**CDL Quantum Bootcamp 2022**

**Cohort Project #1: State preparation and MIS optimization wth neutral atom arrays**

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**Task 1: Adiabatic state preparation with Bloqade**

**(see files: “task1.ipynb”, “task1 - Jupyter Notebook”, “9\*matrix.\*”)**

We followed the predefined procedure here, using Bloqade as suggested. The tutorial has a bit of arbitrariness/wiggle room in terms of the parameters that one may choose for doing the calculation. For definiteness, we settled on the following realistic system parameters:

Lattice spacing: a = 5.48 μm

Rabi frequency: Omega ranges from 0 to 8π MHz

Detuning parameter: Delta ranges from -20π MHz to +20π MHz

Van der Waals constant: C6=2π×862690 MHz μm6

Using bloqade, we performed the adiabatic simulation over time, using the suggested ramping functions for the Rabi and detuning frequencies, in an attempt to generate the Z2 state for a 1D lattice of 9 Rydberg atoms, as suggested. The x-spin expectation values and densities were computed at each lattice site, as was the energy gap between the ground and first excited states. Details may be found in the files listed above.

Now in addition to the above, we implemented a similar simulation using *Andromeda* [1], i.e. our proprietary quantum simulation code from Quantum Galaxies [2]. Our motivation here is to determine if we can address much *larger* and more realistic quantum simulations than might otherwise be the case using other canned codes. Also, *Andromeda* can do so in a way that provides reliable error bars, and also many computed eigenstates (i.e. not just the ground and first excited states), even in situations where coupling/correlation would otherwise result in a calculation that would be considered “challenging”. Finally, since scalability of the problem is not expected to be too great a challenge for *Andromeda*, we emphasize that *all of our* Andromeda *calculations are performed here* without *the blockade assumption/approximation* [3]. Although useful in some cases, there are many scientific, engineering, and business applications—the vast majority in fact—where such an approximation would be inappropriate.

In any event, the bigger and more important goal than simulating the blockade approximation is being able to simulate more general Hamiltonians at realistic scales where quantum advantage might be achieved [3]. On the experimental side, various physical implementations including atomic ions, neutral Rydberg atoms, and superconducting qubits have been constructed, and applied to such problems as Ising spin models, Fermi Hubbard models, and strongly interacting quantum dynamics—with anywhere from 10 to 100 qubits physically realized. This has motivated the commensurate develop of classical algorithms capable of simulating systems of this size, such as *Andromeda*.

The *Andromeda* code is not currently set up to operate as a time-dependent adiabatic quantum simulator in the manner of *bloqade*—although to achieve this, there are plans to merge *Andromeda* with *QuTiP* [4] going forward. Nevertheless, in principle it is sufficient to be able to separatelyu compute the relevant Hamiltonian eigenstates (energies and wavefunctions) for the time-dependent Hamiltonian at various time steps, which Andromeda is perfectly set up to do in its present form. So, for purposes of this exercise, we diagonalized the time-dependent Hamiltonian at three different time steps, corresponding to three separate values of the detuning frequency, as indicated below:

Lattice spacing: a = 5.48 μm

Rabi frequency: Omega = 8π MHz

Detuning parameter: Delta = {-20π MHz, 0 MHz, +20π MHz}

Van der Waals constant: C6 = 2π × 862690 MHz μm6

For task 1, we solved the exact same problem as with bloqade described above, i.e. the 1D lattice of 9 Rydberg atoms. Note that we also used bloqade to solve the Hamiltonian at fixed time steps, as per the above *Andromeda* calculation, in order to confirm that both codes give the same results. Indeed, this was found to be the case, to the level of accuracy to which the *Andromeda* calculation was performed, which was established to be around 3 parts per thousand.

Using *Andromeda* as well, we also computed x-spin expectation values and densities at each of the 9 lattice sites. Also, we computed *all* 29 eigenstates—not just the ground and first excited states. See files listed above for further details.

**Task 2: Larger arrays with the Blockade Approximation**

**(see files: “task2.ipynb”, “task2 - Jupyter Notebook”, “60\*.\*”)**

Here is where we are really able to test the utility of *Andromeda* in the context of the present exercise. Using *bloqade*, we increased the size of the 1D lattice calculation to the largest lattice size that we could. This was found to be a lattice of only 15 or so atoms, corresponding to a basis size of 215 ~ 30,000. Then, in order to push the size limit still further, we introduced the blockade approximation, as suggested. This enabled us to get up to 21 atoms. Without the blockade approximation, this lattice size would corresponding to a basis size of 221 ~ 2 million, though of course the actual basis size is orders of magnitude smaller due to the blockade approximation itself. Further details may be found in “task2.ipynb”. In any event, these simulation limits suggest that experiments, which have already been done with at least 51 qubits [3], would already have achieved quantum advantage.

