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Qiskit Team PiQAOAsso:

Quantum Approximate Optimization Algorithm for constrained optimization problems — Graph coloring

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Qiskit 2019

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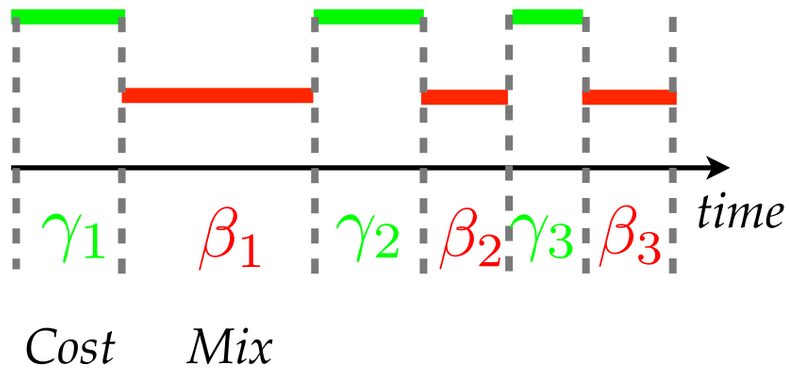
One leading Candidate of quantum heuristics: Quantum Approximate Optimization Algorithms (QAOA) —> Quantum Alternating Operator Ansatz

- One-line summary of the algorithm

$$U = e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \cdots e^{-i\beta_2 H_M} e^{-i\gamma_1 H_C}$$

[Farhi, Goldstone, and Gutmann, arXiv:1411.4028]

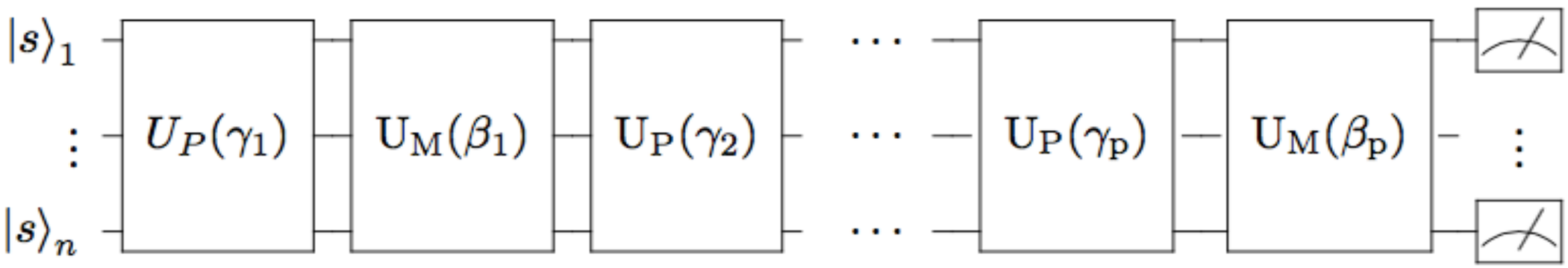


$$H_C = \sum_{j,j',\cdots} (C_j \sigma_j^z + C_{j,j'} \sigma_j^z \sigma_{j'}^z + C_{j,j',j''} \sigma_j^z \sigma_{j'}^z \sigma_{j''}^z, + \cdots)$$

$$H_M = \sum_j \sigma_j^x$$

Approach: $QAOA_p$ circuit:

- Prepare initial state
- Loop p times, and on iteration i apply Hamiltonians
  - (Phase separation) Cost-function-based H_C diag. in Z basis, for time γi
  - (Mixing) Hamiltonian H_M, for time β_i
- Measure in computational basis



QAOA for constrained optimization

[Hadfield et al., from QAOA to QAOA, arXiv 1709.03489];

- How are constrained problems approached?

  Encode the constraints as penalty in the cost function. — Lagrange multipliers

  Commonly practiced in quantum annealing.

Alternative: Use a **mixer** that contains the quantum evolution in the subspace that satisfies the constraints. *[Hen & Spedalieri, '16]*

Advantage: **Smaller search space**!

