VQD Ansatz Analysis

Matrix Qubits	Ansatz Qubits	Ansatz Type	Classical optimizer	Circuit Paramters	Entanglement Type	Entanglement Blocks	Rotation Blocks	Repetitions	Beta
1	1	Two Local	COBYLA	2	N/A	N/A	Rx	1	Default
				2	N/A	N/A	Ry	1	Default
				2	N/A	N/A	Rz	1	Default
			CG	2	N/A	N/A	Rx	1	Default
				2	N/A	N/A	Ry	1	Default
				2	N/A	N/A	Rz	1	Default
			Gradient Descent	2	N/A	N/A	Rx	1	Default
				2	N/A	N/A	Ry	1	Default
				2	N/A	N/A	Rz	1	Default
			L_BFGS_B						
				2	N/A	N/A	Rx	1	Default
				2	N/A	N/A	Ry	1	Default
				2	N/A	N/A	Rz	1	Default
			SPSA						
				2	N/A	N/A	Rx	1	Default
				2	N/A	N/A	Ry	1	Default
				2	N/A	N/A	Rz	1	Default
COMMENTS:	- From the above data, CG and L_BFGS_B perform better than other optimizers. We will go with L_BFGS_B since it's faster than CG and uses less memory.								
	- The Ry gate performs better than the Rx and Rz gate. Let's verify this for a 2-qubit matrix and using different types of ansatz architectures.								
	- SPSA is a stochastic method and is the most suitable optimizer on real quantum hardware according to qiskit documentation.								
2	2	Two Local	L_BFGS_B	4	N/A	CZ	Rx	1	Default
				4	N/A	CZ	Ry	1	Default
				4	N/A	CZ	Rz	1	Default
		Real Amplitudes	L_BFGS_B	4	N/A	CX	Ry	1	Default
		Efficient SU2	L_BFGS_B	4	N/A	CX	Rx	1	Default
				4	N/A	CX	Ry	1	Default
				4	N/A	CX	Rz	1	Default
COMMENTS:	- Next, we analyze ansatzes for 3-qubit matrices. As shown below, more than one rotation gate is necessary to acheive 100% accuracy. The CX and CZ entanglement blocks have relatively the same effect, though the CX ter								
	- The best accuracy is achieved when the Ry is used by with a higher circuit repitition number, e.g., 2. We get exact 0 absolute errors in this case. Interestingly, the acuracy does not improve by using two Ry gates, but it impro Local architecture. Real Amplitude architectures yields better results than two local and efficient SU2.								

Classical Iterations	VQE iterations	Ground State Absolute Error	Excited State Absolute Error
		3.0155	1.2491
		0.0001	0
		3.0155	9.5541
		3.0155	9.5541
		0	0
		3.0155	9.5541
		3.0155	1.2489
		0.0107	0.0001
		3.0155	9.5541
		3.0155	9.5541
3	20	0	0
		3.0155	9.5541
		3.0155	1.2491
		0	0
		3.0155	9.5541
		3.0155	2.1756
19	150	0	0
		3.0155	56.8666
		0	0
		3.0155	56.8666
		0	0
		3.0155	3.9123

nds to be a bit faster than CZ. The CY gate gives the largest error and has been therefore omitted.

oves by simply repiting the circuit with one Ry gate. Linear entanglement yields slightly better results than circular entanglement for the Two

