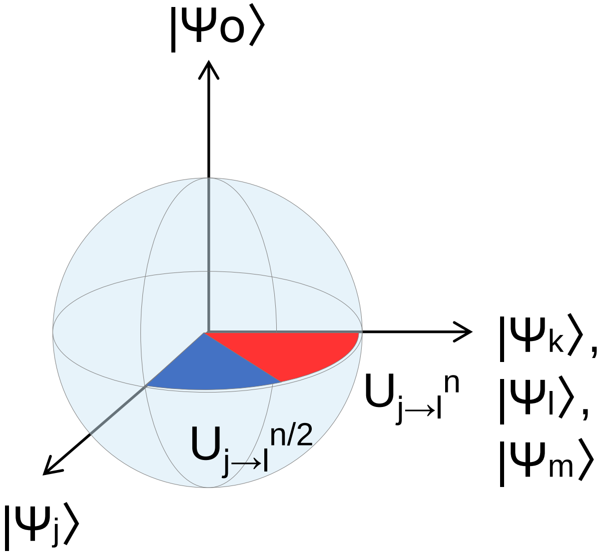
Deriving full energy levels by one Subspace-Search Variational Quantum Eigensolver using frame superposition cluster

Hikaru Wakaura[1], Shoya Yasuda[2], Takao Tomono[3], Yuichiro Minato[4]

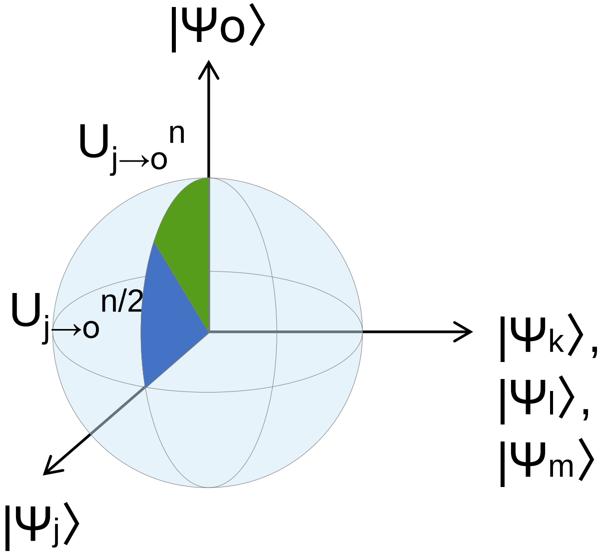
Quantscape, 4-11-18, Meguro, Tokyo, 153-0064, Japan

1) hikaruwakaura@gmail.com, 2) yasuda@vigne-cla.com, 3) takao.tomono@ieee.org, 4) minato@blueqat.com

In case treansition between j and l-th states.



In case treansition between j and o-th states.



Introduction:

Recently, Ion-q rereased a new quantum computer that has 32 qubits of 4 million quantum volume. In addition, 11-qubit quantum computer has been rereased on cloud pratform. It's not long time until coming quantum era.

Variational Quantum Eigensolver (VQE) method is hybrid algorithm that uses quantum computers to derive the energy of quantum systems and uses classical computers to optimize variables. Many kind of VQE methods are developed such as MoG-VQE, MC-VQE, EVQE and Subspace-Search VQE (SSVQE). SSVQE method is one of VQE method that derives multiple energy levels at once. Though, the number of the energy levels that can be derived in high accuracy at once is two. Therefore, we tried to derive the state that can be identical to the good initial parameter by deriving Frame Superposition Clusters(FSCs).

Method:

Frame Superposition Clusters(FSCs) are cluster operators that transit the state to another state by operating given times. For example, Ry(π/2) gate is FSC between |0〉 state and |1〉 state by two operations. It can be expand for the states spanned by multiple qubits.Nothing to say, it is applicable for the states derived by VQE and SSVQE methods as shown in Fig. 1.FSCs $U_{j\rightarrow l}^{n/2}$ are equivalent to the quantum circuit shown in Fig. 2 in the case that j and l-th states are derived at once by SSVQE method.

