GGI - SFT 2022

Many-body physics and quantum computation

- Notes and exercises -

Kareljan Schoutens
Institute of Physics and QuSoft
University of Amsterdam

C.J.M.SCHOUTENS@UVA.NL

1 Qubits and quantum gates - spin systems

Summary of lecture 1

1. Introduction - Quantum Many Body (QMB) systems, Quantum Computing (QC) and Quantum simulation (Q sim). The latter not to be confused with emulating a quantum circuit (with few enough) qubits on a classical computer.

2. QC 101 - basics of qubit states (Bloch sphere), quantum circuits, 1-qubit gates plus CNOT as universal gate set.

3. Spins for qubits - 1-qubit rotations via magnetic field pulses.

4. Spin-spin interactions - Ising (XX), XY ($XX+YY$) and Heisenberg ($XX+YY+ZZ$) as examples. For each you can construct a quantum circuit out of native gates to produce CNOT, establishing universality. For the Heisenberg interaction the circuit features twice the gate HEIS($\pi/2$) which acts as the square root of the SWAP gate.

5. Digression: Krawtchouk XY chain - tuned XY couplings on open chain. Llnear dispersion with equidistant energy levels, Three fun facts about $\frac{\pi}{J}$ or $\frac{\pi}{2J}$ pulses: (i) Perfect State Transfer (PST), (ii) generating GHZ states and (iii) fast generation of a rainbow state with maximal LR block entanglement.

Some references

1. The basis of quantum computation, qubits, quantum circuits and all that are documented in many textbooks, such as the classic *Quantum Computation and Quantum Information* by M.A. Nielsen and I.L. Chuang, Cambridge University Press (10th Anniversary edition published 2010).

2. Nice introduction to the subject and many original results in *Quantum protocols for few-qubit devices*, PhD thesis Koen Groenland, University of Amsterdam (2020), https://pure.uva.nl/ws/files/43833415/Thesis.pdf

3. Compilation into native gates provided by interacting spins, see for example N. Schuch and J. Siewert, Phys. Rev. A **67**, 3 (2003) 032301.

4. Perfect State Transfer via Krawtchouk chain, first described in M. Christandl, N. Datta, A. Ekert and A.J. Landahl, Phys. Rev. Lett. **92**, 18 (2004) 187902.

1.1 Problem: 1-qubit rotations

Express the Hadamard gate as a product of (three) matrices of the form $U_X(t) = \exp(-itX)$ and $U_Z(t) = \exp(-itZ)$, up to an overall phase. Hint: visualise your proposed solution on the Bloch sphere.

1.2 Problem: CNOT from native gates for XY interaction

As discussed in the lecture, a 2-qubit gate that is native to the XY interaction is iSWAP, which swaps the two qubit states but adds a factor i for $|01\rangle$ and $|10\rangle$. Design a circuit for the CNOT gate, using twice the iSWAP gate plus a number of 1-qubit gates. If you are comfortable with programming in Python, extend the Jupyter notebook "CNOT for XXX spin qubits.ipynb" to include this circuit and run it to demonstrate its correctness.

1.3 Problem: generating GHZ states using Krawtchouk chain dynamics

We discussed that a pulse with time $t = \frac{\pi}{J}$ of the Krawtchouk chain Hamiltonian can we used to generate a GHZ state. Work this out for a chain of $N = 2$ or $N = 3$ spins (qubits) and show that

$$|\mathrm{GHZ}\rangle = U_{1-\mathrm{qubit}} \exp(-i\frac{\pi}{J}H^K)|+\rangle^{\otimes N}.$$

In each case, determine the operator $U_{1-\mathrm{qubit}}$, which you should build entirely from 1-qubit rotations.

2 Resonant driving, strategies for multi-qubit gates and basics for Rydberg atoms

Summary of lecture 2

1. (Off-)resonant driving - transitions in 2-level systems with an energy off set are effectively introduced by a driving terms that resonates in sink with the system's eigenfrequency. Detuning this frequency frustrates the transition. The optimal description uses a rotating frame and often requires the 'rotating wave approximation'.

2. Resonant driving on Krawtchouk chain energy eigenstates. Motivation: effective implementation of Toffoli gates with n controls. Protocol uses 'eigengate' which maps computational basis states to Krawtchouk chain energy eigenstates.

3. iToffoli with n controls from resonant driving Ising star states. Here the computational basis provides the energy eigenstates, simplifying the protocol. Details have been worked out for superconducting qubits ($n = 2$, 3) and for trapped ions.

4. Rydberg atoms - basic description with hamiltonian describing coupled 2-level atoms ($|g_i\rangle$, $|r_i\rangle$), featuring driving terms (strength Ω_i), detunings Δ_i and interaction terms V_{ij} falling off like r^{-6}. We distinguish three dynamical regimes: blockade, facilitation and dressing.