QAOA for graph coloring problem

Theory and Simulation:

Wang, Rubin, Dominy, Rieffel. **XY mixer for QAOA on graph coloring problems.** (to-appear)

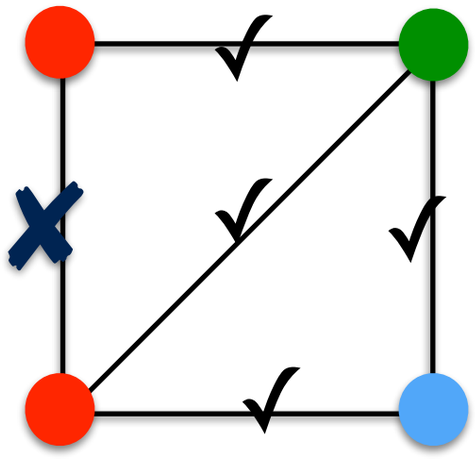
- Goal: Assign colors to vertices to maximize properly-colored edges (connecting two vertices of different color) — NP hard

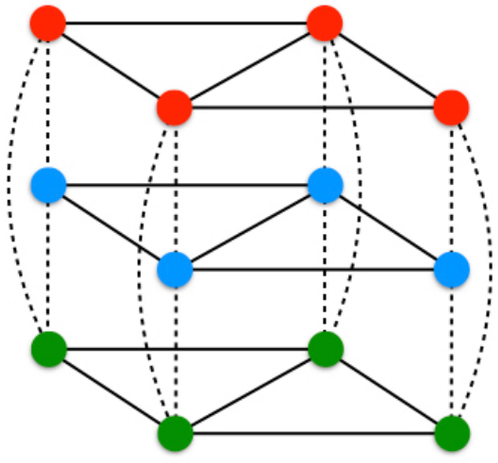
Encoding:

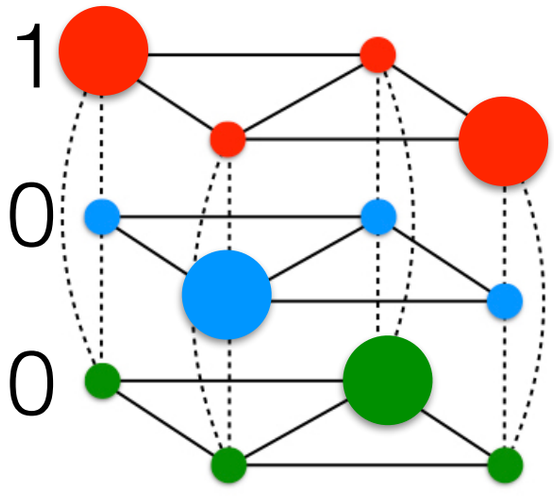
Binary: $x_{v,c} = 1$ whether vertex v is assigned color-c

Constraints:

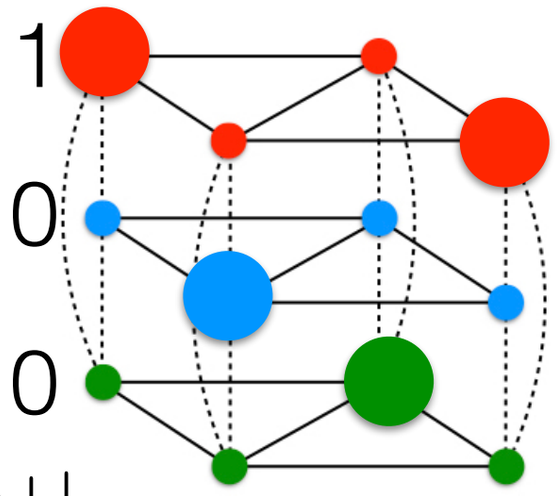
Each vertex should have exactly one color: $\sum_{c=1}^{k} x_{v,c} = 1 \Longleftrightarrow \sum_{c=1}^{k} \sigma_{v,c}^{z} = k - 2$







QAOA for graph coloring problem



Constraints:

Each vertex should have exactly one color: $\sum_{c=1}^{k} \sigma_{v,c}^{z} = k - 2$

Mixer to Stay in the feasible subspace: $|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|$

XY-model

$$\propto \sigma_{v,c}^{x}\sigma_{v,c}^{x} + \sigma_{v,c}^{y}\sigma_{v,c}^{y}$$

- Size of search space

Penalty + X-mixer	Full Hilbert space	2^{nk}
XY mixer	Feasible subspace	k^n
Ratio: $\left(\frac{k}{2^k}\right)^n$	The feasible space **shrinks exponentially** with *n*.	