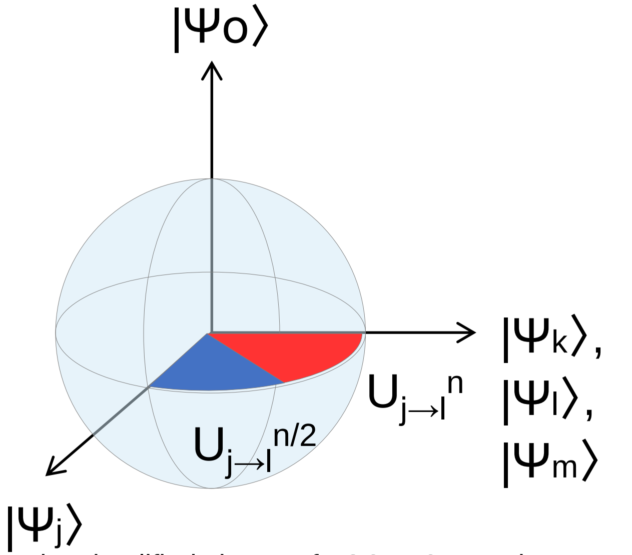
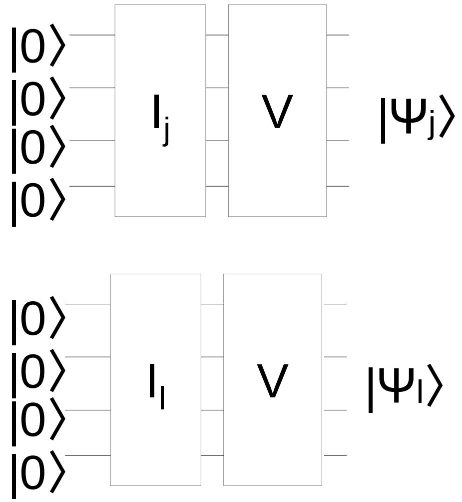


Fig. 1 The simplified picture of FSCs. Constraint Terms must be included because there are some Degenerated states in quantum systems generally. Blue sector indicates the transition angle by $U_{j\rightarrow l}^{n/2}$ and red sector indicates the transition by $U_{j\rightarrow l}^{n}$, respectively.



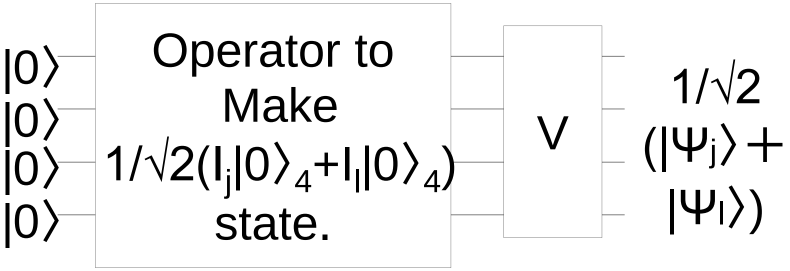


Fig. 2 Quantum circuit that make the equally superpositioned state of j and l-th states. I_j and I_l indicates the operators to generate the initial states of j and l-th state, respectively.

Method:

We derive the FSCs by optimizing equation

$$
\begin{aligned}
F_{j\to l} &= \alpha \mid \langle \Psi_l \mid H \mid \Psi_l \rangle - \langle \Psi_j \mid U_{j\to l}^{n/2\ \dagger} H U_{j\to l}^{n/2} \mid \Psi_j \rangle \mid + E_l^{const.} \\
&= \alpha \mid d_i^{jl} \mid + \sum_{j=0}^{numofconst.} \langle \Phi_j \mid U_{j\to l}^{n\ \dagger}(\langle U_j \rangle - U_j^{const}) U_{j\to l}^{n} \mid \Phi_j \rangle
\end{aligned}
$$

.

Constraint term is necessary for deriving FSC reaches correct state from gegenerated states.

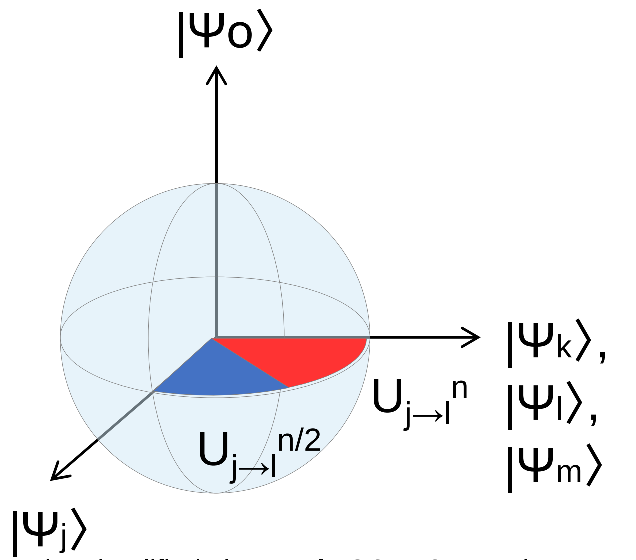
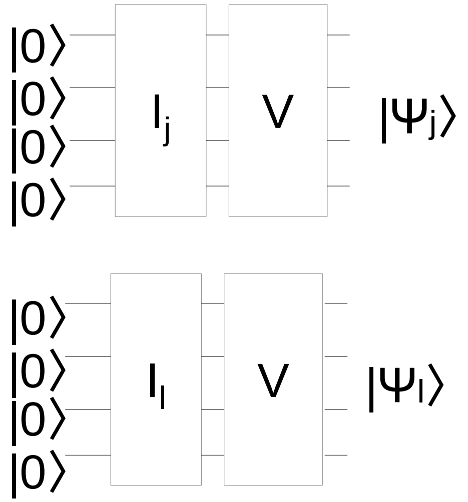


