

Lecture 9: Iterative phase estimationReading: [Whitfield et al arXiv:1001.3855 \(2010\)](#) [Guzik et al, Science \(2005\)](#)**1 Phase estimation for determining ground state energy**

Now we have a quantum problem formulated in a way that a QC can carry out relevant operations. We next need an algorithm that uses these operations to arrive at a desired quantity - for instance, the ground state, thermal averages, or other observable of interest. The most basic desired quantity for a given Hamiltonian is the ground state energy, which means we want to find the smallest eigenvalue of a given Hamiltonian. The most straightforward (but technically challenging to implement) algorithm to obtain this eigenvalue is that of eigenvalue estimation. The algorithm is nearly identical to that presented in any quantum computing textbook so I will just describe the specific steps needed for the BK transformed H_2 Hamiltonian.

The idea of phase estimation is that a controlled unitary is applied to a system register, and the relative phase (corresponding to the eigenvalue of the unitary) is picked up on a control register. Repeated application of $c - U$ along with controlled rotations based on the bits of the eigenvalue measured at each stage yields an estimate of the phase, or equivalently the eigenvalue.

There are a number of practical issues with implementing this algorithm for problems that are classically challenging on near-term devices. First, the complexity of obtaining b bits scales exponentially with b as 2^b applications of $c - U$ are required to obtain the least significant bit, and we have to have the least significant bit to obtain the subsequent bits. That inefficient scaling means that the gate depth for phase estimation is prohibitively large for any QC we presently have. Further, we need to have a state with non-negligible overlap with the ground state in the state register to start, or else the measurement will collapse the state into an eigenstate that is not the ground state. All of these challenges are quite prohibitive for phase estimation in the near term.

However, we can still try out the algorithm to see how it works for the minimal basis H_2 problem. For that problem, there are 4 spin-orbitals: the bonding and anti-bonding orbitals and two spins. The two electrons occupy the spin up and down bonding orbitals. The sums in the Hamiltonian therefore go over 0 to 3. Using the BK transform and removing qubits with only Z operators, we get the Hamiltonian of interest:

$$H = g_0 I + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 X_0 X_1 + g_5 Y_0 Y_1 \quad (1.1)$$

From the above discussion, we see we need to implement the unitary e^{-iHt} . We can do that efficiently by Trotterization:

$$e^{-iHt} = e^{-it \sum_{\gamma} g_{\gamma} H_{\gamma}} \approx U_{\text{trot}}(t) \equiv (\prod_{\gamma} e^{-ig_{\gamma} H_{\gamma} t/n})^n \quad (1.2)$$

where n is the number of Trotter steps. The starting state for the simulation should be a state with good overlap with the actual ground state, which to start we take to be the HF ground state. In the occupation number basis for minimal basis H_2 , the lowest two molecular orbitals are occupied (lowest energy, spin up and down): $|\phi_{\text{occ}}\rangle = |0011\rangle$. If we convert to BK, we have:

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (1.3)$$

Remember that we still have to remove qubits 1 and 3. Therefore, we get the HF state in the BK basis is $|\phi\rangle = |01\rangle$ given in O Malley et al.

The original phase estimation algorithm requires a number of qubits that is too even for the H_2 Hamiltonian. This depth can be reduced using an iterative phase estimation algorithm. Recall that in the traditional phase estimation algorithm we obtain all b bits of the phase by applying $c - U$ 1, 2, 4, ..., 2^b times - measurement of the b -qubit phase register then gives all the b bits at the same time. We can instead set up an iterative phase estimation algorithm where we obtain one bit at a time. Let's write the phase we want $\phi = 0.j_0j_1\dots j_b = j_0/2 + j_1/4 + \dots + j_{b-1}/2^b$.

First, we do $c - U$ 2^{b-1} times and measure the bit to get the least significant bit of the phase, j_{b-1} . Then, we run the circuit again but add in a phase gate on the phase register to rotate off the bit that we just measured. Then we proceed to measure the next most significant bit. If we keep following this procedure we will obtain all b bits in an iterative way without having to apply all the $c - U$ operations at once.

We need to fill in the details to rotate off the preceding bits of phase. If we have measured k bits of the phase, we need to perform a rotation of the overall accumulated phase is $\Phi(k)$ before obtaining the next bit. That phase is $0.0j_{k+1}\dots j_{b-1}$. If you work with the indices starting from the initial definition of the phase, you can find that

$$\Gamma(k) = \sum_{l=2}^{b-k} \frac{j_{l+k-1}}{2^l} \quad (1.4)$$

Note the upper limit of the sum is different by 1 from that given in the Whitfield paper. In that paper I believe they actually were obtaining $b + 1$ bits of phase although they said they were getting b bits, accounting for the extra 1.

This phase should be rotated off before measuring j_k , so we apply a phase gate with $\Phi_k = \exp(2\pi i\Gamma(k))$. This phase then gives an estimate of the final energy.

A final point is that the HF state is not always the optimal state to start the calculation in the sense that it may have poor overlap with the ground state. Such a situation occurs if bonds are close to breaking, for instance. To improve the overlap with the actual ground state, a strategy that can be used is adiabatic state preparation (ASP). This procedure relies on the adiabatic theorem, which loosely states that if a state is in an eigenstate at $t = 0$, the system will remain in that position of the eigenspectrum if the Hamiltonian changes sufficiently slowly. So for ground states, if we start in the ground state of some Hamiltonian, we will stay in the ground state if the Hamiltonian is interpolated to some other one of higher interest. Mathematically, we write the time-dependent Hamiltonian as:

$$H(s) = (1 - s)H_0 + sH_1 \quad (1.5)$$

where $s \in [0, 1]$ is the interpolation parameter and the simulation starts at $s = 0$. Typically H_0 is the initial Hamiltonian for which finding the ground state is easy, while H_1 is the one for which the ground state is desired but not known. We can use this process to start e.g. in a HF ground state and interpolate to one closer to the actual ground state of the full Hamiltonian, then do phase estimation.

A question is how slowly do we need to go for the adiabatic theorem to hold? Loosely, the time is $t_f \sim 1/\Delta^2$, where Δ is the minimum energy gap along the path interpolating the two Hamiltonians. A challenge with ASP and adiabatic quantum computation in general is that we do not a priori know what the gaps are along the path, and hence figuring out the necessary time is not easy.