On the other hand, *Andromeda* appears to be a much more numerically efficient approach. Using *Andromeda*, we have performed calculations for 1D lattice of the following sizes: 9, 18, 36 and 60 atoms, with data reported here just for the largest, 60-atom calculation. The parameters chosen (also for the bloqade calculations) are as specified in Task 1. Note that in the interest of time, however, we did not perform calculations for all three detuning frequency values for all four lattice sizes, but instead concentrated mainly on calculations for delta = 0 MHz. For these calculations we did concentrate on just the lowest two eigenstates (i.e. ground and first excited), and computed the band gap between them as well as the spin expectation and density/occupation values at each lattice site, as requested. Accuracies are again found to be a few parts per thousand. Details may be found in the files listed above.

It must be emphasized that the largest calculation performed here corresponds to a basis size of 260 or about 1018 basis functions. This is about *one trillion* times larger than the largest basis size we were able to achieve using *bloqade*—even with the blockade assumption in place. However, we stress again that no blockade approximation was used in our *Andromeda* calculation. The significance is that *Andromeda* can accommodate simulations of realistic NISQ quantum computer calculations [3], with up to 60 qubits or so. Additionally, this can be done *without* resorting to specific approximations such as the blockade assumption, meaning that such simulations are of relevance for a much broader range of quantum simulations, beyond just Rydberg-atom quantum computing hardware.

Regarding 2D lattice calculations, we did perform some of these using bloqade, but were only able to do so up to a 4x4 lattice of 16 atoms/qubits. This is comparable to the 1D lattice size, in terms of number of atoms/qubits or basis functions. Identical system parameters were used in each case. Note that in the interest of time, we did not perform any 2D lattice calculations, using either *bloqade* or *Andromeda*. However, using *Andromeda* at least, it is not envisioned that 2D calculations would be appreciably more expensive than the corresponding 1D calculations, provided similar system parameters were employed [1]. In any event, *Andromeda*’s performance does not suffer unduly due to strong coupling or correlation.

**Task 3: Maximum Independent Set (MIS) combinatorial optimization (see file: “Task 3 description.docx”)**

The Maximum Independent Set problem is the problem of finding a subset of vertices within a graph such that firstly, no two vertices within said subset are connected by edges (independent set definition), and secondly, there are no other vertices outside of this subset which can be added to it without violating the independent set criteria (hence maximum). This problem has many business applications [5], ranging from problems with direct application to the antenna placement problem (to find the best areas to place antennas for cell networks), to related graph problems like the maximum clique problem (where it can be used for portfolio optimization for finance), to problems in other fields like propositional satisfiability, which is used very commonly in many logistics problems.

Using *bloqade*, we conducted exercises in MIS combinatorial optimization, as suggested for this exercise, specifically for the DUGG problem. Once again, we ran into similar qubit limitations as in Task 2—i.e., we were limited by about 20 qubits total. This is quite a bit smaller than is needed for realistic applications or than can presumably be tackled using current-day NISQ quantum computers. For further details, please see “Task 3 description.docx”.

**Task 4: Business application**

**(see video file:**

**https://www.dropbox.com/s/ulav14ljhx0yd0y/week-1-video.mp4?dl=0)**

**Step 1: Explain the technical problem you solved in this exercise:**

Simulating general quantum computer calculations of realistic size (~60 qubits) on a classical computer, thereby providing accurate and reliable benchmarking data at the cusp of quantum advantage.

**Step 2: Explain or provide examples of the types of real-world problems this**

**solution can solve**

1. Especially in the present NISQ era, quantum hardware and software vendors need accurate and reliable benchmarking data, in order to confirm that their quantum computing calculations are in fact providing (reasonably) correct answers.
2. Such data should be completely *general* and not limited to special cases where classical computing solutions would be comparatively easy, such as weak coupling or blockade approximations. Thus, in addition to the many business-oriented examples provided in the exercise instructions, our solution can be directly applied to many other science, engineering, and business applications such as: i) quantum chemistry and electromagnetic simulation (of key value in drug design and exotic materials development); ii) financial derivative pricing.

**Step 3: Identify at least one potential customer for this solution - ie: a**

**business who has this problem and would consider paying to have this problem solved**

Note: some of the examples below are actually current clients or collaborators of Quantum Galaxies Corporation.