Some references [references for dynamics constrained by Rydberg atom blockade, facilitation or dressing to follow later]

1. Resonant driving, see again *Quantum protocols for few-qubit devices*, PhD thesis Koen Groenland, University of Amsterdam (2020), https://pure.uva.nl/ws/files/43833415/Thesis.pdf

2. Multi-qubit gates via resonant driving on Krawtchouk chain eigenstates: K. Groenland and K. Schoutens, Phys. Rev. A **97** (2018) 042321.

3. Single-step implementation of Toffoli gate with n controls using Ising star interaction: S.E. Rasmussen, K. Groenland, R. Gerritsma, K. Schoutens and N.T. Zinner, Phys. Rev. A **101** (2) (2020) 022308.

2.1 Problem: $n = 2$ Toffoli gate compiled into CNOTs

Find in the literature (or derive by you own means) a quantum circuit compiling the $n = 2$ Toffoli gate into CNOT gates and 1-qubit rotations. The optimal way to do this uses 6 CNOT gates. As another exercise, you can build the circuit in the Cirq notebook and check its workings.

2.2 Problem: Rabi oscillations for Rydberg blocked atoms

As clearly observed in, for example, Fig 1d in H. Bernien et al, Nature 551 (2017) 579-584, https://arxiv.org/abs/1707.04344v2, the Rabi frequency of '2-level' Rydberg atoms is enhanced by a factor of $\sqrt{N}$ as soon as the atoms form groups of N atoms that are within each other's Rydberg blockade radius R_b. Explain why this is.

2.3 Problem: Rydberg dressing

Reproduce the leading r dependent term in the effective potential $W(r)$ that arises from 'Rydberg dressing' as explained in the lectures. The expression is

$$W(r) = \frac{\Omega^4 V(r)}{8\Delta^3(2\Delta + V(r))}.$$

Hint: you can do this using perturbation theory to fourth order. Alternative approach is to write the Schrödinger equation based on the Hamiltonian as a 4×4 matrix on the basis $|gg\rangle$, $|gr\rangle$, $|rg\rangle$, $|rr\rangle$, *and to adjust the state vector such that the 'small' components (*gr, rg *and* rr*) are stationary.This then determines the effective potential for the* gg *component, which leads to* $W(r)$.

3 Quantum computing and simulation with Rydberg atoms

Summary of lecture 3

1. Rydberg atoms as qubits - demonstrating how a CNOT gate can be realized for two atoms in blockade regime.

2. Q Sim with Rydberg atoms I - blockade regime.

   - Atom chain in Rydberg blockade regime. Adiabatic preparation of crystalline states (such as $\mathbb{Z}_2$ state). Observation of revivals of these states in after-quench dynamics, later understood in terms of Quantum Many Body Scars (QMBS).
   - Rydberg atoms on 2D kagome lattice as Q Sim of topological quantum spin liquid.

3. Q Sim with Rydberg atoms II - facilitation regime. Open chain with $\Delta = -V_{NN}$. The number of clusters of atoms in the $|r\rangle$ state is conserved - the corresponding Hilbert space has the topology of a hypercube in $d = 2N_{cl}$ dimensions, allowing the comparison of scars in the quantum many-body dynamics with classical, 1-particle scars.

4. Q Sim with Rydberg atoms III - dressing regime. Describing proposal for simulation of M_1 model which has manifest $N = 2$ supersymmetry and connects to first minimal model of $N = 2$ superconformal field theory. The proposal employs Rydberg dressed interactions to mediate NN constraint and tuned value of NNN repulsion. The proposed observables are arrival time characteristics of kinks and skinks traversing the system.

Some references

1. Rydberg atom chain: H. Bernien et al, Nature **551**, 579-584 (2017), https://arxiv.org/abs/1707.04344v2.

2. Rydberg atoms on kagome lattice: G. Semighini et al, Science **374**, 6572 (2021), https://arxiv.org/abs/2104.04119.

3. Rydberg atom chain in facilitation regime: M. Marcuzzi et al, Phys. Rev. Lett. **118**, 063606 (2017), https://arxiv.org/abs/1607.06295 and B. van Voorden et al, Phys. Rev. B **103**, 220301 (2021), https://arxiv.org/abs/2012.05310.

4. Supersymmetric M_1 model first proposed in: P. Fendley, K. Schoutens, and J. de Boer. Phys. Rev. Lett. **90**, 120402 (2003), https://arxiv.org/abs/hep-th/0210161. Proposal for quantum simulation of this model: J. Minar, B. van Voorden and K. Schoutens, Phys. Rev. Lett. **128** (2022) 050504, https://arxiv.org/abs/2005.00607. News item on this paper: https://phys.org/news/2022-02-kinks-skinks-supersymmetry.html.

3.1 Problem: $d = 4$ hypercube for $N_{cl} = 2$

For a Ryberg atom chain, work out the topology for the $N_{cl} = 2$ states that are degenerate under the facilitation condition $\Delta = -V_{NN}$. Can you picture this as a truncated 4d hypercube?