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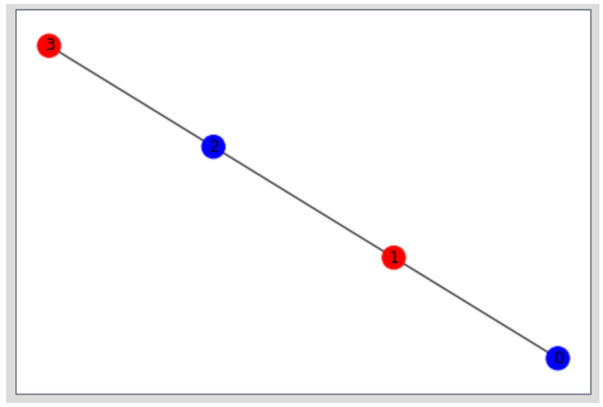
Pseudo code for qiskit to incorporate arbitrary mixer for QAOA

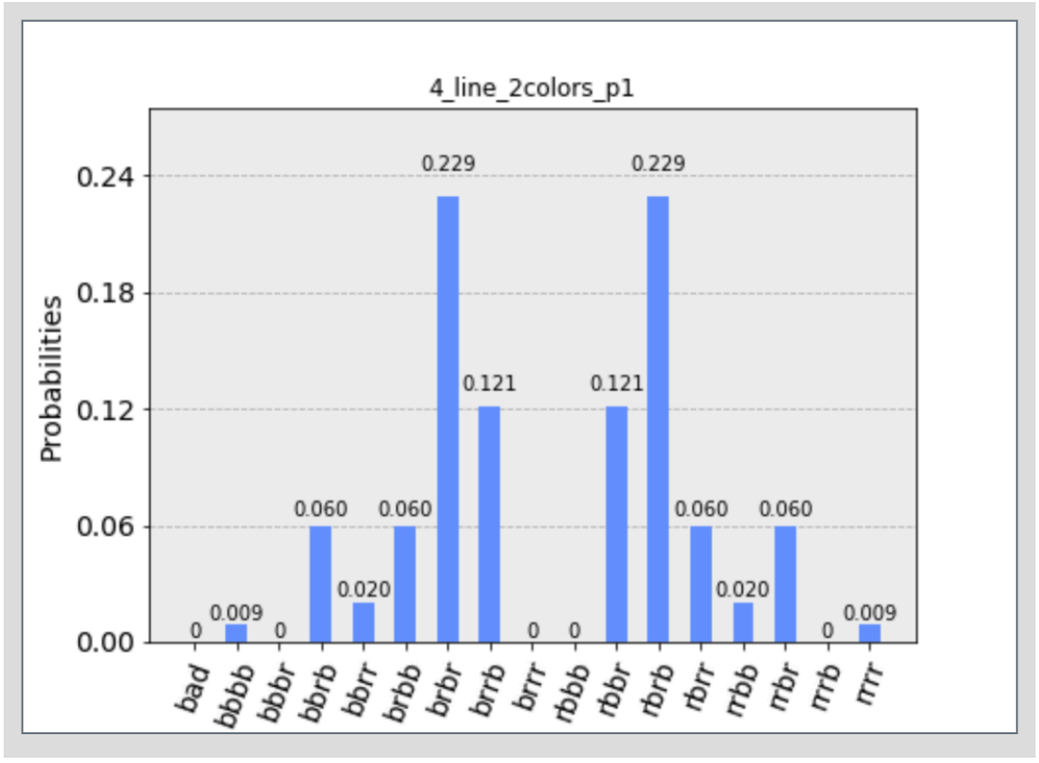
Pseudo-Code

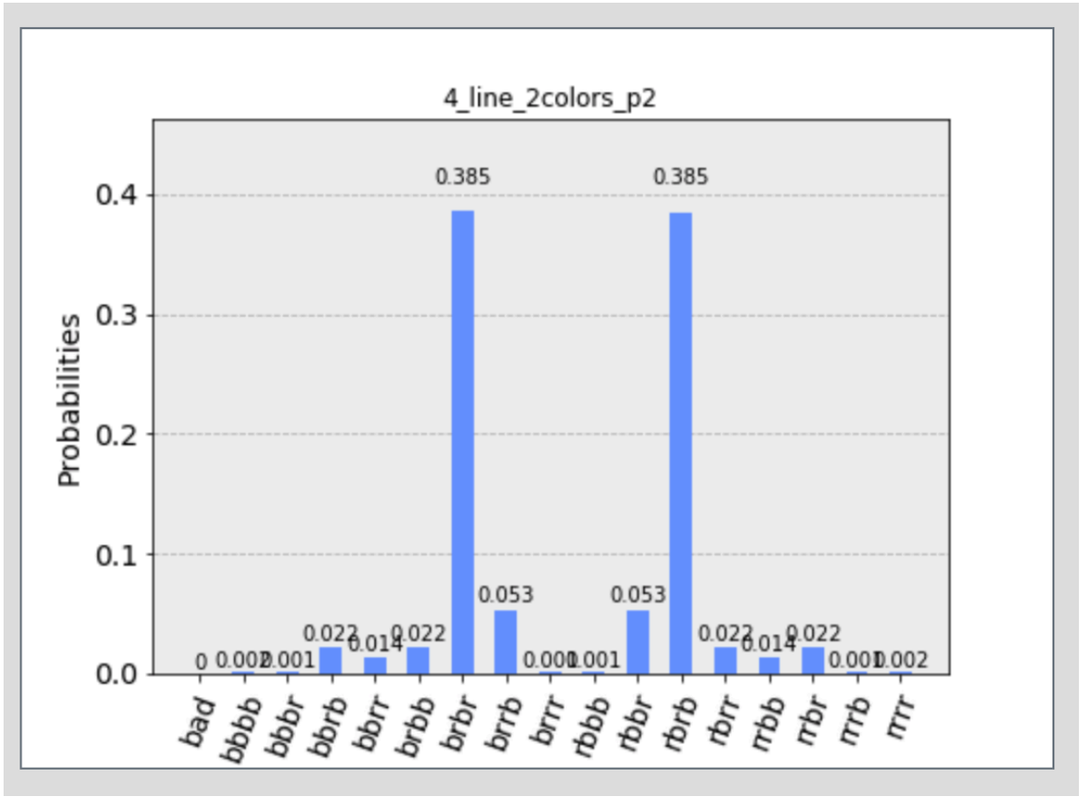
```
class constrainedQAOA(VQE):
    def __init__(cost, mixer, optimizer, initial_state, p, ...):

        # remove old mixer construction

        var_form = constrainedQAOAVarForm(cost, p, mixer, initial_state)

        super().__init__(cost, var_form, optimizer)
```