Fig. 1 The simplified picture of FSCs. Constraint Terms must be included because there are some Degenerated states in quantum systems generally. Blue sector indicates the transition angle by $U_{j\to l}^{n/2}$ and red sector indicates the transition by $U_{j\to l}^{n}$, respectively.



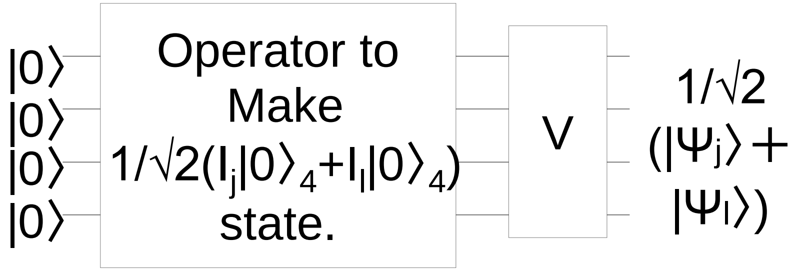


Fig. 2 Quantum circuit that make the equally superpositioned state of j and l-th states. I_j and I_l indicates the operators to generate the initial states of j and l-th state, respectively.

Result:

We show the result of calculation in case n=2 on hydrogen molecule by SSVQE two timesin the case that diatomic bond length is 0.7 (Å) in Table. 1. In case that probability coefficients are near to equal between j and l-th states, FSCs transit j-th state to l-th state correctly. Table. 2 shows the overlap between j-th state that is operated $U_{j\to l}^{n/2}$ and $U_{j\to l}^{n}$, and superposition-ed state between j and l-th states made by the circuit in Fig. 2. It also shows that j-th state that is operated FSC matches the genuine equally superpositioned state of them. Next problem is to derive the FSC equivalent to the initial parameter set that can succeed the derivation of all states at once.

Table. 1 (left) probability of j-th state of $U_{j\to l}^{n/2}|\Psi_j\rangle$ state.
(right) Match terms of each sampling.

Probability	Iter. 1	Iter. 2
c_0^{12}	0.1649	0.2362
c_0^{13}	0.5647	0.48
c_0^{31}	0.3932	0.5134
c_0^{14}	0.4992	0.6021
c_0^{23}	0.0245	0.568
c_0^{24}	0.0641	0.8716
c_0^{34}	0.5836	0.4585

Level	$\mid d_1^{jk} \mid$	$\mid d_2^{jk} \mid$
$\mid d^{12} \mid$	0.252	0.1433
$\mid d^{13} \mid$	0.0128	0.0084
$\mid d^{31} \mid$	0	0
$\mid d^{14} \mid$	0	0
$\mid d^{23} \mid$	0.1463	0.1493
$\mid d^{24} \mid$	0.3299	0.3974
$\mid d^{34} \mid$	0	0

$$|\Phi_{jl}\rangle = 1/\sqrt{2}(|\Psi_j\rangle + |\Psi_l\rangle)$$

Table. 2 Matching of j-th state operated $U_{j\to l}^{n/2}$ and $U_{j\to l}^{n}$ to $|\Phi_{jl}\rangle$.

$j\to l$	c_0^{jl}	S_{jl}	$E^{const.}_l$	$\mid\langle\Psi_j\mid U_{j\to l}^{n/2\dagger}\mid\Phi_{jl}\rangle\mid$	$\mid\langle\Psi_j\mid U_{j\to l}^{n\dagger}\mid\Phi_{jl}\rangle\mid$
1→2	0.2349	0	0.6828	0.0751	0.5996
3→4	0.3022	0	0	0.0036	0.4261