3	3	Two Local	L_BFGS_B	6	Linear	CX	Ry	1	Default
		Two Local	L_BFGS_B	9	Linear	CX	Ry	2	Default
		Two Local	L_BFGS_B	6	Full	CZ	Ry	1	Default
		Two Local	L_BFGS_B	12	Linear	CX	Ry, Ry	1	Default
		Two Local	L_BFGS_B	9	Circular	CX	Ry	2	Default
		Two Local	L_BFGS_B	12	Linear	CX	Rx, Ry	1	Default
		Real Amplitudes	L_BFGS_B	6	Linear	CX	Ry	1	Default
		Real Amplitudes	L_BFGS_B	9	Linear	CX	Ry	2	Default
		Real Amplitudes	L_BFGS_B	9	Circular	CX	Ry	2	Default
		Efficient SU2	L_BFGS_B	6	Circular	CX	Ry	1	Default
		Efficient SU2	L_BFGS_B	6	Linear	CX	Ry	1	Default
		Efficient SU2	L_BFGS_B	9	Linear	CX	Ry	2	Default
		Efficient SU2	L_BFGS_B	12	Linear	CX	Rx, Ry	1	Default
COMMENTS:	Now, let's analyze =>4-qubit matrices, which correspond to 16 x 16 matrices. We will follow the same pattern above and add more repititions for the larger matrices.								
4	4	Real Amplitudes	L_BFGS_B	12	Linear	CX	Ry	2	Default
		Real Amplitudes	L_BFGS_B	16	Linear	CX	Ry	3	Default
		Real Amplitudes	L_BFGS_B	16	reverse linear	CX	Ry	3	Default
		Real Amplitudes	L_BFGS_B	16	circular	CX	Ry	3	Default
		Real Amplitudes	L_BFGS_B	16	pairwise	CX	Ry	3	Default
		Real Amplitudes	L_BFGS_B	16	sca	CX	Ry	3	Default
		Two Local	L_BFGS_B	16	Linear	CX	Rx, Ry	1	Default
		Two Local	L_BFGS_B	8	Linear	CX	Ry	1	Default
		Two Local	P_BFGS	8	circular	CX	Ry	1	Default
		Two Local	L_BFGS_B	8	Full	CZ	Ry	1	Default
		Two Local	P_BFGS	8	circular	CX	Ry	1	Default
		Two Local	L_BFGS_B	12	Linear	CX	Ry	2	Default
		Two Local	L_BFGS_B	12	sca	CX	Ry	2	Default
		Two Local	L_BFGS_B	16	Linear	CX	Ry	3	Default
		Two Local	L_BFGS_B	16	circular	CX	Ry	3	Default
		Two Local	L_BFGS_B	20	circular	CX	Ry	4	Default
		Two Local	L_BFGS_B	24	full	CX	Ry	5	Default
		Two Local	L_BFGS_B	24	circular	CX	Ry	5	Default
		Two Local	L_BFGS_B	36	linear	CZ	Ry	8	Default
		Efficient SU2	L_BFGS_B	8	Linear	CX	Ry	1	Default
		Efficient SU2	L_BFGS_B	12	Linear	CX	Ry	2	Default

139	1400	0	1.4999
128	2000	0	0
100	1200	0	0.198
		0	1.4999
		0.0001	0
		0	1.2141
		0	1.4999
		0	0
		0	0
		0	1.9911
		0	1.9911
		0	0
		2.521	3.1229
		1.0461	1.974
		0.0072	2.5378
		1.0985	2.1605
		0.9787	4.6958
		1.0726	2.1607
		1.0951	1.9775
		1.1598	4.2669
		1.1424	3.1958
96	1000	0.0002	2.8163
500	6000	0.9556	2.9775
96	1000	0	2.8163
		0.938	0.7248
		0.0003	1.9789
		0.0002	2.6409
		0.0185	2.8316
		0.0745	0.2091
546	14000	0.0181	0.5732
533	14000	0.0507	2.6027
248	16000	0	6.8016
		1.1597	4.2315
		1.0877	1.1748

		Efficient SU2	L_BFGS_B	12	circular	CX	Ry	2	Default
		Efficient SU2	L_BFGS_B	16	Linear	CX	Ry	3	Default
		Efficient SU2	L_BFGS_B	16	Circular	CX	Ry	3	Default
		Efficient SU2	L_BFGS_B	12	sca	CX	Ry	2	Default
		Two local + Efficient SU2	L_BFGS_B	24	sca/circular	CX,	Ry	2,2	Default
		Two local + RA+ Efficient SU2		24	full	CX, CZ	Ry, Ry, Rz	1,1,1	Default
		TL+RA+ESU2	P_BFGS	48	linear/sca/circular	CZ, CX, CX	Ry, Ry, Ry	3,3,3	Default

		1.0149	2.1572						
		1.0797	1.2372						
		3.3052	0.517						
		1.0841	2.973						
		0.056	1.615						
500	14000	1.1322	3.2714						
269	14000	0.1379	1.4632						