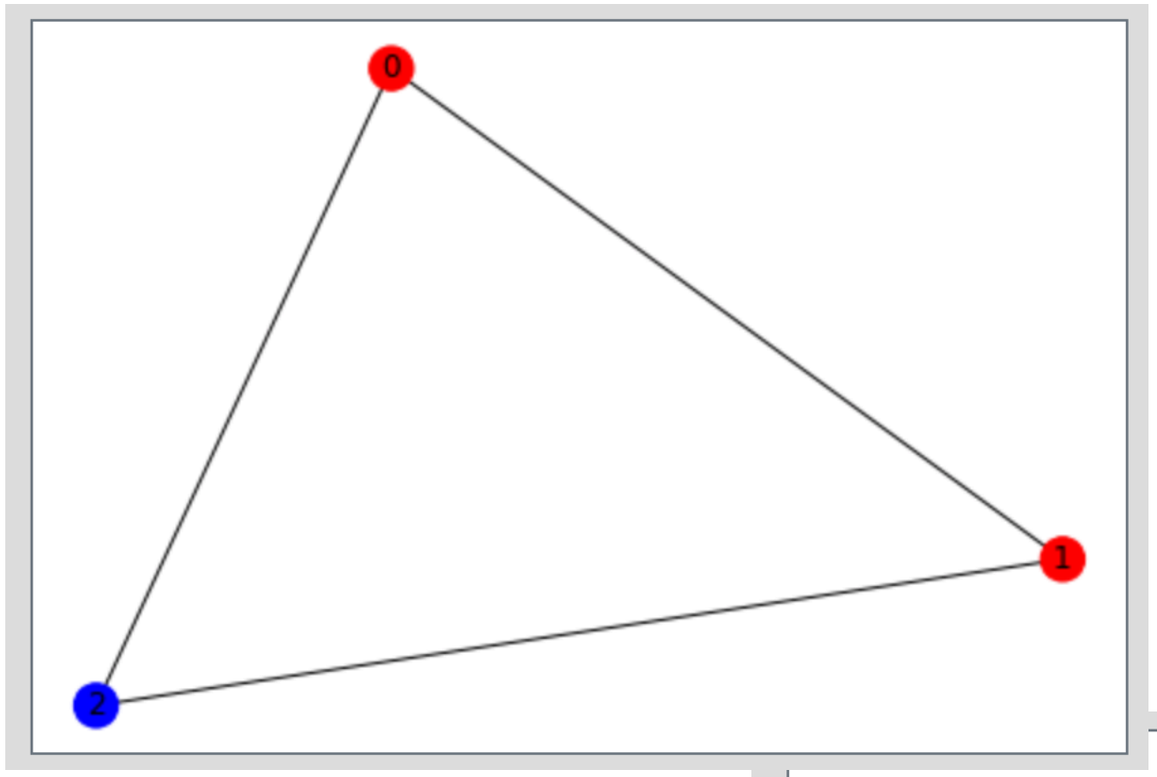
Pseudo-Code

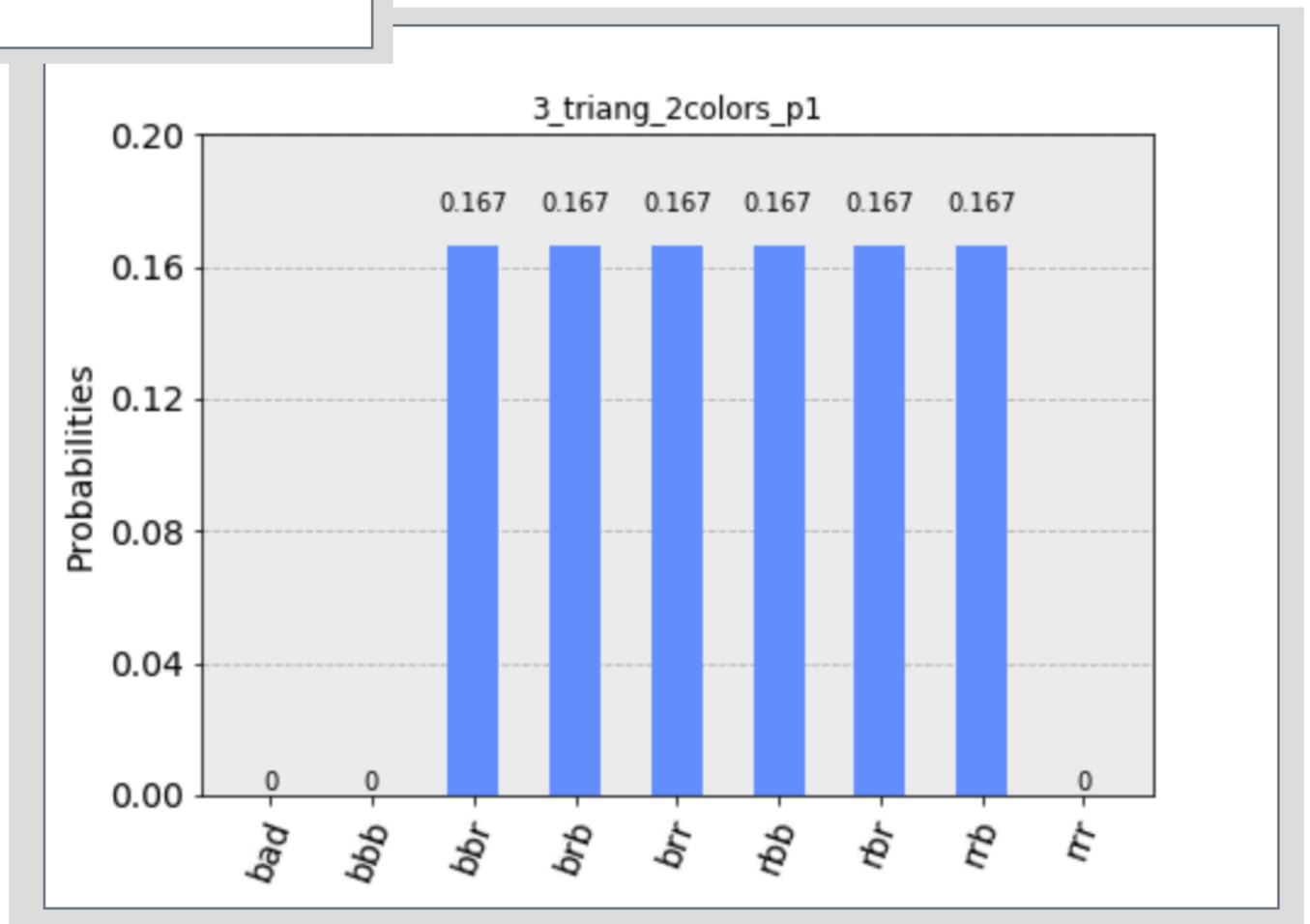
```
class constrainedQAOAVarForm(QAOAVarForm):
    def __init__(self, cost, mixer, initial_state, p, optimizer):
        # remove old mixer construction

    U_c = cost.evolve(gamma)
    U_m = mixer.evolve(beta)
    U_qaoa = U_c*U_m

    VQE(initial_state, U_qaoa, optimizer)
```


