HighTemperatureSuperConductorExample

March 21, 2024

1 Fermi Hubbard Ground State Energy Estimation with Quantum Circuits

Consider the two orbital tight binding Fermi Hubbard Model for cuprate superconductors (seen for example here) on a square lattice:

$$
\begin{aligned}
H_{TB} = &-t_1 \sum_{i,\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i+\hat{y},x,\sigma} + d^{\dagger}_{i,y,\sigma} d_{i+\hat{x},y,\sigma} + h.c. \right) \\
&- t_2 \sum_{i,\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i+\hat{x},x,\sigma} + d^{\dagger}_{i,y,\sigma} d_{i+\hat{y},y,\sigma} + h.c. \right) \\
&- t_3 \sum_{i,\hat{\mu},\hat{\nu},\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i+\hat{\mu}+\hat{\nu},x,\sigma} + d^{\dagger}_{i,y,\sigma} d_{i+\hat{\mu}+\hat{\nu},y,\sigma} + h.c. \right) \\
&+ t_4 \sum_{i,\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i+\hat{x}+\hat{y},y,\sigma} + d^{\dagger}_{i,y,\sigma} d_{i+\hat{x}+\hat{y},x,\sigma} + h.c. \right) \\
&- t_4 \sum_{i,\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i+\hat{x}-\hat{y},y,\sigma} + d^{\dagger}_{i,y,\sigma} d_{i+\hat{x}-\hat{y},x,\sigma} + h.c. \right) \\
&- \mu \sum_{i} \left(n^x_i + n^y_i \right)
\end{aligned}
\tag{1}
$$

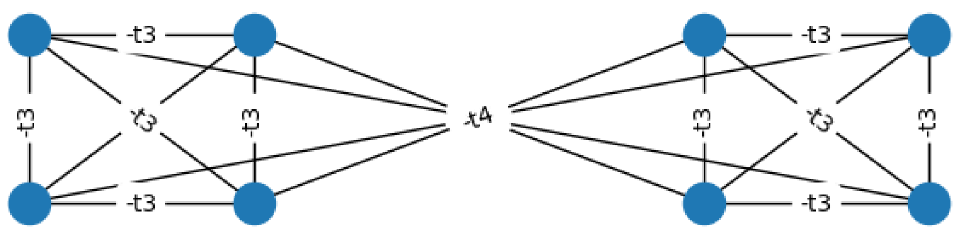
where $t_1 = -1.0, t_2 = 1.3, t_3 = t_4 = -0.85$ with operators $d^{\dagger}_{i,\alpha,\sigma}$ and $d_{i,\alpha,\sigma}$ respectively create or annihilate electrons on an atom at site i, with orbital α, and spin σ. The operator n^{α}_i represents the number operator of an atom at a given orbital, i.e. $n^x_i = \sum_{\sigma} \left(d^{\dagger}_{i,x,\sigma} d_{i,x,\sigma} \right)$. The indices in the Hamiltonian are assigned in the following manner: the index i will correspond to a 2-tuple (m, n) indicating the x and y coordinates of the atom in the lattice. Since there are 2 orbitals, $\alpha \in \{x, y\}$. Lastly, $\sigma \in \{\uparrow, \downarrow\}$. For the sake of simplicity of coding, we will remap these labels to integer values, meaning we will assign indices $m \in L_x, n \in L_y, a \in \mathbb{Z}^2, s \in \mathbb{Z}^2$ where L_x is the x dimension of the square lattice, and L_y is the y dimension of the square lattice. In the summations, $\hat{x}$ and $\hat{y}$ correspond to adjacent sites in the lattice, rather than the orbitals. The summation over unit vectors $\hat{\mu}$ and $\hat{\nu}$ correspond to the summing over unit vectors in all 8 cardinal and intercardinal directions without double counting.