3.2 Problem: Witten index for M_1 model

The Witten index is defined as

$$\mathrm{Tr}[(-1)^F],$$

with F the number of particles (fermions) in a state. Prove that, for the M_1 model on a chain of length $L = 3l$ and with periodic boundary conditions (PBC), $W = 2$. What is the value for $L = 3l - 1$ or $L = 3l + 1$. And for open boundary conditions?

4 Quantum Computing for Quantum Many Body - QPE

Summary of lecture 4

1. Basic strategies: Quantum Phase Estimation (QPE) and Variational Quantum Eigensolvers (VQE).
2. Hamiltonian simulation is goal in itself (quantum dynamics) as well as building block in QPE circuits.
3. QPE explained on basis of examples with $s = 1$ and $s = 2$ binary digits.
4. Quantum Fourier Transform (QFT) as key ingredient to QPE circuit as well as other quantum algorithms such as Shor's algorithm for factoring.
5. Demo in Cirq with 2-site Fermi-Hubbard model as (partially) worked example. The original choice $U = \frac{3}{4}$, $t = \frac{1}{4}$ gives eigenvalues $\pm\frac{3}{8}$ and $\pm\frac{5}{8}$, which happen to be degenerate in the representation as phases where you count numbers modulo 1. I therefore changed the parameters to $U = \frac{3}{8}$, $t = \frac{1}{8}$ and added some explanation.
6. Brief on Hamiltonian simulation (Lie-Trotter-Suzuki and alternatives such as qubitization).

Some references

1. QPE and QFT are well-explained in the Nielsen-Chuang textbook.
2. For Hamiltonian simulation, see for example: A.M. Childs et al, Proceedings of the National Academy of Sciences 115, 9456-9461 (2018), https://arxiv.org/abs/1711.10980.

4.1 Problem: controled unitaries

In the Cirq demo, the simplest example of a QPE circuit need a rotation gate controled by one of the binary qubits. Assuming that the only 2-qubit gate at your disposal is the CNOT, design a circuit that implements this controled rotation gate. [The circuit shown in the lecture was not correct - see lecture 5 for correct version.] Same question for a controled-Y gate. Can you envision a scheme to handle a general 1-qubit gate controled by a single qubit?

PS In the Cirq demo we added a version of the QPE circuit for unitary $Z^{2\theta}$ where the controled rotations are compiled into CNOT's and 1-qubit gates.

4.2 Problem: rounding errors in QPE

QPE is not exact if the phase can not be represented exactly using the s auxiliary qubits. Assuming $s = 2$ and an unknown phase $1/2 \leq \phi \leq 3/4$, determine the probability for measurement outcomes $\phi = 1/2$ and $\phi = 3/4$. Are other outcomes possible?

4.3 Problem: quantum circuit for QFT

In the lecture we flashed the quantum circuit for QFT without explanation or detail. Study the Cirq demo, or any textbook on this, to see how the QFT is implemented. What is the 2-qubit gate count for QFT on n qubits?

5 Quantum Computing for Quantum Many Body - VQE

Summary of lecture 5

1. Basics of Variational Quantum Eigensolvers (VQE).
2. Warm up example: Heisenberg XXX chain with Hamiltonian Variational Ansatz (HVA); demo in Cirq.
3. Ingredients of QC^2 (Quantum Chemistry on Quantum Computer): choice of orbital basis, fermion-to-qubit mapping, Hartree-Fock and Unitary Coupled Cluster (UCC) Ansatz. Worked example: H_2 molecule.
4. Heisenberg XXX on kagome lattice as target for near term hardware. Using a 2D superconducting qubit architecture, the HVA for this problem is 'hardware efficient' in a number of ways (no fermon-to-qubit mapping, qubit geometry similar to system geometry, HEIS(α) gate near native).

Some references

1. VQE for Heisenberg XXX chain and kagome lattice, J. Kattemölle and J. van Wezel, https://arxiv.org/abs/2108.02175, see also J.L. Bosse and A. Montanaro, https://arxiv.org/abs/2108.08086.
2. Review *Quantum Computational Chemistry*, S. McArdle et al, Rev. Mod. Phys. **92**, 15003 (2020), https://arxiv.org/abs/1808.10402v3.

5.1 Problem: improving the Cirq VQE code

The Cirq code we provided for the XXX chain has a highly primitive optimizer (simply looping over a grid of angles), which can be improved in many ways. Give this a try and see if you can improve the accuracy.

5.2 Problem: HVA for small size systems

The HVA for the XXX chain on $L = 4$ sites is exact after two layers (one even, one odd). The angles α, β are given in the notebook. Prove that for these values the circuit builds the exact ground state, with energy $E_{GS} = -8$.

5.3 Problem: quantum circuit for QCCSD Ansatz for H_2

The UCCSD operator for the H_2 molecule is given in eq. (104) of the Rev. Mod. Phys. paper cited in the above, and the corresponding quantum circuit is displayed in FIG. 11 of that same paper. Show that the circuit indeed implements the UCCSD operator. The operators $R_x(\theta)$ and $R_z(\theta)$ are defined in eq. (6) of that paper (note the factor 1/2 in the exponent!).