary' levels similar to the site Hamiltonians, i.e.

$$\hat{H}_{penalty} = \sum_i \Big(|i\rangle\langle i| \otimes \hat{I} + \hat{I} \otimes |i\rangle\langle i| \Big), \text{where } |i\rangle \text{ are the auxiliary levels.}$$

Adding this penalty Hamiltonian solves the problem, and adds a stronger constraint of the final state being within the effective levels. My guess is that this can then also help reduce the number of 'auxiliary' levels needed since the final state is more constrained.

Note that this Hamiltonian should only be applied for variational methods. There is no need to add this for dynamics simulation since it is effectively ignored by the fidelity definition that I have set previously.

3 Possible new encodings

Advantage of any new encoding for variational method should be that it can entangle the two cavities in a similar fashion to the nearest-neighbor interaction or it can access the possible ground states easier.

One encoding that I thought of might be interesting for strongly correlated Hubbard model is to use the encoding $\begin{pmatrix} |21\rangle \\ |41\rangle \\ |31\rangle \\ |42\rangle \\ |32\rangle \\ |43\rangle \end{pmatrix} \otimes \begin{pmatrix} |43\rangle \\ |32\rangle \\ |42\rangle \\ |31\rangle \\ |41\rangle \\ |21\rangle \end{pmatrix}$. In this encoding, all of the states that the two cavities are in the same level are have no double occupied sites. If the initial state is the two cavities both in the ground state, then only applying the two-mode squeezer control does not bring out any states that have double occupied sites.

4 Variational method results

When using symmetric initial state and finding the ground state for [2,2], it is observed that applying identical quadrature controls with two-mode squeezer control or beam-splitter control performs roughly equal. In Figure 1, it shows the performance of variational method at different U/t ratios.

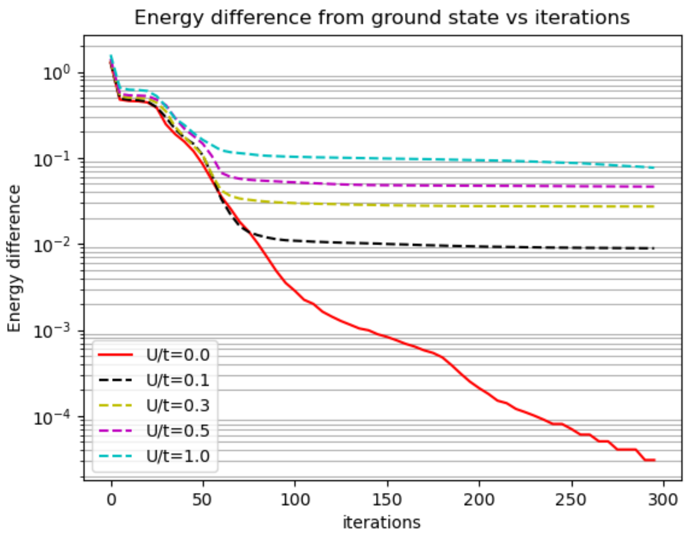

Figure 1: Absolute energy difference compared to ground state energy vs GRAPE iterations for variational method with identical quadrature controls and two-mode squeezer controls.

4.1 Anti-symmetric initial states

When using anti-symmetric initial states, the optimized control pulse seems to need to access more auxiliary levels than currently granted, i.e. the energy obtained from propagating the state in a Hilbert space dimension of 10 and 20 gives results that differ not negligibly. Some sample data is shown in Table 1.

U/t	Symmetric	Anti-symmetric
0.1	-1.3478(-1.3474)	-1.3564(-1.2853)
0.3	-1.2825(-1.2825)	-1.3055(-1.2681)
0.5	-1.2277(-1.2273)	-1.2557(-1.2220)
1.0	-1.0878(-1.0815)	-1.1367(-1.1056)

Table 1: Optimized final state energies of symmetric and anti-symmetric states. The energies inside the bracket is one computed from propagating in a much larger Hilbert space. Here symmetric beam splitter control is used for both symmetric and anti-symmetric initial states.

4.2 Strongly correlated Hubbard model

It have been derived for strongly correlated Hubbard model, the energy of the ground state should tend to $-12\frac{t^2}{U}$. However, it seems that GRAPE is having trouble reaching the ground state, which is slightly below the zero energy state. My estimate is that GRAPE is only approaching the state with zero energy. Some data is shown in table 2.

U/t	Symmetric beam splitter controls	Mode squeezer controls	Ground state energy
10.0	1.6747e-07	1.1367e-07	-0.0380

Table 2: Optimized final state energies for strongly correlated Hubbard model.

This can be a result of lacking enough controls to entangle the two cavities strong enough as the Hubbard model with $U \gg t$.