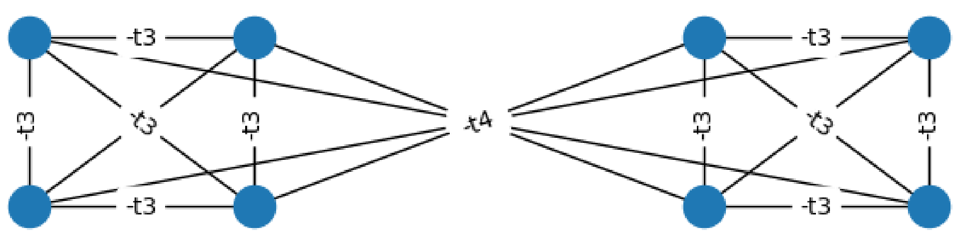
[1]:
```
import time
import numpy as np
from qca.utils.utils import circuit_estimate
from pyLIQTR.PhaseEstimation.pe import PhaseEstimation
from networkx import get_node_attributes, draw, draw_networkx_edge_labels
```

```
from qca.utils.hamiltonian_utils import generate_two_orbital_nx,␣
↪nx_to_two_orbital_hamiltonian
```

```
/Users/jonhas/anaconda3/lib/python3.11/site-packages/attr/_make.py:918:
RuntimeWarning: Running interpreter doesn't sufficiently support code object
introspection.  Some features like bare super() or accessing __class__ will not
work with slotted classes.
  set_closure_cell(cell, cls)
```

[2]:
```
g_example = generate_two_orbital_nx(2,2)
pos = get_node_attributes(g_example, 'pos')
edge_labels = dict([((n1, n2), d['label']) for n1, n2, d in g_example.
↪edges(data=True)]);
draw(g_example, pos)
draw_networkx_edge_labels(g_example,pos, edge_labels = edge_labels);
```





[3]:
```
t1 = -1
t2 = 1.3
t3 = 0.85
t4 = 0.85
mu = 1
```

```
nx_to_two_orbital_hamiltonian(g_example, t1, t2, t3, t4, mu)
```

[3]:
```
-1.0 [0^ 0] +
-0.85 [0^ 4] +
-0.85 [0^ 8] +
-0.85 [0^ 12] +
0.85 [0^ 14] +
-1.0 [1^ 1] +
-0.85 [1^ 5] +
-0.85 [1^ 9] +
-0.85 [1^ 13] +
0.85 [1^ 15] +
-1.0 [2^ 2] +
-0.85 [2^ 6] +
-0.85 [2^ 10] +
0.85 [2^ 12] +
-0.85 [2^ 14] +
-1.0 [3^ 3] +
-0.85 [3^ 7] +
-0.85 [3^ 11] +
0.85 [3^ 13] +
-0.85 [3^ 15] +
-0.85 [4^ 0] +
-1.0 [4^ 4] +
-0.85 [4^ 8] +
-0.85 [4^ 10] +
-0.85 [4^ 12] +
-0.85 [5^ 1] +
-1.0 [5^ 5] +
-0.85 [5^ 9] +
-0.85 [5^ 11] +
-0.85 [5^ 13] +
-0.85 [6^ 2] +
-1.0 [6^ 6] +
-0.85 [6^ 8] +
-0.85 [6^ 10] +
-0.85 [6^ 14] +
-0.85 [7^ 3] +
-1.0 [7^ 7] +
-0.85 [7^ 9] +
-0.85 [7^ 11] +
-0.85 [7^ 15] +
-0.85 [8^ 0] +
-0.85 [8^ 4] +
-0.85 [8^ 6] +
-1.0 [8^ 8] +
-0.85 [8^ 12] +
```

```
-0.85 [9^ 1] +
-0.85 [9^ 5] +
-0.85 [9^ 7] +
-1.0 [9^ 9] +
-0.85 [9^ 13] +
-0.85 [10^ 2] +
-0.85 [10^ 4] +
-0.85 [10^ 6] +
-1.0 [10^ 10] +
-0.85 [10^ 14] +
-0.85 [11^ 3] +
-0.85 [11^ 5] +
-0.85 [11^ 7] +
-1.0 [11^ 11] +
-0.85 [11^ 15] +
-0.85 [12^ 0] +
0.85 [12^ 2] +
-0.85 [12^ 4] +
-0.85 [12^ 8] +
-1.0 [12^ 12] +
-0.85 [13^ 1] +
0.85 [13^ 3] +
-0.85 [13^ 5] +
-0.85 [13^ 9] +
-1.0 [13^ 13] +
0.85 [14^ 0] +
-0.85 [14^ 2] +
-0.85 [14^ 6] +
-0.85 [14^ 10] +
-1.0 [14^ 14] +
0.85 [15^ 1] +
-0.85 [15^ 3] +
-0.85 [15^ 7] +
-0.85 [15^ 11] +
-1.0 [15^ 15]
```

