Lecture 14: Density matrix dynamics
Reading: Lamm and Lawrence PRL (2018).

1 Introduction

The problem of preparing a thermal state on a quantum processor has traditionally been considered challenging and not tractable for near-term devices. QITE and QMETTS appear to have mitigated the problem by not requiring the preparation of a thermal state, but rather evolving in imaginary time and sampling in a Markov chain process to yield a thermal average of an observable. However, combined real-time and imaginary time dynamics have not yet been implemented in conjunction with the QMETTS algorithm, although there appears to be no barrier to doing so. In any case, before these algorithms were first reported, other schemes have been described to compute dynamics and thermal averages on quantum processors.

One of those recent schemes is Evolving density matrices on qubits algorithm by Lamm and Lawrence. It is a hybrid quantum-classical algorithm to simulate the dynamics of a quantum many-body system at a finite temperature. It works by first computing a classical approximation to the thermal density matrix, which is necessarily sparse, and then time evolving each element of this density matrix on a quantum processor. Observables can then be computed using this time-evolved density matrix. The advantage of this scheme is that the computation of the thermal state is performed on a classical computer, avoiding the challenging state preparation step. Then, evolving the mixed thermal state reduces to evolving multiple pure states.

2 Density Matrix Quantum Monte Carlo (DMQMC)

To begin, we first need a sparse approximation of the density matrix at a given temperature. A stochastic algorithm to do that is DMQMC in which a population of imaginary particles known as psips explore configuration space via random walks in imaginary time, $\beta = it$. As $\beta \to \infty$, the psips density approximates that of the ground state. For finite β, the psips density approximates that of the density matrix at $T \sim \beta^{-1}$.

We begin by deriving the symmetric Bloch equation for the imaginary time evolution of the density matrix $\rho = \exp(-\beta H)$. Using a resolution of the identity to express

$$rho(\beta) = \exp(-\beta H/2) \sum_{\alpha} |\alpha\rangle \langle\alpha| \exp(-\beta H/2) \tag{2.1}$$

we get,

$$\frac{d\rho}{d\beta} = -\frac{1}{2}(H\rho + \rho H) \tag{2.2}$$

with the initial condition $\rho(\beta = 0) = I$ where I is the identity matrix corresponding to infinite temperature. DMQMC stochastically implements a first-order Euler difference approximation to this equation with ρ represented by psips. Each psips is associated with a matrix element $|b_p\rangle \langle a_p|$ and sign χ_p so that the approximate density matrix is $\tilde{\rho} = \sum_p \chi_p |b_p\rangle \langle a_p|$.

The algorithm starts by randomly placing psips along the diagonal of ρ with positive sign $\chi_p = 1$. The psips density is evolved in steps of $\Delta\beta$ for a total number of steps $N_{step} = \beta/\Delta\beta$. At each step, a psip can undergo one of four operations that are described in the paper and I won't reproduce here. The main point is that after evolution in β following these steps, we obtain a sparse approximation

to $\rho(\beta)$. As expected for a stochastic algorithm, the expectation values converge as $P^{-1/2}$ where P is the number of psips.

3 Dynamics on a quantum processor

Now that we have a classical approximation to the thermal density matrix, we want to perform quantum simulation of dynamics. We can get observables at a given time as:

$$\langle O(t)\rangle = \frac{Tr(Oe^{-iH_1t}\rho e^{iH_1t})}{Tr\rho} \tag{3.1}$$

where H_1 is the perturbing Hamiltonian that turns on at $t = 0$. To ensure the density matrix is Hermitian in the presence of stochastic noise, we use the density matrix $\rho = (\tilde{\rho} + \tilde{\rho}^\dagger)/2$ so that

$$\langle O(t)\rangle = \frac{1}{Tr\rho}\sum_p Tr\left(\frac{1}{2}Oe^{-iH_1t}(\chi_p |b_p\rangle\langle a_p| + \chi_p^* |a_p\rangle\langle b_p|)e^{iH_1t}\right) \tag{3.2}$$

where the sum is over psips forming the sparse approximation of the density matrix. Note that from this equation, the dynamics of each psips can be obtained independently from all the others - no mixed state required!

The only remaining task is to actually evaluate the individual terms. If we have a diagonal term for which $a_p = b_p$, then computing $\langle a_p|O(t)|a_p\rangle$ is straightforward as a normal measurement. If the psips is non-diagonal, e.g. $|b_p\rangle\langle a_p|$, it must be diagonalized. Taking χ_p to be real, then

$$|b_p\rangle\langle a_p| + |a_p\rangle\langle b_p| = |u_p\rangle\langle u_p| - |v_p\rangle\langle v_p| \tag{3.3}$$

$$|u_p\rangle = \frac{1}{\sqrt{2}}(|a_p\rangle + |b_p\rangle) \tag{3.4}$$

$$|v_p\rangle = \frac{1}{\sqrt{2}}(|a_p\rangle - |b_p\rangle) \tag{3.5}$$

Therefore, we prepare the states $|u_p\rangle$ and $|v_p\rangle$, measure the operator, and take the difference to get the off-diagonal terms. Note that I think Eq. 5 in the Lamm paper is missing a factor of $1/2$ and χ_p. The $1/2$ factor is because in the arxiv version they defined the states $|u_p\rangle$ and $|v_p\rangle$ without a factor of $\sqrt{2}$ and I guess forgot to update equation 5 in the PRL version. The χ_p I think should still be there but am not sure what happened to it.

How do we prepare the states $|u_p\rangle$ and $|v_p\rangle$? I don't really understand the method proposed on p3 of the paper. Here is a scheme I came up with instead. Start with an ancilla qubit in a superposition state. Apply anti-CNOT, controlled by the ancilla, to flip the qubit corresponding to $|a_p\rangle$. Similarly, apply CNOT to flip the qubit corresponding to $|b_p\rangle$. Apply H to the ancilla. The resulting state is:

$$\frac{|0\rangle\otimes(|a_p\rangle + |b_p\rangle) + |1\rangle\otimes(|a_p\rangle - |b_p\rangle)}{\sqrt{2}} \tag{3.6}$$

Now measure the ancilla. If we measure 0, the system is in state $|u_p\rangle$ and we proceed. If we measure 1, the system is in state $|v_p\rangle$ and we add its contribution to the expectation value with a minus sign.

To summarize the steps to be performed:

1. After obtaining the DMQMC density matrix, prepare the state $|a_p\rangle$, $|u_p\rangle$, or $|v_p\rangle$.

2. Time-evolve the density matrix element by Trotterization

3. Measure O and other observables

The nice feature of this algorithm is that one can perform quantum dynamics over the full Hilbert space on the various components of the thermal density matrix. On the other hand, I wonder how much time must be simulated before the dynamics is not tractable classically given the sparse initial condition.