Intel® Quantum SDK Tutorials

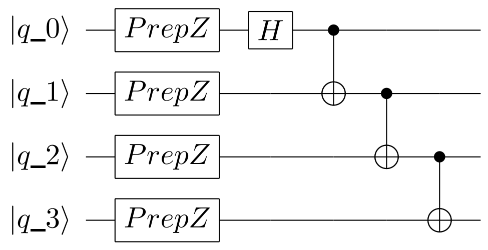
February 15, 2024

Release Version 1.1

Contents:

1.0 A Tour of GHZ examples

This tutorial provides some basic introduction to programming quantum algorithms and working with the `FullStateSimulator` through three implementations of the following circuit



and the accompanying classical logic. The executable will manage running the above quantum circuit and retrieving the data in the `FullStateSimulator` to confirm the instructions are producing what is intended. This circuit produces a Greenberger-Horne-Zeilinger (GHZ) state for 4 qubits. In other words, the qubits will be in a super-position of two states, one with all qubits in the $|0\rangle$ state and one with all qubits in the $|1\rangle$ state, and each with equal chance of being measured.

The source code for each implementation is available in the `quantum_examples/` directory of the Intel® Quantum SDK.

1.1 Ideal GHZ

To begin writing the program, get access to the quantum data types and methods by including the `quintrinsics.h` and the `quantum_full_state_simulator_backend.h` headers into the source as shown in Listing 1.

Listing 1: The headers required to use the quantum gates or `FullStateSimulator`.

```
#include <clang/Quantum/quintrinsics.h>

/// Quantum Runtime Library APIs
#include <quantum_full_state_simulator_backend.h>
```

As described in Getting Started Guide (Writing New Algorithms), next declare an array of qubits (`qbit`) in the global namespace as show in Listing 2

Listing 2: Declaration of the `qbit` type variables in global namespace.

```
const int total_qubits = 4;
qbit qubit_register[total_qubits];
```

Next, implement the quantum algorithm by writing the functions or classes that contain the quantum logic. The `quantum_kernel` keyword should be in front of each function that builds the quantum algorithm. Shown in Listing 3, all the quantum instructions are placed in a single `quantum_kernel`. The first instruction is to initialize the state of each qubit by utilizing a `for` loop to call `PrepZ()` on the elements of the `qbit` array. Next, apply a Hadamard gate (`H()`) on the first qubit to set it into a superposition. And lastly, apply Controlled Not gates (`CNOT()`) on pairs of qubits to create entanglement between them.

Listing 3: `quantum_kernel` to prepare a Greenberger-Horne-Zeilinger state.

```
quantum_kernel void ghz_total_qubits() {
  for (int i = 0; i < total_qubits; i++) {
    PrepZ(qubit_register[i]);
  }

  H(qubit_register[0]);

  for (int i = 0; i < total_qubits - 1; i++) {
    CNOT(qubit_register[i], qubit_register[i + 1]);
  }
}
```

In the `main` function of the program, instantiate a `FullStateSimulator` object and use its `ready()` method, as shown in Listing 4. Do that as described in Developer Guide and Reference (Configuring the FullStateSimulator), by first creating an `IqsConfig` object, changing it to be verbose (not required), and then using it as an argument to the `FullStateSimulator` constructor. Then use the return of the `ready()` method to trigger an early exit if something is wrong.

Listing 4: Setup of the FullStateSimulator. See Developer Guide and Reference (Configuring the FullStateSimulator) for a more detailed explanation.

```
int main() {
  iqsdk::IqsConfig settings(total_qubits, "noiseless");
  settings.verbose = true;
  iqsdk::FullStateSimulator quantum_8086(settings);
  if (iqsdk::QRT_ERROR_SUCCESS != quantum_8086.ready())
    return 1;
```

Next, prepare the classical data structures for working with simulation data. Create a set of `id` values to refer to the qubits of interest as shown in Listing 5. This is important because `qbit` variables do not necessarily specify a constant physical qubit in hardware; this mapping can be created and changed at various stages during program execution according to the compiler optimizations.

Listing 5: Declare and fill a `std::vector` with references to the elements of the `qbit` array.

```
  // get references to qbits
  std::vector<std::reference_wrapper<qbit>> qids;
  for (int id = 0; id < total_qubits; ++id) {
    qids.push_back(std::ref(qubit_register[id]));
  }
```

Now that the backend simulator is ready, call the `quantum_kernel`.

Listing 6: Call the `quantum_kernel`.

```
ghz_total_qubits();
```

After this line during execution, the `FullStateSimulator` contains the state-vector data describing the qubits. Although there are facilities to conveniently specify every possible state for a set of qubits, this could be an overwhelming amount of data. Where possible, use the available constructors described in API Reference to configure a `QssIndex` object to refer to only the states of interest and store them in a vector. In Listing 7, two explicit strings formatted for 4 qubits are used to specify the two states.

Listing 7: Specifying the states of interest; this will be an argument used to collect data from the simulation.

```
// use string constructor of Quantum State Space index to choose which
// basis states' data is retrieved
iqsdk::QssIndex state_a("|0000>");
iqsdk::QssIndex state_b("|1111>");
std::vector<iqsdk::QssIndex> bases;
bases.push_back(state_a);
bases.push_back(state_b);
```

Now access the probabilities for these two states through `FullStateSimulator`'s `getProbabilities()` method. Remember that ideally the GHZ state would only be in $|0000\rangle$ or $|1111\rangle$. So for this simulated circuit, when summing the probabilities of measuring in either $|0000\rangle$ or $|1111\rangle$, the sum should be 1.0.

Listing 8: The classical logic that checks a property of the state in the qubit register. This gets quantum results from simulation data at runtime.

```
iqsdk::QssMap<double> probability_map;
probability_map = quantum_8086.getProbabilities(qids, bases);

double total_probability = 0.0;
for (auto const & key_value : probability_map) {
  total_probability += key_value.second;
}
std::cout << "Sum of probability to measure fully entangled state: "
          << total_probability << std::endl;
```

Alternatively, display a formatted summary of the states to the console output with `displayProbabilities()` or `displayAmplitudes()`.

Listing 9: Generate a quick, formatted display of the probabilities for the two states of interest printed to the console.

```
quantum_8086.displayProbabilities(probability_map);
```

This program can be compiled with the default options. Configuring the qubit simulation in the Intel® Quantum Simulator creates a set of qubits with no limitation on their connectivity, in other words two-qubit operations (gates) can be applied between any pair of qubits.

```
$  <path to Intel Quantum SDK>/intel-quantum-compiler ideal_GHZ.cpp
```

Running the executable produces a line describing each quantum instruction because the verbose option was set to true when configuring the `FullStateSimulator`. That is followed by the line showing that `total_-probability` is equal to 1 and the summary produced by `displayProbabilities()`.

```
$ ./ideal_GHZ

- Run noiseless simulation (verbose mode)
Instruction #4 : ROTXY(phi = 1.5707, gamma = 1.57075)  on phys Q 0
Instruction #5 : ROTXY(phi = 0, gamma = 3.14154)  on phys Q 0
Instruction #6 : ROTXY(phi = 4.71229, gamma = 1.57075)  on phys Q 1
Instruction #7 : CPHASE(gamma = 3.1415) on phys Q0 and phys Q1
Instruction #8 : ROTXY(phi = 1.5707, gamma = 1.57075)  on phys Q 1
Instruction #9 : ROTXY(phi = 4.71229, gamma = 1.57075)  on phys Q 2
Instruction #10 : CPHASE(gamma = 3.1415) on phys Q1 and phys Q2
Instruction #11 : ROTXY(phi = 1.5707, gamma = 1.57075)  on phys Q 2
Instruction #12 : ROTXY(phi = 4.71229, gamma = 1.57075)  on phys Q 3
Instruction #13 : CPHASE(gamma = 3.1415) on phys Q2 and phys Q3
Instruction #14 : ROTXY(phi = 1.5707, gamma = 1.57075)  on phys Q 3
Sum of probability to measure fully entangled state: 1
Printing probability map of size 2
|0000>  : 0.5                           |1111>  : 0.5
```

The complete code is available as `ideal_GHZ.cpp` in the `quantum_examples/` directory of the Intel® Quantum SDK.

1.2 Sampled GHZ

As discussed in Developer Guide and Reference (Measurements & FullStateSimulator), the state-vector probabilities that the above program uses are not data that quantum hardware is capable of returning. Consider the hypothetical scenario in which you now need to know how many times the quantum circuit must be run and evaluated in order to find the probability with the desired numerical accuracy. This can be done efficiently by using the simulation data.