[4]:
```
g_current_limit = generate_two_orbital_nx(6,7)
g_ideal = generate_two_orbital_nx(10,10)

##### START UNCOMMENT FOR TESTING
#n_test = 2
#g_current_limit = generate_two_orbital_nx(n_test,n_test)
#g_ideal = generate_two_orbital_nx(n_test,n_test)
##### END UNCOMMENT FOR TESTING
n_qubits_current_limit = len(g_current_limit)
n_qubits_ideal = len(g_ideal)
```

[5]:
```python
ham_current_limit = nx_to_two_orbital_hamiltonian(g_current_limit,t1,t2,t3,t4,mu)
ham_ideal = nx_to_two_orbital_hamiltonian(g_ideal,t1,t2,t3,t4,mu)
trotter_order_current_limit = 2
trotter_steps_current_limit = 1

trotter_order_ideal = 2
trotter_steps_ideal = 1

#note that we would actually like ~10 bits of precision, it just takes a really long time to run
bits_precision_ideal = 1
bits_precision_current_limit = 1

current_limit_args = {
    'trotterize' : True,
    'mol_ham'    : ham_current_limit,
    'ev_time'    : 1,
    'trot_ord'   : trotter_order_current_limit,
    'trot_num'   : trotter_steps_current_limit
}

ideal_args = {
    'trotterize' : True,
    'mol_ham'    : ham_ideal,
    'ev_time'    : 1,
    'trot_ord'   : trotter_order_ideal,
    'trot_num'   : trotter_steps_ideal
}
```

[6]:
```python
E_min_ideal = -len(ham_ideal.terms)
E_max_ideal = 0
ideal_omega = E_max_ideal-E_min_ideal
t_ideal = 2*np.pi/ideal_omega
ideal_phase_offset = E_max_ideal*t_ideal

E_min_current_limit = -len(ham_current_limit.terms)
E_max_current_limit = 0
limited_omega = E_max_current_limit-E_min_current_limit
limited_t = 2*np.pi/limited_omega
limited_phase_offset = E_max_current_limit*limited_t

init_state_ideal = [0] * n_qubits_ideal
init_state_current_limit = [0] * n_qubits_current_limit

print('starting')
t0 = time.perf_counter()
```

```
gse_inst_current_limit = PhaseEstimation(
    precision_order=bits_precision_current_limit,
    init_state=init_state_current_limit,
    phase_offset=limited_phase_offset,
    include_classical_bits=False, # Do this so print to openqasm works
    kwargs=current_limit_args)
gse_inst_current_limit.generate_circuit()
t1 = time.perf_counter()
print(f'current limit time to generate high level: {t1 - t0}')

t0 = time.perf_counter()
gse_inst_ideal = PhaseEstimation(
    precision_order=bits_precision_ideal,
    init_state=init_state_ideal,
    phase_offset=ideal_phase_offset,
    include_classical_bits=False, # Do this so print to openqasm works
    kwargs=ideal_args)
gse_inst_ideal.generate_circuit()
t1 = time.perf_counter()
print(f'ideal time to generate high level: {t1 - t0}')

gse_circuit_ideal = gse_inst_ideal.pe_circuit
gse_circuit_current_limit = gse_inst_current_limit.pe_circuit
```

```
starting
current limit time to generate high level: 0.18624829200052773
ideal time to generate high level: 0.9717117079999298
```