1. Google, Quantinuum, IBM, HP, Xanadu
2. i) Gaussian, Qchem, Schrödinger, Maxwell Labs, Lumionics, ORCA

b) ii) Goldman Sachs, Multiverse Computing

**Step 4: Prepare a 90 second video explaining the value proposition of your innovation to this potential customer in non-technical language**

**(see video file: https://www.dropbox.com/s/ulav14ljhx0yd0y/week-1-video.mp4?dl=0)**

**Additional Challenges Addressed by this Exercise:**

**Challenge 1:**

Given that our *Andromeda* calculations automatically use tensor networks (albeit of a very simple and straightforward sum-of-products kind), our work addresses Challenge 1. However, unlike other popular approaches such as Matrix Product States, which are rather arbitrary in terms of how they are structured and in the choice of parameters such as the bond dimension, our tensor decomposition is a mathematically natural one—with no real arbitrary parameters besides the tensor rank (which is treated as a numerical convergence parameter). As a result, we are able to extend our calculation up to the equivalent of 60 qubits, and completely bypass the blockade approximation—thus enabling us to directly tackle situations where such an approximation is not appropriate. Further questions are considered below.

*How large can you trust your results using tensor networks?*

60 qubits, without breaking too much of a sweat. Our main limitation is *not* RAM or the number of qubits that we can represent. Rather, it is the slow convergence of our iterative Krylov-subspace methods, that tends to set in when our basis sizes get up to around 1018 or so (i.e. around 60 qubits). However, we have rigorous self-consistent error-checking in place, that can tell us the accuracy of our calculations. In this case, our 60-qubit calculation is accurate to a few parts per thousand at present—although with more time available, we could converge more cycles and compute more accurate results.

*How does this compare with current experimental capabilities?*

The fact that we can handle 60 qubits explicitly (in some cases, even more than that) is extremely important for NISQ-era quantum computing, because it means that we can provide crucially important reliable benchmark data for quantum computing experiments. Currently quantum computing hardware can accommodate up to 100 or so qubits reliably. However, quantum hardware is not always reliable at the upper limits of its capabilities, meaning that the computed results may or may not be correct. Accurate benchmark data for numerically challenging applications on the verge of quantum advantage is therefore in great demand. Our *Andromeda* methodology allows us to provide such benchmarks using classical computers.

*Can you prepare a 2D state of size comparable to current experiments?*

Due to time constraints, we did not consider the 2D case here explicitly. However, we imagine performance benchmarks to be similar to those encountered for the 1D case that we did consider here, at least if similar system parameters (e.g. lattice sizes) are used. In particular, *Andromeda* is not unduly limited by strong correlation or coupling. Again, regardless of context, it seems that the main limitation is around 60 qubits, but due to Krylov subspace convergence rather than RAM limits *per se*.

*If tensor networks are state-of-the-art, what do they imply about quantum advantage in Rydberg devices?*

Of course, providing quantum computing benchmarks for challenging numerical applications runs directly counter to the idea of achieving “quantum advantage”. To be sure, the existence of accurate and reliable classical tensor-network codes such as *Andromeda* raises the threshold where quantum advantage will be attained. But this give and take has been a part of the quantum computing framework for many years now, leading “quantum inspired” algorithms that push the envelope on the classical computing side.

**Challenge 2:**

*In addition to adiabatic protocols, other state preparation protocols are currently being explored on quantum computing hardware. A leading variational protocol is the Quantum Approximate Optimization Algorithm (QAOA), in which time evolution occurs via rapidly switching between a cost and mixer Hamiltonian. For your problems above, particularly your Business Application, attempt a QAOA solution and compare your results to the adiabatic approach.*

This was done as part of our Task 3. See file “Task 3 description.docx”.

[1] B. Poirier, PRX Quantum, Submitted (2022).

J. Jerke, J. Karwowski, and B. Poirier, Mol. Phys. 117, 1264 (2018).

J. Jerke and B. Poirier, J. Chem. Phys. 148, 104101 (2018).

J. Jerke, Y. Lee, and C. J. Tymczak, J. Chem. Phys. 143, 064108 (2015).

[2] <https://cepheus.quantumgalaxies.com/company>

[3] H. Bernien et al, Nature 551, 579–584 (2017).

A. Browaeys and T. Lahaye, arXiv:2002.07413 [cond-mat.quant-gas] (2020).

J. Wurtz, P. Lopes, N. Gemelke, A. Keesling, and S. Wang, arXiv:2205.08500 [quant-ph] (2022).

T. Monz, Phys. Rev. Lett. 106, 130506 (2011).

R. Islam, R. et al, Science 340, 583–587 (2013).

C. Song, Phys. Rev. Lett. 119, 180511 (2017).

M. Gärttner, M. et al, Nat. Phys. 13, 781–786 (2017).

[4] <https://qutip.org>.

[5] J. Wurtz, et al., arXiv:2205.08500 (2022).