Only the non-`quantum_kernel` sections of the `ideal_GHZ.cpp` program need changed to accomplish this. This can be done by using a different `FullStateSimulator` method after calling the `quantum_kernel`, as shown in Listing 10

Listing 10: code_samples/sample_GHZ.cpp

```
  // use sampling technique to simulate the results of many runs
  std::vector<std::vector<bool>> measurement_samples;
  unsigned total_samples = 1000;
  measurement_samples = quantum_8086.getSamples(total_samples, qids);
```

Each `std::vector<bool>` represents the observation of a state, each individual value represents the outcome of that qubit as arranged in the `qids` vector. The `FullStateSimulator` has a helper method to conveniently calculate the number of times a given state appears in an ensemble of observations.

Listing 11: code_samples/sample_GHZ.cpp

```
// build a distribution of states
iqsdk::QssMap<unsigned int> distribution =
        iqsdk::FullStateSimulator::samplesToHistogram(measurement_samples);
```

From this `QssMap`, calculate the estimate of the probability of observing each state.

Listing 12: The classical logic inspecting the results of sampling many simulated measurements.

```
// print out the results
std::cout << "Using " << total_samples
          << " samples, the distribution of states is:" << std::endl;
for (const auto & entry : distribution) {
  double weight = entry.second;
  weight = weight / total_samples;

  std::cout << entry.first << " : " << weight << std::endl;
}
```

This program can be compiled with the same command as the previous program.

```
$ <path to Intel Quantum SDK>/intel-quantum-compiler sample_GHZ.cpp
```

In addition to the same output from `ideal_GHZ.cpp`, the result of the `samplesToHistogram()` method is also printed out:

```
Using 1000 samples, the distribution of states is:
|0000> : 0.496
|1111> : 0.504
```

Because the `IqsConfig` used the default setting of a random seed (by not specifying one), this simulation will produce a different sequence of samples on subsequent executions and thus a slightly different estimate of the probability of observing each state.

The complete code is available as `sample_GHZ.cpp` in the `quantum_examples/` directory of the Intel® Quantum SDK.

1.3 GHZ state on Quantum Dot Simulator

It takes the change of only a few lines of code to target another backend, as you can see by comparing `sample_-GHZ.cpp` and `qd_GHZ.cpp` (e.g. using the `diff` CLI tool). As described in Developer Guide and Reference (Quantum Dot (QD) Simulator), the Quantum Dot Simulator (`QD_Sim`) adds to the state vector simulation by including details from the control signals that interact with quantum dot qubits. This creates additional computational overhead compared to the Intel® Quantum Simulator. The first change in this program is to reduce the size of the circuit to just a pair of qubits so the execution stays around a few seconds.

QD_Sim treats running sequential quantum_kernels and measurement gates differently than the Intel® Quantum Simulator (see Developer Guide and Reference (Important Points on the Quantum Dot Simulator)). Although some programs could require alteration of their logic, the above program's quantum_kernel and simulator usage is compatible with either backend. To change the qubit simulator, instead of the IqsConfig object switch to a DeviceConfig constructed with the argument "QD_SIM" as shown in Listing 13 (note the all capitals for the argument string).

Listing 13: Configuring the FullStateSimulator to use the Quantum Dot Simulator backend.

```
int main() {
  iqsdk::DeviceConfig qd_config("QD_SIM");
  iqsdk::FullStateSimulator quantum_8086(qd_config);
```

With this change of backend qubit simulation, the program must now be compiled with non-default options. The file intel-quantum-sdk-QDSIM.json points to a file describing a 6-qubit linear array. Use the -c flag to give the file's location to the compiler, and specify placement and scheduling options with -p and -S.

```
$ <path to Intel Quantum SDK>/intel-quantum-compiler -c <path to Intel Quantum SDK>/intel-
↪quantum-sdk-QDSIM.json -p trivial -S greedy qd_GHZ.cpp
```

QD_Sim produces its own output in addition to the output explicitly designed into the behavior of the program.

```
$ ./qd_GHZ.cpp

1688766838 time dependent evolution start time
sweep progress: calculation point=0 0%
sweep progress: calculation point=18199 10%
sweep progress: calculation point=36398 20%
sweep progress: calculation point=54597 30%
sweep progress: calculation point=72796 40%
sweep progress: calculation point=90994 50%
sweep progress: calculation point=109193 60%
sweep progress: calculation point=127392 70%
sweep progress: calculation point=145591 80%
sweep progress: calculation point=163790 90%
Time evolution took 2.568378 seconds
Fri Jul  7 14:54:01 2023
1688766841 time dependent evolution end time
Sum of probability to measure fully entangled state: 0.999983
Printing probability map of size 2
|00>    : 0.4998                        |11>    : 0.5002

Using 1000 samples, the distribution of states is:
|00> : 0.519
|11> : 0.481
```

The output starts with the backend's simulation progress, followed by the familiar output in the program's implementation. The probabilities reported by the FullStateSimulator are slightly different from the exact 0.50 because the Quantum Dot Simulator includes the simulation of the electronics controlling the quantum dots.

The complete code is available as qd_GHZ.cpp in the quantum_examples/ directory of the Intel® Quantum SDK.

2.0 Using `release_quantum_state()`

Using `release_quantum_state()` to indicate the intention to effectively abandon operating on the qubits can lead to greater reduction of the total operations when combined with `-O1` optimization. Inconsequential operations can be removed, and in some cases this can include a measurement operation. Consider the following sample code. The first three `quantum_kernel` blocks build up the preparation and measurement of a state with three angles as input parameters.

```
#include <clang/Quantum/quintrinsics.h>
#include <quantum_full_state_simulator_backend.h>

qbit q[2];

quantum_kernel void PrepAll() {
  PrepZ(q[0]);
  PrepZ(q[1]);
}

//nothing special about this ansatz
quantum_kernel void Ansatz_Heisenberg (double angle0, double angle1, double angle2) {
  RX(q[0], angle0);
  RY(q[1], angle1);
  S(q[1]);
  CNOT(q[0], q[1]);
  RZ(q[1], angle2);
  CNOT(q[0], q[1]);
  Sdag(q[1]);
}

quantum_kernel double Measure_Heisenberg(){
  cbit c[3];

  CNOT(q[0], q[1]);
  MeasX(q[0], c[0]); // XX term
  MeasZ(q[1], c[1]); // ZZ term
  CZ(q[0], q[1]);
  MeasX(q[0], c[2]); //-YY term
  CZ(q[0], q[1]);
  CNOT(q[0], q[1]);

  release_quantum_state();

  return (1. -2. * (double) c[0]) + (1. -2. * (double) c[1]) + (1. + 2. * (double) c[2]);

}
```

The next `quantum_kernel` function calls the prior three blocks. This fourth function contains the `release_-quantum_state()` call from above. The `main()` function calls `VQE_Heisenberg()` after setting up a `FullStateSimulator`.

```
quantum_kernel double VQE_Heisenberg(double angle0, double angle1, double angle2) {
  PrepAll();
  Ansatz_Heisenberg (angle0, angle1, angle2);

  return Measure_Heisenberg();  //note this QK will inherit the release for this function
}

int main(){
  iqsdk::IqsConfig settings(2, "noiseless");
  iqsdk::FullStateSimulator quantum_8086(settings);
  if (iqsdk::QRT_ERROR_SUCCESS != quantum_8086.ready())
    return 1;

  double debug1 = 1.570796;
  double debug2 = debug1 / 2;
  double debug3 = debug2 / 2;
  VQE_Heisenberg(debug1, debug2, debug3);
}
```

If this is compiled with `-O0` flag and no optimization is performed, we expect each of the 3 measurement operations (`MeasX`, `MeasZ`, `MeasX`) to be called. Looking at the resulting `.qs` file confirms this:

```
        .globl        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub" // -- Begin␣
↪function _Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub
        .type        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub",@function
"_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub": // @"_Z45VQE_Heisenberg(double,␣
↪double, double).QBB.3.v.stub"
// %bb.0:                                   // %aqcc.quantum
        quprep QUBIT[0] (slice_idx=1)
        quprep QUBIT[1] (slice_idx=0)
        qurotxy QUBIT[0], @shared_variable_array[4], @shared_variable_array[0] (slice_idx=0)
        qurotxy QUBIT[1], @shared_variable_array[5], @shared_variable_array[1] (slice_idx=0)
        qurotz QUBIT[1], 1.570796e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 1.570796e+00 (slice_idx=0)
        qurotz QUBIT[1], @shared_variable_array[6] (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 1.570796e+00 (slice_idx=0)
        qurotz QUBIT[1], 4.712389e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 1.570796e+00 (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qumeasz QUBIT[0] @shared_cbit_array[0] (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 1.570796e+00 (slice_idx=0)
        qumeasz QUBIT[1] @shared_cbit_array[1] (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qumeasz QUBIT[0] @shared_cbit_array[2] (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 1.570796e+00 (slice_idx=0)
```

(continues on next page)

(continued from previous page)

```
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 1.570796e+00 (slice_idx=2)
        return
.Lfunc_end3:
        .size        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub", .Lfunc_end3-"_
↪Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub"
                                        // -- End function
        .section        ".note.GNU-stack","",@progbits
```

However, compiling with -O1 will cause the optimizer to remove operations. Here in addition to combining and removing gates, the optimizer will remove a measurement operation because its outcome can be deduced from the other two measurements' outcomes. The cbit used to store the now-missing measurement outcome will have its value correctly set by the Quantum Runtime.

```
        .globl        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub" // -- Begin␣
↪function _Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub
        .type        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub",@function
"_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub": // @"_Z45VQE_Heisenberg(double,␣
↪double, double).QBB.3.v.stub"
// %bb.0:                                // %aqcc.quantum
        quprep QUBIT[1] (slice_idx=1)
        quprep QUBIT[0] (slice_idx=0)
        qurotxy QUBIT[1], @shared_variable_array[4], @shared_variable_array[1] (slice_idx=0)
        qurotxy QUBIT[0], @shared_variable_array[5], @shared_variable_array[0] (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 0.000000e+00 (slice_idx=0)
        qucphase QUBIT[0], QUBIT[1], 3.141593e+00 (slice_idx=0)
        qurotxy QUBIT[0], 1.570796e+00, 0.000000e+00 (slice_idx=0)
        qumeasz QUBIT[0] @shared_cbit_array[0] (slice_idx=0)
        qurotxy QUBIT[1], 1.570796e+00, 4.712389e+00 (slice_idx=0)
        qumeasz QUBIT[1] @shared_cbit_array[1] (slice_idx=2)
        return
.Lfunc_end3:
        .size        "_Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub", .Lfunc_end3-"_
↪Z45VQE_Heisenberg(double, double, double).QBB.3.v.stub"
                                        // -- End function
        .section        ".note.GNU-stack","",@progbits
```

3.0 Writing Variational Algorithms

3.1 Introduction

Variational algorithms are considered to be one of the most promising applications to allow quantum advantage using near-term systems [CABB2021]. The Intel® Quantum SDK has many features that are geared for coding variational algorithms with a focus on performance. The Hybrid Quantum Classical Library (HQCL) [HQCL2023] is a collection of tools that will help a user increase productivity when programming variational algorithms. This example combines these tools with `dlib` (a popular C++ library for solving optimization problems [DLIB2023]), to applying the variational algorithm to the generation of thermofield double (TFD) states [PRMA2020] [SPKR2021]. Previous implementations [KWPH2022] included the latter workload with a hard-coded version of the cost function expression, which was pre-calculated. Fig. 1 (reproduced from [KWPH2022]) shows the full circuit that is used for the variational algorithm execution.

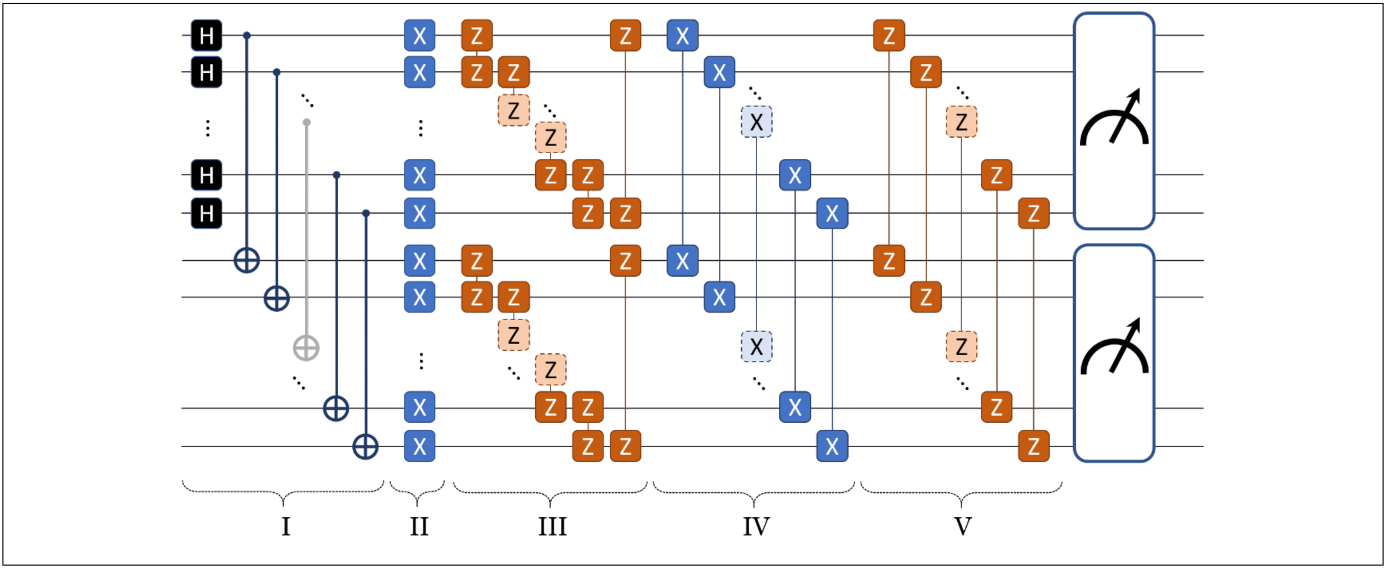


Fig. 1: The quantum circuit for single-step TFD state generation. Stages:(I) preparing infinite temperature TFD state, (II) Intra-system R_X operation, (III) Intra-system ZZ operation, (IV) Inter-system XX operation, (V) Inter-system ZZ operation. A and B represent the two subsystems, each containing N_{sub} qubits. (reproduced from [KWPH2022])

In this implementation, HQCL will symbolically construct the cost function expression, and use qubit-wise commutation (QWC) [YEVI2020] to group terms and reduce the number of circuit repetitions required to calculate the cost function. HQCL will also automatically populate the necessary mapping angles at runtime, to facilitate measurements of the system along different axes.

The classical optimization in this workload will be handled using the `dlib` C++ library. The `dlib` library contains powerful functions performing local as well as global optimizations. Here, the `find_min_bobyqa` function for the minimization of the cost function performs quite well for the chosen workload. The choice of the optimization technique can heavily influence the number of iterations required for convergence of certain variational algorithms. The Intel Quantum Simulator [GHBS2020] will be used as the backend in this example.

3.2 Code

3.2.1 Preamble

In the preamble of the source file shown in Listing 14 below, the header files for the IQSDK, `dlib`, and HQCL are included first.

Listing 14: The preamble of the source file.

```
1  // Intel Quantum SDK header files
2  #include <clang/Quantum/quintrinsics.h>
3  #include <quantum.hpp>
4
5  #include <vector>
6  #include <cassert>
7
8  // Library for optimizations
9  #include <dlib/optimization.h>
10 #include <dlib/global_optimization.h>
11
12 // Libraries for automating hybrid algorithm
13 #include <armadillo>
14 #include "SymbolicOperator.hpp"
15 #include "SymbolicOperatorUtils.hpp"
16
17 // Define the number of qubits needed for compilation
18 const int N_sub = 2;  // Number of qubits in subsystem (thermal state size)
19 const int N_ss = 2; // Number of subsystems (Not a general parameter to be changed)
20 const int N = N_ss * N_sub; // Total number of qubits (TFD state size)
21
22 qbit QReg[N];
23 cbit CReg[N];
24
25 const int N_var_angles = 4;
26 const int N_map_angles = 2 * N;
27
28 double QVarParams[N_var_angles]; // Array to hold dynamic parameters for quantum algorithm
29 double QMapParams[N_map_angles]; // Array to hold mapping parameters for HQCL
30
31 typedef dlib::matrix<double, N_var_angles, 1> column_vector;
32 namespace hqcl = hybrid::quantum::core;
```

A data structure within `dlib` is defined (using a `typedef`) in line 31 for convenience in passing the set of parameters into the optimization loop. This algorithm will use four variational parameters and two mapping angles per qubit (a total of eight).

3.2.2 Construction of the Ansatz

Listing 15 contains the operations corresponding to the stages II, III, IV, and V from Fig. 1 (stage I will be discussed later in Listing 16). These are the four core stages that define the operations for the TFD algorithm. A future version of the IQSDK will support `quantum kernel expressions` which can be used to conveniently construct quantum kernels in a modular way [PAMS2023] [SCHM2023].

Listing 15: The core set of operations to implement the TFD algorithm.

```
quantum_kernel void TFD_terms () {
  int index_intraX = 0, index_intraZ = 0, index_interX = 0, index_interZ = 0;

  // Single qubit variational terms
  for (index_intraX = 0; index_intraX < N; index_intraX++)
    RX(QReg[index_intraX], QVarParams[0]);

  // Two-qubit intra-system variational terms (adjacent)
  for (int grand_intraZ = 0; grand_intraZ < N_sub - 1; grand_intraZ++) {
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      CNOT(QReg[grand_intraZ + N_sub * index_intraZ + 1], QReg[grand_intraZ + N_sub * index_
↪intraZ]);
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      RZ(QReg[grand_intraZ + N_sub * index_intraZ], QVarParams[1]);
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      CNOT(QReg[grand_intraZ + N_sub * index_intraZ + 1], QReg[grand_intraZ + N_sub * index_
↪intraZ]);
  }

  if (N_sub > 2) {
    // Two-qubit intra-system variational terms (boundary term)
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      CNOT(QReg[N_sub * index_intraZ], QReg[N_sub * index_intraZ + (N_sub - 1)]);
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      RZ(QReg[N_sub * index_intraZ + (N_sub - 1)], QVarParams[1]);
    for (index_intraZ = 0; index_intraZ < N_ss; index_intraZ++)
      CNOT(QReg[N_sub * index_intraZ], QReg[N_sub * index_intraZ + (N_sub - 1)]);
  }

  // two-qubit inter-system XX variational terms
  for (index_interX = 0; index_interX < N_sub; index_interX++) {
    RY(QReg[index_interX + N_sub], -M_PI_2);
    RY(QReg[index_interX], -M_PI_2);
  }
  for (index_interX = 0; index_interX < N_sub; index_interX++)
    CNOT(QReg[index_interX + N_sub], QReg[index_interX]);
  for (index_interX = 0; index_interX < N_sub; index_interX++)
    RZ(QReg[index_interX], QVarParams[2]);
  for (index_interX = 0; index_interX < N_sub; index_interX++)
    CNOT(QReg[index_interX + N_sub], QReg[index_interX]);
  for (index_interX = 0; index_interX < N_sub; index_interX++) {
    RY(QReg[index_interX + N_sub], M_PI_2);
    RY(QReg[index_interX], M_PI_2);
```

(continues on next page)

(continued from previous page)

```
  }

  // two-qubit inter-system ZZ variational terms
  for (index_interZ = 0; index_interZ < N_sub; index_interZ++)
    CNOT(QReg[index_interZ], QReg[index_interZ + N_sub]);
  for (index_interZ = 0; index_interZ < N_sub; index_interZ++)
    RZ(QReg[index_interZ + N_sub], QVarParams[3]);
  for (index_interZ = 0; index_interZ < N_sub; index_interZ++)
    CNOT(QReg[index_interZ], QReg[index_interZ + N_sub]);
```

There are three supporting quantum kernels that are used (see Listing 16), in addition to the core set of operations. `PrepZAll()` is used to prepare all the qubits in the ground state at the beginning of every iteration. `BellPrep()` is used to prepare Bell pairs between corresponding qubits of the two subsystems, effectively resulting in the infinite temperature TFD state. The `DynamicMapping()` quantum kernel is used to hold the mapping operations that HQCL will implement for basis changes during runtime.

Listing 16: The supporting quantum kernels to implement the TFD algorithm.

```
quantum_kernel void PrepZAll () {
  // initialize the qubits
  for (int Index = 0; Index < N; Index++)
    PrepZ(QReg[Index]);
}

quantum_kernel void BellPrep () {
  // prepare the Bell pairs (T -> Infinity)
  for (int Index = 0; Index < N_sub; Index++)
    H(QReg[Index]);
  for (int Index = 0; Index < N_sub; Index++)
    CNOT(QReg[Index], QReg[Index + N_sub]);
}

quantum_kernel void DynamicMapping () {
  // Not part of the ansatz
  // Rotations to map X to Z or Y to Z
  for (int qubit_index = 0; qubit_index < N; qubit_index++) {
    int map_index = 2 * qubit_index;
    RY(QReg[qubit_index], QMapParams[map_index]);
    RX(QReg[qubit_index], QMapParams[map_index + 1]);
  }
}
```

The supporting quantum kernels (Listing 16) and the core TFD quantum kernel (Listing 15) are combined to form the full quantum circuit in Listing 17.

Listing 17: The full TFD quantum kernel to run during optimization loop.

```
quantum_kernel void TFD_full() {
```

(continues on next page)

(continued from previous page)

```
  PrepZAll();
  BellPrep();
  TFD_terms();
  DynamicMapping();
}
```

3.2.3 Functions for Constructing the Cost Expression and the Cost Calculation

Listing 18: Construction of the full symbolic operator for the cost function expression.

```
hqcl::SymbolicOperator constructFullSymbOp(double inv_temp) {
  hqcl::SymbolicOperator symb_op;
  hqcl::pstring sym_term;

  // Single qubit variational terms
  for (int index_intraX = 0; index_intraX < N; index_intraX++) {
      sym_term = {std::make_pair(index_intraX, 'X')};
      symb_op.addTerm(sym_term, 1.00);
  }

  // Two-qubit intra-system variational terms (adjacent)
  for (int grand_intraZ = 0; grand_intraZ < N_sub - 1; grand_intraZ++) {
      for (int index_intraZ = 0; index_intraZ < N_ss; index_intraZ++) {
          int qIndex0 = grand_intraZ + N_sub * index_intraZ;
          int qIndex1 = grand_intraZ + N_sub * index_intraZ + 1;
          sym_term = {std::make_pair(qIndex0, 'Z'), std::make_pair(qIndex1, 'Z')};
          symb_op.addTerm(sym_term, 1.00);
      }
  }

  // Two-qubit intra-system variational terms (boundary term)
  if (N_sub > 2) {
      for (int index_intraZ = 0; index_intraZ < N_ss; index_intraZ++) {
          int qIndex0 = N_sub * index_intraZ;
          int qIndex1 = N_sub * index_intraZ + (N_sub - 1);
          sym_term = {std::make_pair(qIndex0, 'Z'), std::make_pair(qIndex1, 'Z')};
          symb_op.addTerm(sym_term, 1.00);
      }
  }

  // two-qubit inter-system XX variational terms
  for (int index_interX = 0; index_interX < N_sub; index_interX++) {
      int qIndex0 = index_interX;
      int qIndex1 = index_interX + N_sub;
      sym_term = {std::make_pair(qIndex0, 'X'), std::make_pair(qIndex1, 'X')};
      symb_op.addTerm(sym_term, -pow(inv_temp, -1.00));
  }

  // two-qubit inter-system XX variational terms
```

(continues on next page)

(continued from previous page)

```
  for (int index_interZ = 0; index_interZ < N_sub; index_interZ++) {
      int qIndex0 = index_interZ;
      int qIndex1 = index_interZ + N_sub;
      sym_term = {std::make_pair(qIndex0, 'Z'), std::make_pair(qIndex1, 'Z')};
      symb_op.addTerm(sym_term, -pow(inv_temp, -1.00));
  }

  return symb_op;
}
```

Programmatic construction of the cost expression is necessary for HQCL to form the QWC groups, to generate the necessary circuits to run per optimization iteration, and to correctly evaluate the cost at each iteration. In Listing 18, we generate symbolic terms (`sym_term`) for every expression present, and add it to the full symbolic operator `symb_op`. The full cost expression to be coded is given by

$$C(\beta) = \sum_{i=1}^{N_{\text{sub}}} X_i^A + \sum_{i=1}^{N_{\text{sub}}} X_i^B + \sum_{i=1}^{N_{\text{sub}}} Z_i^A Z_{i+1}^A + \sum_{i=1}^{N_{\text{sub}}} Z_i^B Z_{i+1}^B - \beta^{-1} \left(\sum_{i=1}^{N_{\text{sub}}} X_i^A X_i^B + \sum_{i=1}^{N_{\text{sub}}} Z_i^A Z_i^B \right)$$

where the subscript represents the qubit index and the superscript represents the subsystem the qubit belongs to (A or B) [KWPH2022].

Listing 19: A function to calculate the cost at each iteration during optimization.

```
double runQuantumKernel(iqsdk::FullStateSimulator &sim_device, const column_vector& params,
                        hqcl::SymbolicOperator &symb_op, hqcl::QWCMap &qwc_groups) {
  double total_cost = 0.0;

  for (auto &qwc_group : qwc_groups) {
    std::vector<double> variable_params;
    variable_params.reserve(N * 2);

    hqcl::SymbolicOperatorUtils::applyBasisChange(qwc_group.second, variable_params, N);

    std::vector<std::reference_wrapper<qbit>> qids;
    for (int qubit = 0; qubit < N; ++qubit)
      qids.push_back(std::ref(QReg[qubit]));

    // Set all the mapping angles to the default of 0.
    for (int map_index = 0; map_index < N_map_angles; map_index++)
      QMapParams[map_index] = 0;

    for (auto indx = 0; indx < variable_params.size(); ++indx)
      QMapParams[indx] = variable_params[indx];

    // Perform the experiment, Store the data in ProbReg
    TFD_full();
    std::vector<double> ProbReg = sim_device.getProbabilities(qids);

    double current_pstr_val = hqcl::SymbolicOperatorUtils::getExpectValSetOfPaulis(
```

(continues on next page)

(continued from previous page)

```
        symb_op, qwc_group.second, ProbReg, N);
    total_cost += current_pstr_val;
  }

  return total_cost;
}
```

The function `runQuantumKernel` encompasses all the functionality that is required to calculate the cost, when running a single optimization iteration with `dlib`. It takes the already formulated set of QWC groups, and run the ansatz with the same set of variational parameters but with different basis mapping parameters (each time mapping from the different bases, as demanded by the cost expression). The full cost is then returned for consideration by the classical optimization loop within `dlib`.

Listing 20: The `main` function.

```
int main() {
    // Setup quantum device
    iqsdk::IqsConfig sim_config(N, "noiseless", false);
    iqsdk::FullStateSimulator sim_device(sim_config);
    assert(sim_device.ready() == iqsdk::QRT_ERROR_SUCCESS);

    // initial starting point. Defining it here means I will reuse the best result
    // from previous temperature when starting the next temperature run
    column_vector starting_point = {0, 0, 0, 0};

    // calculate the actual inverse temperature that is used during calculations
    double inv_temp = 1.0;

    // Fully formulated Cost Function Expression
    hqcl::SymbolicOperator cost_expr = constructFullSymbOp(inv_temp);

    // Qubitwise Commutation (QWC) Groups Formation
    hqcl::QWCMap qwc_groups = hqcl::SymbolicOperatorUtils::getQubitwiseCommutationGroups(cost_
↪expr, N);

    // Construct a function to be used for a single optimization iteration
    // This function is directly called by the dlib optimization routine
    auto ansatz_run_lambda = [&](const column_vector& var_angs) {

      // Set all the variational angles to input values.
      for (int q_index = 0; q_index < N_map_angles; q_index++)
          QVarParams[q_index] = var_angs(q_index);

      // run the kernel to compute the total cost
      double total_cost = runQuantumKernel(sim_device, var_angs, cost_expr, qwc_groups);

      return total_cost;
    };

    // run the full optimization for a given temperature
    auto result = dlib::find_min_bobyqa(
```

(continues on next page)

(continued from previous page)

```
                                ansatz_run_lambda, starting_point,
                                2 * N_var_angles + 1, // number of interpolation points
                                dlib::uniform_matrix<double>(N_var_angles, 1, -7.0), // lower bound␣
↪constraint
                                dlib::uniform_matrix<double>(N_var_angles, 1, 7.0), // upper bound␣
↪constraint
                                1.5, // initial trust region radius
                                1e-5, // stopping trust region radius
                                10000 // max number of objective function evaluations
    );

    return 0;
}
```

The main function shown in Listing 20 will initialize the IQSDK backend, construct the cost expression, and kick off the optimization. The lambda function `ansatz_run_lambda` is used since `dlib` requires the function used during optimization to take a column vector as an input and to return a double. This function essentially wraps the previously-defined `runQuantumKernel` function.

3.3 Results

The execution of the above program can be tracked with a log of the angles and the cost function at each iteration. The summarized results are shown in Fig. 2 and Fig. 3. These plots demonstrate that 95 steps are required for convergence to the requested tolerance level.

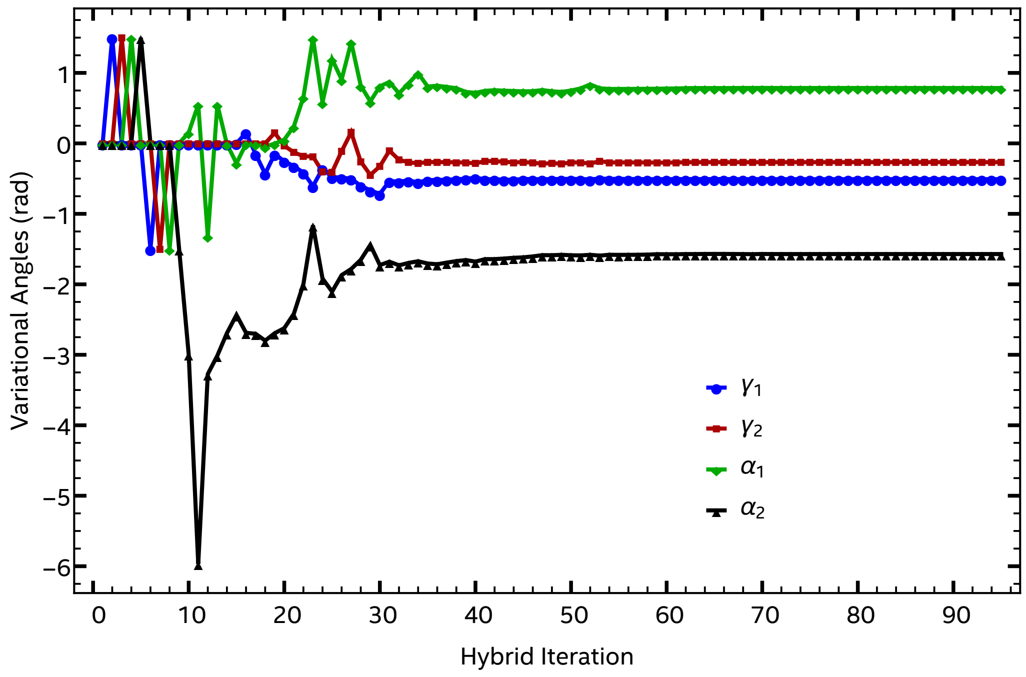


Fig. 2: Convergence behavior for the four variational angles (see [PRMA2020] [SPKR2021] for details on the notation).

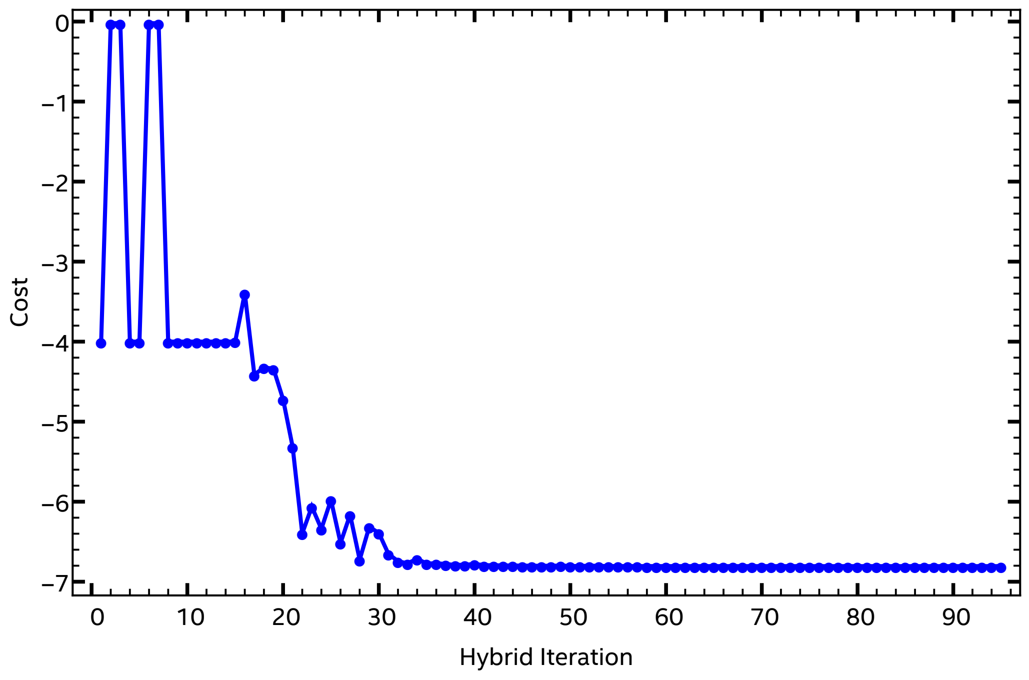


Fig. 3: Convergence of the evaluated cost during the variational algorithm execution.

4.0 Using `qbit` variables

`qbit` is the data type for representing qubits. Variables of `qbit` type can be declared in the global namespace or locally within a `quantum_kernel` function. Similar to locally declared classical C++ variables, locally declared `qbit` variables' scope is limited to the `quantum_kernel` function they are declared in.

When a locally declared `qbit` variable goes out of scope, the quantum state is not automatically released. This means in subsequent computation, the physical qubit associated to this variable might be reassgined to a different `qbit` while still holding the now out-of-scope variable's quantum state. Without proper handling, this could lead to unreliable results. One option is to use `release_quantum_state()` at the end of the `quantum_kernel` in which local `qbit` variables are declared. See Developer Guide and Reference (Local `qbit` Variables). Examples can be found below:

```
qbit global_qbit;

void quantum_kernel exampleReleaseOnMeasurement(){
   qbit local_3[3];     // declare a quantum array with 3 qbits

   // Prep the local qbit variables
   PrepZ(local_3[0]);
   PrepZ(local_3[1]);
   PrepZ(local_3[2]);

   RY(local_3[0], 0.5);
   RY(local_3[1], 0.5);
   RY(local_3[2], 0.5);

   // Measuring the qbit variables
   MeasX(local_3[0]);
   MeasX(local_3[1]);
   MeasX(local_3[2]);
   // After the measurements, the physical qubits assigned to local_3 are released
}

void quantum_kernel exampleExplicitRelease() {
   qbit q0;
   qbit q1;

   PrepZ(q0);
   PrepZ(q1);

   RZ(q0);
   RZ(q1);
   RZ(global_qbit);

   release_quantum_state();
   // After the call to release_quantum_state(), all qubits, including the global qbit,
   // are released from this point onwards and the physical qubits can be
   // reused in a new ``quantum_kernel``
```

(continues on next page)

(continued from previous page)

```
}

void quantum_kernel badExampleNoRelease() {
   // In this example, the local qubits are not properly released at the end of the kernel
   qbit q0;
   qbit q1;

   PrepZ(q0);
   PrepZ(q1);

   RZ(q0);
   RZ(q1);
}

void quantum_kernel badExample() {

   // This program will not cause a compilation error
   // However the computed results might be incorrect
   // as the second call to badExampleNoRelease() might be using the same
   // physical qubits which are in unknown states
   badExampleNoRelease();
   badExampleNoRelease();
}
```

`qbit` variables can be passed as arguments of `quantum_kernel` functions with the exception of top level `quantum_kernel` functions, which do not take quantum-type parameters. `qbit` variables must be passed by reference. If passed by value, a local copy of the input `qbit` variables will be made, just as for classical variables. Since quantum states cannot be copied, passing a `qbit` by value has no physical meaning and will cause an error when compiling, . Examples of how to pass `qbit` variables as inputs to `quantum_kernel` functions are shown below.

```
qbit global_qbit;

// Pass by pointer - accepted behaviour
void quantum_kernel passQubitArrayByPtr(qbit qubit_array[], int num_ele){
   for (int i=0; i < num_ele; i++)
      H(qubit_array[i]);
}

// Pass by pointer - accepted behaviour
void quantum_kernel passQubitArrayByPtr2(qbit *qubit_array, int num_ele){
   for (int i=0; i < num_ele; i++)
      H(qubit_array[i]);
}

// Pass by reference - accepted behaviour
void quantum_kernel passQubitByRef(qbit &q){
   Z(q);
}

// Pass by value - will result in a compilation error
```

(continues on next page)

(continued from previous page)

```
void quantum_kernel passQubitByValue(qbit q){
   Z(q);
}

// Note that the top level quantum_kernel does not take quantum arguments
void quantum_kernel top_level_kernel() {
   qbit qubit_array[3];

   passQubitArrayByPtr(qubit_array, 3);
   passQubitArrayByPtr2(qubit_array, 3);
   passQubitByRef(global_qbit);
   passQubitByValue(global_qbit);   // Pass by value - will result in a compilation error
}
```

The minimum number of physical qubits required in a program is the sum of all global `qbit` variables plus the maximum width of local `qbit` variables. In the following example, the minimum number of physical qubits needed is 8, comprising the 3 global `qbit` and the 5 `qbit` inside `circuitWidth5`.

```
qbit global_qbit[3];

void quantum_kernel circuitWidth2(){
   qbit array[2];
}

void quantum_kernel circuitWidth5(){
   qbit array[5];
}

void quantum_kernel circuits(){
   circuitWidth2();
   circuitWidth5();
}
```

When compiling with a configuration file, the `qbit` variables will be mapped to physical qubits using the placement method set by the `-p` flag. All `qbit` variables, both global and locally declared, will be mapped using the same method, with the exception that only global `qbit` variables can be mapped by user defined mapping. See Developer Guide and Reference (Qubit Placement and Scheduling).

5.0 Quantum Teleportation with FLEQ

This tutorial introduces the main concepts of FLEQ using quantum teleportation. Quantum teleportation [NICH2010] allows one actor, Alice, to send quantum information to another actor, Bob, in the form of a qubit state. The protocol proceeds as follows:

1. Alice and Bob each start with one half of a Bell pair in the state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.
2. Alice prepares her state $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$, resulting in the three-qubit system $|\varphi\rangle \otimes \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$.
3. Alice entangles her state with her half of the Bell pair and measures both qubits, producing bits x and y, and leaving Bob's half of the Bell pair in one of the following four states:

Table 1: Bob's state after Alice's local measurement

x	y	**State**
0	0	$\alpha\|0\rangle + \beta\|1\rangle$
0	1	$\alpha\|0\rangle - \beta\|1\rangle$
1	0	$\alpha\|1\rangle + \beta\|0\rangle$
1	1	$\alpha\|1\rangle - \beta\|0\rangle$

4. Finally, Alice sends the classical bits x and y to Bob, who uses that information to correct his state to Alice's original $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$.

5.1 One-qubit teleportation with quantum kernel expressions

We start by including the necessary header files: `quintrinsics.h` for use of the Intel® Quantum SDK, `quantum_full_state_simulator_backend.h` for a simulator backend, and `qexpr.h` for quantum kernel expressions. In addition, we include several headers from the C++ standard library that will be useful.

Listing 21: Header files.

```cpp
#include <clang/Quantum/quintrinsics.h>
#include <quantum_full_state_simulator_backend.h>
#include <clang/Quantum/qexpr.h>
#include <qexpr_utils.h>

#include <iostream>
#include <cassert>
#include <vector>
#include <random>
```

To prepare a Bell state using quantum kernel expressions, we write a function that takes as input two qubits, and returns the quantum kernel expression that prepares those qubits in a Bell state.

Listing 22: Quantum kernel expression implementing the Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

```
QExpr bell00(qbit& a, qbit& b) {
    return qexpr::_PrepZ(a)
         + qexpr::_PrepZ(b)
         + qexpr::_H(a)
         + qexpr::_CNOT(a,b);
}
```

Notice that this function **returns** an expression representing a quantum program; unlike the non-FLEQ `quantum_kernel` functions in the rest of the SDK, FLEQ does not **call** quantum gates. Instead, it focuses on constructing a quantum kernel **expression** or `QExpr`.

In a similar vein, Alice can prepare her state φ by calling a `QExpr`-returning function `prepPhi()` on a qubit q, which prepares q by performing an X rotation around a randomly generated angle. The `PROTECT` modifier prevents inlining, and must be included whenever a `QExpr` function uses local variables.

Listing 23: Prepare Alice's state $|\varphi\rangle$.

```
double randomDoubleBetweenZeroAndTwoPi() {
    std::random_device rd;  // Used to seed the random number generator
    std::mt19937 gen(rd()); // Mersenne Twister PRNG
    std::uniform_real_distribution<double> dis(0.0, 2.0 * M_PI);
    return dis(gen);
}
// Prepare a state |phi> by performing an X rotation around a random angle
PROTECT QExpr prepPhi(qbit& q) {
    double theta = randomDoubleBetweenZeroAndTwoPi();
    std::cout << "Using angle " << theta << "\n";
    return qexpr::_PrepZ(q) + qexpr::_RX(q, theta);
}
```

Next, we implement Alice's half of the teleportation protocol, where she entangles her prepared qubit with her half of the Bell pair. She writes the results to two boolean references x and y.

Listing 24: Entangle q and a and measure both, writing the results to x and y respectively.

```
QExpr alice(qbit& q, qbit& a, bool& x, bool& y) {
    return qexpr::_CNOT(q, a)
         + qexpr::_H(q)
         + qexpr::_MeasZ(q, x)
         + qexpr::_MeasZ(a, y);
}
```

Finally, we implement Bob's piece of the protocol, which uses x and y to apply corrections to his qubit, b.

Listing 25: Use x and y to apply corrections to Bob's qubit b.

```
PROTECT QExpr bob(qbit& b, bool &x, bool &y) {
    return qexpr::cIf(y, qexpr::_X(b), qexpr::identity())
         + qexpr::cIf(x, qexpr::_Z(b), qexpr::identity());
}
```

Unlike the other `QExpr` functions up until now, `bob()` does not correspond to a straightforward quantum circuit. Instead, it uses the classical conditional blocks `cIf` to change which quantum kernel expression will be applied based on the runtime values of x and y. In particular, if y and x are both `true` at runtime, evaluating `bob()` will invoke the quantum operation `X(b)` followed by the operation `Z(b)`. On the other hand, if y is `false` but x is `true`, evaluating `bob()` will only invoke `Z(b)`. See the FLEQ Guide and Reference (Branching) for more details on classical conditionals.

To put all of these components together, we will implement 1-qubit teleportation in a top-level classical function, `teleport1()`.

Listing 26: Implement the 1-qubit teleportation protocol

```
void teleport1(iqsdk::FullStateSimulator& device) {

    qbit q;
    qbit a;
    qbit b;

    // Prepare qubits a and b in a bell state
    qexpr::eval_hold(bell00(a,b));

    // Alice prepares her qubit q in the state |phi>
    qexpr::eval_hold(prepPhi(q));

    // Record the state Alice prepared
    auto q_ref = to_ref_wrappers(qlist::QList(q));
    auto probabilitiesBefore = device.getProbabilities(q_ref);

    // Alice entangles her state q with a, and sends measurement
    // results x and y to Bob
    bool x;
    bool y;
    qexpr::eval_hold(alice(q, a, x, y));

    // Bob uses x and y to correct his qubit b
    qexpr::eval_hold(bob(b, x, y));

    // At the end, b should be in the state |phi>, up to a global phase
    auto b_ref = to_ref_wrappers(qlist::QList(b));
    auto probabilitiesAfter = device.getProbabilities(b_ref);

    std::cout << "Before teleportation, qubit q has distribution:\n";
    iqsdk::FullStateSimulator::displayProbabilities(probabilitiesBefore, q_ref);
    std::cout << "After teleportation, qubit b has distribution:\n";
```

(continues on next page)

(continued from previous page)

```
    iqsdk::FullStateSimulator::displayProbabilities(probabilitiesAfter, b_ref);
}
```

The function takes as input a full state simulator device, which we assume has been properly initialized. Lines 3-5 of `teleport1()` declare three local qubits: q is Alice's state; a is Alice's half of the Bell pair; and b is Bob's half of the Bell pair. The variables a and b are initialized in line 8 by evaluating the quantum kernel expression `bell00` with the `eval_hold()` function.

Line 11 prepares Alice's qubit q in state $|\varphi\rangle$ by evaluating the quantum kernel expression `prepPhi(q)`. Because this state is different every iteration, line 15 calls `getProbabilities()` to record what $|\varphi\rangle$ is before teleportation. The function `getProbabilities()` produces a data structure that maps qubit states to the probability associated with that state at the current point in the computation. The argument to `getProbabilities()` specifies the subset and order of qubits whose probabilities should be considered. In this case, we are asking for only the qubit q. See the Developer Guide and Reference (Measurements & FullStateSimulator) for more details.

To achieve quantum teleportation, in line 21, Alice measures her qubits to boolean values x and y by evaluating the `QExpr` function `alice()`. On line 24, Bob uses these values to correct his state b by evaluating `bob()`. Finally, line 28 invokes `getProbabilities()` once more to determine the state of b after teleportation, and prints out both probability distributions to compare them for equality.

The output of running `teleport1()` is the following:

```
$ ./qexpr_teleport
  Using angle 4.75947
  Bob received 1 and 0.
  Before teleportation, qubit q has distribution:
  Printing probability register of size 2
  |0⟩   : 0.5236                        |1⟩   : 0.4764

  After teleportation, qubit b has distribution:
  Printing probability register of size 2
  |0⟩   : 0.5235                        |1⟩   : 0.4765
```

Line 2 indicates that Alice's state $|\varphi\rangle$ was prepared with angle 4.75947. Line 3 indicates that Alice measured bits x and y as 1 and 0, respectively. Finally, lines 4-10 show that Bob's state after teleportation matches Alice's state before teleportation (up to a rounding error).

5.2 A single quantum kernel expression

The function `teleport1()` above contains multiple evaluation calls to `eval_hold()`; it itself is a classical function that interacts with the quantum runtime. If a user does not need to report the output of the first state, can they implement teleportation as a single `QExpr` function?

An initial **incorrect** attempt in doing this is to write a `QExpr` function that simply joins the three modular components of the teleportation protocol:

Listing 27: Incorrect attempt to implement teleportation as a single quantum kernel expression.

```
PROTECT QExpr teleport1_join(qbit& q, qbit& a, qbit& b) {
    bool x = false;
    bool y = false;
    return bell00(a,b)
            + alice(q, a, x, y)
            + bob(b,x,y);
}
```

To use this function, Alice prepares her qubit q in state $|\varphi\rangle$ and combines that with the teleportation procedure. Below, Alice prepares the state $|1\rangle$.

Listing 28: Incorrect attempt to implement teleportation as a single quantum kernel expression.

```
void teleport1_bad(iqsdk::FullStateSimulator& device) {
    qbit q;
    qbit a;
    qbit b;

    qexpr::eval_hold(qexpr::_PrepZ(q) + qexpr::_X(q) + teleport1_join(q,a,b));

    // At the end, b should be in the state |1>
    auto b_ref = to_ref_wrappers(qlist::QList(b));
    auto probabilitiesAfter = device.getProbabilities(b_ref);

    std::cout << "Expecting state |1>\n";
    std::cout << "After teleportation, Bob obtains state:\n";
    iqsdk::FullStateSimulator::displayProbabilities(probabilitiesAfter, b_ref);
}
```

When we try to run this algorithm, half the time we will observe b in the state $|0\rangle$ and half the time we will observe it in the state $|1\rangle$. This is an indication that the corrections in Bob's part of the protocol are not being applied correctly. Indeed, if we were to print out the values of x and y before Bob performs his corrections, we would see that the values of x and y are always 0.

The reason for this is that the measurement in Alice's protocol (inside the `QExpr` function `alice()`) is occurring within the same Quantum Basic Block (QBB) as the conditional in `bob()`. However, measurement results are not written to classical variables x and y until the end of a QBB. Thus, the measurement results do not propagate to x and y before Bob tries to use them. See FLEQ Guide and Reference (Barriers and binding) for more details.

The solution is to insert a barrier between Alice's protocol and Bob's protocol to ensure they happen within separate QBBs. This can be achieved via the `bind` function, an analogue of the usual `join` function that combines two quantum kernel expressions. Where `join` takes two quantum kernel expressions and combines them sequentially in the same quantum basic block, `bind` produces separate QBBs, executing one after the other. Analogous to the notation `e1 + e2` for joining quantum kernel expressions in sequence, users can write `e1 << e2` for binding quantum kernel expressions in sequence. See FLEQ Guide and Reference (Barriers and binding) for more details.

In this case, the `QExpr` teleportation function `teleport1_join()` should be replaced by a version that uses << in place of +.

Listing 29: A quantum kernel function that implements quantum teleportation using `bind()`.

```
PROTECT QExpr teleport1_bind(qbit& q, qbit& a, qbit& b) {
    bool x = false;
    bool y = false;
    return (bell00(a,b) + alice(q, a, x, y))
            << bob(b,x,y);
}
```

We can now invoke this algorithm by evaluating `teleport1_bind()` after Alice has prepared her qubit in state $|1\rangle$. In this case we find that no matter how many times we run the algorithm, Bob always results in a qubit in state $|1\rangle$, as expected.

5.3 Multi-qubit teleportation

In this section we will extend single-qubit quantum teleportation to a protocol that teleports N qubits for an arbitrary N. The protocol requires N pairs of qubits in a Bell state and performs the single-qubit teleportation sequence for each qubit.

A first attempt at multi-qubit teleportation would be just to call the `teleport1()` function N times in sequence. However, with this approach Alice would prepare N single-qubit states, and it would not allow for an entangled state to be teleported.

A next attempt would be for Alice to prepare her qubit state and then evaluate `teleport1_bind()` N times on each successive qubit. This can be achieved via a recursive function that returns a quantum kernel expression (see FLEQ Guide and Reference (Recursion)).

Listing 30: A function that returns a recursive quantum kernel expression applying the quantum teleportation protocol to each triple of qubits in `qs`, `as`, and `bs`.

```
QExpr teleport_sequential(qlist::QList qs, qlist::QList as, qlist::QList bs) {
    return qexpr::cIf(qs.size() == 0,
                        // if qs is empty:
                            qexpr::identity(),
                        // if qs is non-empty:
                            teleport1_bind(qs[0], as[0], bs[0])
                            << teleport_sequential(qs+1, as+1, bs+1)
    );
}
```

The recursive function `teleport_sequential` uses a classical conditional `cIf` to distinguish between a base case (when the `QList` `qs` is empty) and a recursive case (when `qs` is non-empty). It assumes that all three `QList` inputs have the same length. When they are all empty (have size 0), teleportation should do nothing and so returns the `qexpr::identity()` quantum kernel expression. In the recursive case, we will apply single-qubit teleportation (in the form of the `teleport1_bind()` function) on `qs[0]`, `as[0]`, and `bs[0]` and then recursively call `teleport_sequential` on the tails of the three qubit lists (`qs+1`, `as+1`, and `bs+1`).

