

Tutorial Sheet-5

PHN-640

QUANTUM COMPUTING

SPRING 2024

1. For the three encodings- one-hot (OH) encoding with Jordan-Wigner (JW) transformation, Bravyi-Kitaev (BK) encoding, and Gray code (GC) encoding, the Hamiltonian H_2 for a central potential with the basis size $N = 2$ are given below

$$H_{JW(2)} = 7.858535I + 0.00257Z_0 - 7.861105Z_1 - 0.37778(X_0X_1 + Y_0Y_1),$$

$$H_{BK(2)} = 7.858535I + 0.00257Z_0 - 7.861105Z_0Z_1 - 0.37778(X_0 - X_0Z_1),$$

$$H_{GC(2)} = 7.858535I - 7.863675Z_0 - 0.75556X_0,$$

- Create a quantum circuit (ansatz) for each of the Hamiltonian.
 - Define a subroutine `minimization` using an optimizer `COBYLA` to find the minimum energy eigenvalue E of each Hamiltonian.
 - For shots $S = [5e2, 6e3, 7e4, 8e5, 9e6]$, use the subroutine `minimization` to find E and store it in an array `E_shots`. Plot `E_shots` vs S .
 - Execute the code for 20 runs taking 1000 shots and store the result in an array `E_runs`.
 - Find the median M and median absolute deviation (MAD) for `E_runs`. Plot M vs N showing the error bar (MAD).
2. Repeat the Q. No. 1 for $N = 3$ for the following Hamiltonians

$$H_{JW(3)} = H_{JW(2)} + 15.92676(I - Z_2) - 3.6989(X_0Z_1X_2 + Y_0Z_1Y_2) + 4.123715(X_1X_2 + Y_1Y_2),$$

$$H_{BK(3)} = H_{BK(2)} + 15.92676(I - Z_2) - 3.6989(X_0Y_1Y_2 - Y_0Y_1X_2) + 4.123715(X_1X_2 + Z_0Y_1Y_2),$$

$$H_{GC(3)} = 11.892645I - 11.895215Z_0 - 4.03411Z_1 + 4.03154Z_0Z_1 - 3.6989(X_0X_1 - Y_0Y_1) \\ + 4.123715(X_1 - Z_0X_1) - 0.37778(X_0 + X_0Z_1).$$

3. Find E for $H_{JW(2)}$ and $H_{BK(2)}$ taking $runs = 20$ using

- `StatevectorEstimator` to find the ideal value of E
- Noise model of *QASM* simulator
- Noise model with mitigation

Plot the histogram of *Counts* (*runs*) vs E in each case.

4. Repeat the Q. No. 3 for H_{GC} taking $N = 2$ and $N = 4$.
5. Solve the integration I using Monte Carlo integration.

$$I = \int_1^4 (x^2 + 1)dx$$

For shots $S = [500, 1000, 2000, 4000, 8000, 10000]$, store the result each time in an array for 100 runs and plot the histogram for each value of S .