3
2
1
0


4_line_2colors_p1
Probabilities
0.00
0.06
0.12
0.18
0.24
0
0.009
0
0.060
0.020
0.060
0.229
0.121
0
0
0.121
0.229
0.060
0.020
0.060
0
0.009
bad
bbbb
bbbr
bbrb
bbrr
brbb
brbr
brrb
brrr
rbbb
rbbr
rbrb
rbrr
rrbb
rrbr
rrrb
rrr

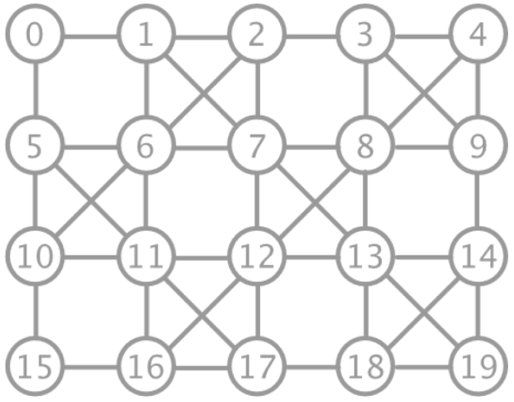

4_line_2colors_p2
Probabilities
0.0
0.1
0.2
0.3
0.4
0
0.002
0.001
0.022
0.014
0.022
0.385
0.053
0.001
0.001
0.053
0.385
0.022
0.014
0.022
0.001
0.002
bad
bbbb
bbbr
bbrb
bbrr
brbb
brbr
brrb
brrr
rbbb
rbbr
rbrb
rbrr
rrbb
rrbr
rrrb
rrr

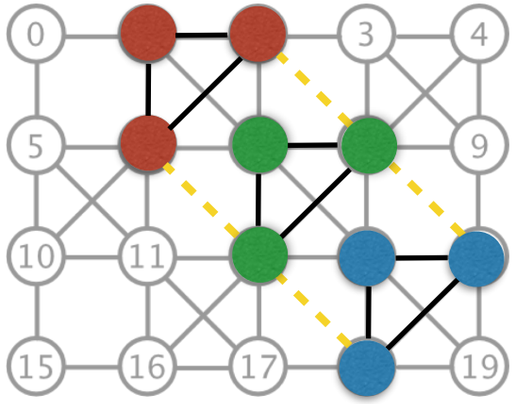

0
1
2

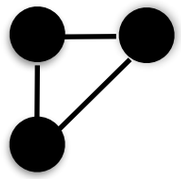

3_triang_2colors_p1
Probabilities
0.20
0.16
0.12
0.08
0.04
0.00
0.167
0.167
0.167
0.167
0.167
0.167
0
0
0
bad
bbb
bbr
brb
brr
rbb
rbr
rrb
rrr

On the hardware IBM Q 20 Tokyo:

3-coloring of a triangle



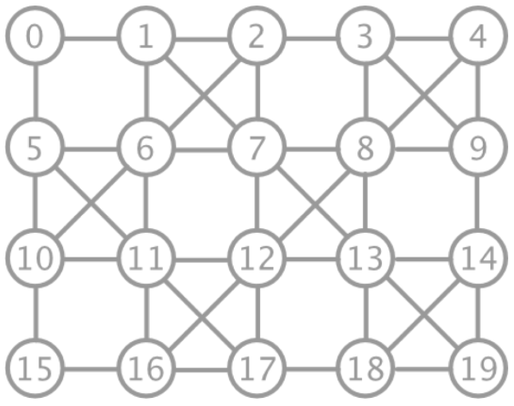


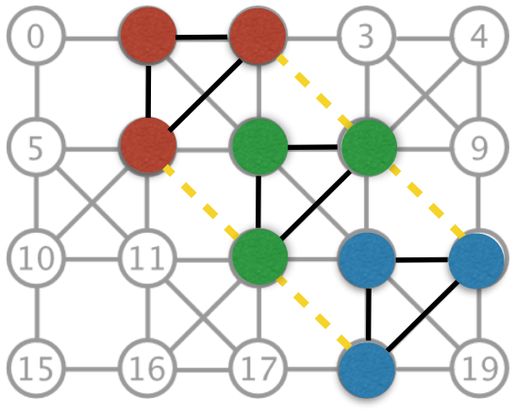


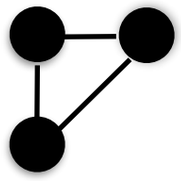
missing connections: SWAP gates needed

On the hardware IBM Q 20 Tokyo:

3-coloring of a triangle





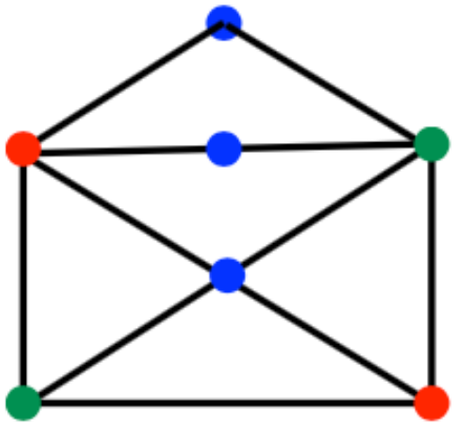


missing connections: SWAP gates needed

> Hi. We get "ERROR_RUNNING_JOB". It seems that your circuit is too long.
>
> I see there are so many CNOT gates. They result in bad fidelity because of CNOT gate errors.

What we could be seeing:

(previous simulation results)



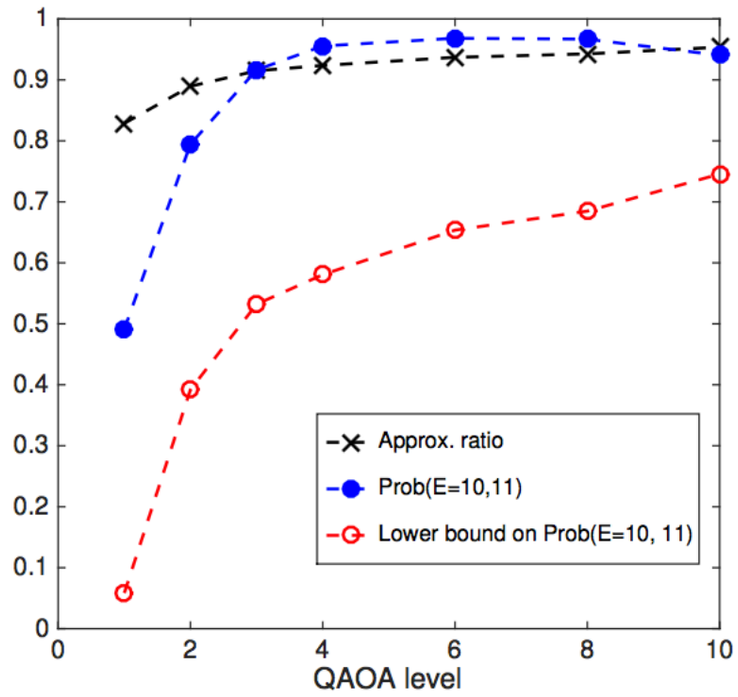
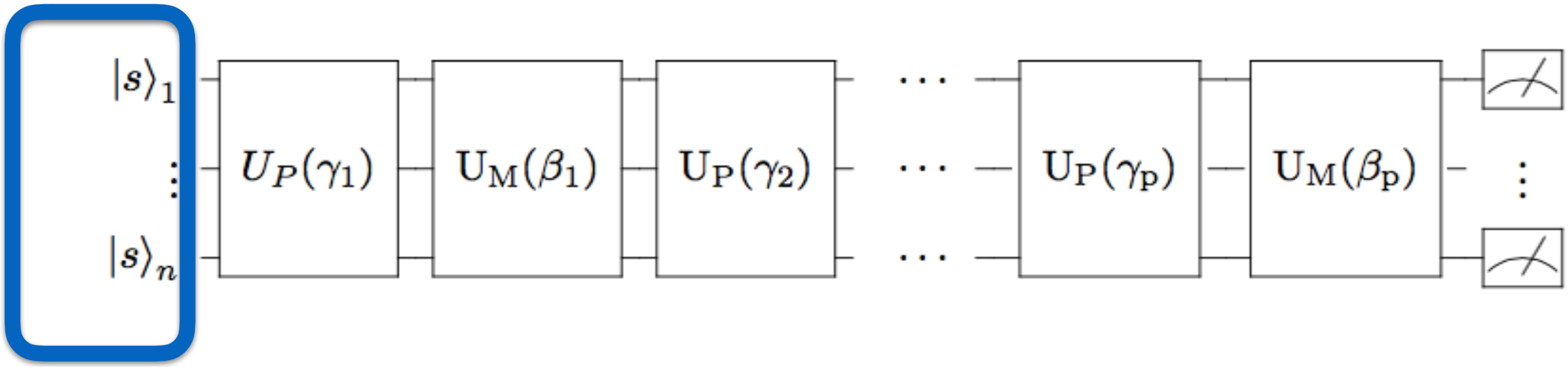


Figure 8. 3-coloring of Envelope graph (11 edges). QAOA with simultaneous ring-mixer. For each QAOA level, the probability of getting the top two highest approximate results (cost 11 and 10) is shown in comparison to the bound given by Eq. (1) with the observed approximation ratio as parameter.

Wang, Rubin, Dominy, Rieffel. **XY mixer for QAOA on graph coloring problems.** (to-appear)



Initial state: W-state

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Conclusion

- QAOA on constraint problems — Explore symmetries in the system, use a smart mixer!

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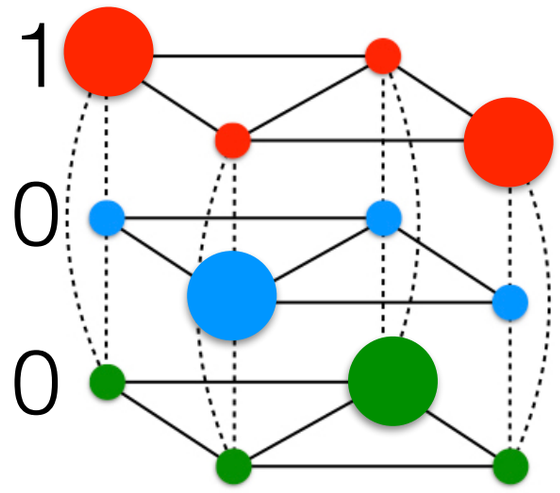
QAOA for graph coloring problem

Cost function

$$f_C = m - \sum_{c=1}^{k} \sum_{\{v,v'\} \in E} x_{v,c} x_{v',c}$$

Cost Hamiltonian

$$H_C = \sum_{c=1}^{k} \sum_{\{v,v'\} \in E} \sigma^z_{v,c} \sigma^z_{v',c}$$



Results

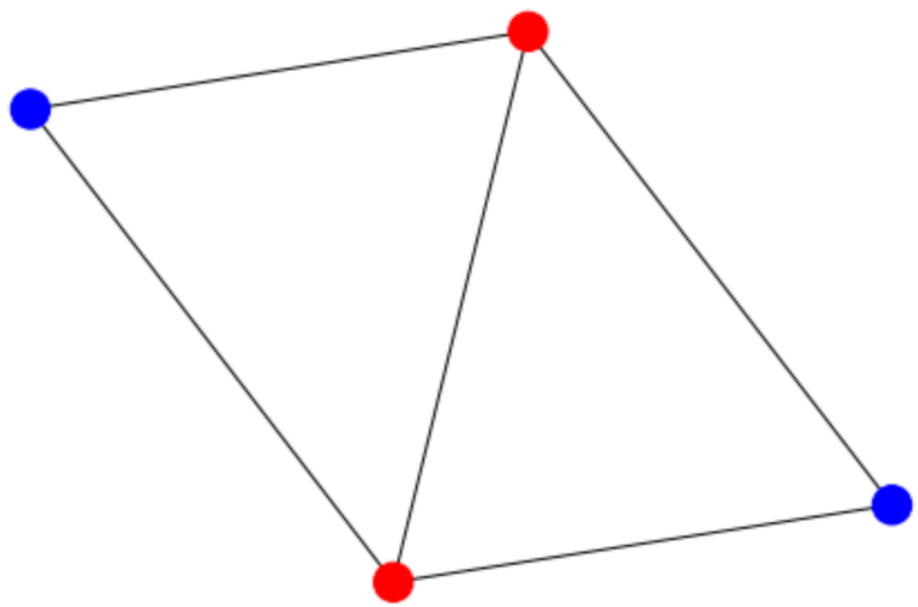
Graphs with 2 colors

In [4]:
```
for graph, structure in zip(to_graph_2colors, structures_2colors):
    probs = get_probs('results/' + graph)
    print('---------------' + graph[:-11] + '---------------')
    draw_best_coloring_2colors(probs, graphs[structure])
    plt.show()
```

```
---------------4_square1diag_2colors_p1---------------
Probability of coloring: 0.2202

---------------4_square1diag_2colors_p2---------------
Probability of coloring: 0.4327


---------------4_square1diag_2colors_p3---------------
Probability of coloring: 0.4644
```



Graphs with 4 colors

In [5]:
```
for graph, structure in zip(to_graph_4colors, structures_4colors):
    probs = get_probs('results/' + graph)
    print('---------------' + graph[:-11] + '---------------')
    draw_best_coloring_4colors(probs, graphs[structure])
    plt.show()
```

```
---------------3_triang_4colors_p1---------------
Probability of coloring: 0.0278
```