For example, if the length of the three qubit lists is 2, then `teleport_sequential(qs, as, bs)` will be unrolled to the following sequence:

```
teleport1_bind(qs[0], as[0], bs[0]) + teleport_sequential(qs+1, as+1, bs+1)
```

Then, because `(qs+1).size() == 1`, the call to `teleport_sequential()` will be unrolled again:

```
teleport1_bind(qs[0], as[0], bs[0])
  + teleport1_bind((qs+1)[0], (as+1)[0], (bs+1)[0])
  + teleport_sequential(qs+2, as+2, bs+2)
```

where `(qs+1)[0]` is the same as `qs[1]`. Finally, because `(qs+2).size() == 0`, the final call to `teleport_-sequential()` will unroll to the identity. Thus all together the call `teleport_sequential(qs,as,bs)` becomes

```
teleport1_bind(qs[0], as[0], bs[0]) + teleport1_bind(qs[1], as[1], bs[1])
```

Putting this all together, the top-level evaluation call would prepare Alice's state $|\phi\rangle$ and call `teleport_-sequential`. Here, we will prepare Alice's state to be the GHZ state $\frac{1}{\sqrt{2}}(|0\cdots0\rangle + |1\cdots1\rangle)$ as illustrated in the example `qexpr_ghz.cpp` (see Developer Guide and Reference (Samples)).

Listing 31: An evaluation call of `teleport_sequential` after preparing $|\varphi\rangle$ as a GHZ state.

```
    const int N = 2;
    qbit listable(qs, N);
    qbit listable(as, N);
    qbit listable(bs, N);

    qexpr::eval_hold(ghz(qs) // Prepare |phi>
                    + teleport_sequential(qs, as, bs));
```

5.4 Minimizing barriers and `map`

Because each call to `teleport1_bind` has a barrier in the form of a `bind`, `teleport_parallel(qs, as, bs)` will result in more than n quantum basic blocks (QBBs) (see FLEQ Guide and Reference (Barriers and binding)). While such barriers are logically valid, they prevent the compiler from optimizing across boundaries, which can make compilation redundant and expensive. It can also result in less-ideal placements (which are determined for each QBB individually) and scheduling. Logically, the n-qubit teleportation protocol really should have three separate components:

1. First, Alice and Bob prepare their joint Bell states.
2. Second, Alice prepares her state $|\varphi\rangle$ and measures her qubits.
3. Finally, Bob receives Alice's measurements and performs his own corrections.

These three states could be achieved using their own recursive functions over the qubit lists, as in `teleport_-sequential()`. But each of these three cases has a similar structure that we can exploit. Consider:

1. Preparing the joint Bell states takes as input two `QList` values `as` and `bs` and maps `bell00()` over each pair `as[i]` and `bs[i]`.
2. Alice's preparations involve first preparing the state $|\varphi\rangle$ and then mapping the function `QExpr alice(qbit& q, qbit& a, bool& x, bool& y)` over `qs[i]`, `as[i]`, and two boolean arrays `xs[i]` and `ys[i]`.

3. Bob's corrections involve mapping the function `QExpr bob(qbit& b, bool x, bool y)` over `bs[i]`, `xs[i]`, and `ys[i]`.

Each of these three cases (as well as `teleport_sequential()` itself) involves mapping a single-qubit `QExpr` function over one or more `QList` values or arrays. In fact, this is such a commonly occurring pattern that FLEQ provides a higher-order functional utility called `qexpr::map()` in the header file `qexpr_utils.h` (see FLEQ Guide and Reference (Higher-order `QExpr` functions)).

The first argument to `qexpr::map(f, qs, ...)` is a function pointer `f`, which takes at least one qubit argument and returns a `QExpr`. The next argument is a `QList` `qs`, and the remaining arguments are either additional `QList` variables, array variables, or non-arrays, each of which is passed as an additional argument to `f`.

The `qexpr::map()` utility is best understood via example.

1. `qexpr::map(bell00, as, bs)` maps `bell00()` over each pair of qubits in the `QList` values `as` and `bs`.
2. `qexpr::map(alice, qs, as, xs, ys)` maps `alice()` over each tuple `(qs[i], as[i], xs[i], ys[i])`.
3. `qexpr::map(bob, bs, xs, ys)` maps `bob()` over each tuple `(bs[i], xs[i], ys[i])`.

Thus, we can lift each component of quantum teleportation to n qubits easily, without even writing any additional `QExpr` functions, and put them together smoothly as follows:

Listing 32: A version of n-qubit teleportation with only two total barriers.

```
PROTECT
QExpr teleport_parallel(QExpr phi, qlist::QList qs, qlist::QList as, qlist::QList bs) {
    bool xs[qs.size()];
    bool ys[qs.size()];

    return qexpr::map(bell00, as, bs)
        << (phi + qexpr::map(alice, qs, as, xs, ys))
        << qexpr::map(bob, bs, xs, ys);
}
```

To test our implementation, we will have Alice prepare a GHZ state on `qs` and then analyze Bob's qubits after teleportation. If teleportation succeeds, Bob's qubits will then be in the original GHZ state.

Listing 33: Evaluating n-qubit teleportation via `teleport_parallel` on the Intel® Quantum Simulator.

```
void teleportN(iqsdk::FullStateSimulator& device) {

    const int N = 3;
    qbit listable(qs, N);
    qbit listable(as, N);
    qbit listable(bs, N);

    // Teleportation with |phi>=1/sqrt(2)(|0...0> + |1...1>)
    qexpr::eval_hold(teleport_parallel(ghz(qs), qs, as, bs));

```

(continues on next page)

(continued from previous page)

```
    // At the end, bs should be in the state |phi>=1/sqrt(2)(|0...0> + |1...1>)
    // (up to a global phase)
    auto outputRefs = to_ref_wrappers(bs);
    auto probsAfter = device.getProbabilities(outputRefs, {}, 0.01);

    std::cout << "Expecting GHZ state |0...0> + |1...1>\n";
    std::cout << "Qubits bs after teleportation:\n";
    iqsdk::FullStateSimulator::displayProbabilities(probsAfter);
}
```

The result of this evaluation call is, as expected:

```
$ ./qexpr_teleport
  Expecting GHZ state |0...0> + |1...1>
  Qubits bs after teleportation:
  Printing probability map of size 2
  |000⟩ : 0.5                           |111⟩ : 0.5
```

Bibliography

[CABB2021] M. Cerezo, A. Arrasmith, R. Babbush, S. C. Benjamin, S. Endo, K. Fujii, J. R. McClean, K. Mitarai, X. Yuan, L. Cincio, and P. J. Coles, Nature Reviews Physics 3, 625 (2021). https://doi.org/10.1038/s42254-021-00348-9

[HQCL2023] Hybrid Quantum-Classical Library, https://github.com/IntelLabs/Hybrid-Quantum-Classical-Library, Accessed : 2023-03-26.

[DLIB2023] dlib C++ library, http://dlib.net/, Accessed : 2023-03-26.

[PRMA2020] S. P. Premaratne and A. Y. Matsuura, in 2020 IEEE International Conference on Quantum Computing and Engineering (QCE) (IEEE, 2020). https://doi.org/10.1109/QCE49297.2020.00042

[SPKR2021] R. Sagastizabal, S. P. Premaratne, B. A. Klaver, M. A. Rol, V. Neĝırneac, M. S. Moreira, X. Zou, S. Johri, N. Muthusubramanian, M. Beekman, C. Zachariadis, V. P. Ostroukh, N. Haider, A. Bruno, A. Y. Matsuura, and L. DiCarlo, npj Quantum Information 7, 10.1038/s41534-021-00468-1 (2021). https://doi.org/10.1038/s41534-021-00468-1

[VEYI2020] V. Verteletskyi, T.-C. Yen, and A. F. Izmaylov, The Journal of Chemical Physics 152, 124114 (2020). https://doi.org/10.1063/1.5141458

[YEVI2020] T.-C. Yen, V. Verteletskyi, and A. F. Izmaylov, Journal of Chemical Theory and Computation 16, 2400 (2020). https://doi.org/10.1021/acs.jctc.0c00008

[GHBS2020] Gian Giacomo Guerreschi, Justin Hogaboam, Fabio Baruffa and Nicolas P D Sawaya, 2020 Quantum Sci. Technol. 5 034007. (2020). https://dx.doi.org/10.1088/2058-9565/ab8505

[PAMS2023] J. Paykin, A. Y. Matsuura, and A. T. Schmitz, in 2023 APS March Meeting, RR08.00007 (2023). https://meetings.aps.org/Meeting/MAR23/Session/RR08.7

[SCHM2023] A. T. Schmitz, in 2023 APS March Meeting, RR08.00008 (2023). https://meetings.aps.org/Meeting/MAR23/Session/RR08.8

[KWPH2022] Khalate, P., Wu, X.-C., Premaratne, S., Hogaboam, J., Holmes, A., Schmitz, A., Guerreschi, G. G., Zou, X. & Matsuura, A. Y., arXiv:2202.11142 (2022). https://doi.org/10.48550/arXiv.2202.11142

[NICH2010] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information: 10th Anniversary Edition (Cambridge University Press, 2010). https://doi.org/10.1017/CBO9780511976667