[7]:

```
print('Estimating Ideal')
t0 = time.perf_counter()
circuit_estimate(gse_circuit_ideal,
                 outdir='GSE/',
                 circuit_name='ideal',
                 trotter_steps=trotter_steps_ideal,
                 write_circuits=True)
t1 = time.perf_counter()
print(f'Time to estimate Ideal: {t1-t0}')

print('Estimating Current Limit')
t0 = time.perf_counter()
circuit_estimate(gse_circuit_current_limit,
                 outdir='GSE/',
                 circuit_name='current_limit',
                 trotter_steps=trotter_steps_current_limit,
                 write_circuits=True)
t1 = time.perf_counter()
print(f'Time to estimate Current Limit: {t1-t0}')
```

```
Estimating Ideal
   Time to decompose high level <class 'cirq.ops.common_gates.HPowGate circuit:
0.00017020799896272365 seconds
   Time to transform decomposed <class 'cirq.ops.common_gates.HPowGate circuit
to Clifford+T: 2.499999936844688e-05 seconds
   Time to decompose high level <class 'cirq.ops.identity.IdentityGate circuit:
6.779099931009114e-05 seconds
   Time to transform decomposed <class 'cirq.ops.identity.IdentityGate circuit
to Clifford+T: 4.666999302571639e-06 seconds
   Time to decompose high level <class
'pyLIQTR.PhaseEstimation.pe_gates.PhaseOffset circuit: 0.0001875830002973089
seconds
   Time to transform decomposed <class
'pyLIQTR.PhaseEstimation.pe_gates.PhaseOffset circuit to Clifford+T:
0.00044433299990487285 seconds
   Time to decompose high level <class
'pyLIQTR.PhaseEstimation.pe_gates.Trotter_Unitary circuit: 162.3568995000005
seconds
   Time to transform decomposed <class
'pyLIQTR.PhaseEstimation.pe_gates.Trotter_Unitary circuit to Clifford+T:
94.940695416999 seconds
   Time to decompose high level <class
'cirq.ops.measurement_gate.MeasurementGate circuit: 0.2753461669999524 seconds
   Time to transform decomposed <class
'cirq.ops.measurement_gate.MeasurementGate circuit to Clifford+T:
8.658299884700682e-05 seconds
Time to estimate Ideal: 363.3271536249995
Estimating Current Limit
   Time to decompose high level <class 'cirq.ops.common_gates.HPowGate circuit:
0.00010029199984273873 seconds
   Time to transform decomposed <class 'cirq.ops.common_gates.HPowGate circuit
to Clifford+T: 1.849999898695387e-05 seconds
   Time to decompose high level <class 'cirq.ops.identity.IdentityGate circuit:
3.937499968742486e-05 seconds
   Time to transform decomposed <class 'cirq.ops.identity.IdentityGate circuit
to Clifford+T: 3.0829996831016615e-06 seconds
   Time to decompose high level <class
'pyLIQTR.PhaseEstimation.pe_gates.PhaseOffset circuit: 0.0001780420006980421
seconds
   Time to transform decomposed <class
'pyLIQTR.PhaseEstimation.pe_gates.PhaseOffset circuit to Clifford+T:
0.0001404169997840654 seconds
   Time to decompose high level <class
'pyLIQTR.PhaseEstimation.pe_gates.Trotter_Unitary circuit: 27.900314915999843
seconds
   Time to transform decomposed <class
'pyLIQTR.PhaseEstimation.pe_gates.Trotter_Unitary circuit to Clifford+T:
31.835247708999304 seconds
```

```
   Time to decompose high level <class
'cirq.ops.measurement_gate.MeasurementGate circuit: 0.056535290999818244 seconds
   Time to transform decomposed <class
'cirq.ops.measurement_gate.MeasurementGate circuit to Clifford+T:
9.570899965183344e-05 seconds
Time to estimate Current Limit: 93.05950350000057
```

[ ]: