Modified Diffusion Quantum Monte Carlo for Approximating Helium Ground State Energy

Reilly Cannon [1]

[1] Reed College, Portland, Oregon

Diffusion Quantum Monte Carlo (DQMC)

Diffusion Quantum Monte Carlo is a stochastic method that gives an approximate upper bound for ground state energies of multiple-bodied quantum systems [1,2].

This poster compares the average numerical results of two different DQMC algorithms: the one as presented in class (labeled here as "Basic") and one with an enhancement to reduce the error due to finite time step (labeled here as "Modified"). The enhancement works as follows.

Note that we can write our propagator $G(\mathbf{R}_f|\mathbf{R}_i;dt)$ as the product of a weight matrix W and stochastic matrix P, representing the transition from position $\mathbf{R}_i$ to $\mathbf{R}_f$:

$$G(\mathbf{R}_f|\mathbf{R}_i;dt) = P(\mathbf{R}_f|\mathbf{R}_i)W(\mathbf{R}_f|\mathbf{R}_i), \tag{1}$$

where $W(\mathbf{R}_f|\mathbf{R}_i) = e^{-((E_{local}(\mathbf{R}_f+E_{local}(\mathbf{R}_i)/2-E_{trial})}$ is the weight matrix and $P(\mathbf{R}_f|\mathbf{R}_i) = (2\pi dt)^{-3N/2}e^{-(\mathbf{R}_f-\mathbf{R}_i-F(\mathbf{R}_i dt)^2/2dt}$ is the stochastic matrix [3]. In the limit as $dt \to 0$, G becomes the exact stochastic matrix with stationary distribution corresponding to the ground state [4]. With a finite time step, however, the stationary distribution is not exactly the ground state. To remedy this, we make the modification

$$P(\mathbf{R}_f|\mathbf{R}_i) = P_{acc}(\mathbf{R}_f|\mathbf{R}_i)P_{prop}(\mathbf{R}_f|\mathbf{R}_i), \tag{2}$$

where we have renamed the stochastic matrix P in (1) to be the proposal probability matrix P_{prop}, and

$$P_{acc}(\mathbf{R}_f|\mathbf{R}_i) = \min\{1, A(\mathbf{R}_f|\mathbf{R}_i)\} \tag{3}$$

with

$$A(\mathbf{R}_f|\mathbf{R}_i) = \frac{|\Phi(\mathbf{R}_f)|^2 P_{prop}(\mathbf{R}_i|\mathbf{R}_f)}{|\Phi(\mathbf{R}_i)|^2 P_{prop}(\mathbf{R}_f|\mathbf{R}_i)}. \tag{4}$$

Here, Φ is our trial wavefunction [3]. With this modification, we ensure that (4) is unity, as in the $dt \to 0$ limit, and G has no time step error as a result of the stochastic matrix $P(\mathbf{R}_f|\mathbf{R}_i)$ for any timestep size [4].

However, error due to time step still shows up in the weight matrix $W(\mathbf{R}_f|\mathbf{R}_i)$. However, a clear improvement results from this modification since we now have a diffusion process with an effective timestep strictly less than the original timestep [3].

Setup, Parameters, and Initial Conditions

No changes to the program parameters from the homework were made. The only modifications to the program can be seen on the right. We ran the modified and unmodified DQMC ten each times to determine average performance. We initialized the algorithm with a total of 4000 walkers and a time step of 0.005. We set the initial positions of the two particles to be the six-dimensional vector $(0, 0, 1/\alpha, 0, 0, -1/\alpha)$, where $\alpha = 1.8$. We performed thermalization for 500 steps and measurement for 1000 steps.

Modified Code

```
ProposalProbability[rf_, ri_, dt_] := Exp[-1/(4*dt) (rf - ri - F[ri] dt).(rf - ri - F[ri] dt)];
```

```
MCStep[positions_, dt_] :=
 Module[{i, r, rp, w, weights, newpositions, eta, ψψ, trialψψ, prf, pri, pacc,
   bdist, b, wNoAcc},
  weights = Table[0, Length[positions]];
  newpositions = positions;
  For[
   i = 1, i ≤ Length[positions], i++,
   r = positions[[i]];
   rp = MoveWalker[r, dt];
   pacc = Min[1, ProposalProbability[r, rp, dt]*Abs[ψTrial[rp]]^2 /
       ProposalProbability[rp, r, dt]*Abs[ψTrial[r]]^2];
   eta = RandomReal[{0, 1}];
   If[pacc > eta,
    newpositions[[i]] = rp;
    weights[[i]] = WeighWalker[rp, r, dt],
    weights[[i]] = WeighWalker[r, r, dt];
   ];
  ];
  Return[RepackWalkers[weights, newpositions]];
 ]
```

Figure 1: Above is the definition of the proposal probability. Below is the program that performs a single step of the Monte Carlo simulation.

Results

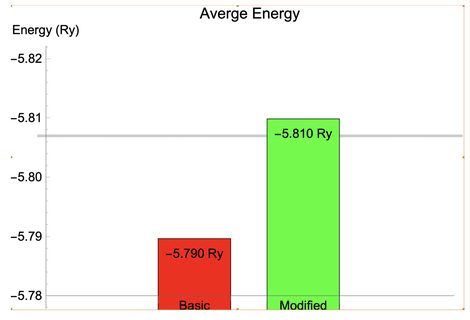

Figure 2: The average energy of the modified algorithm is closer to the numerically exact energy then that of the basic algorithm.

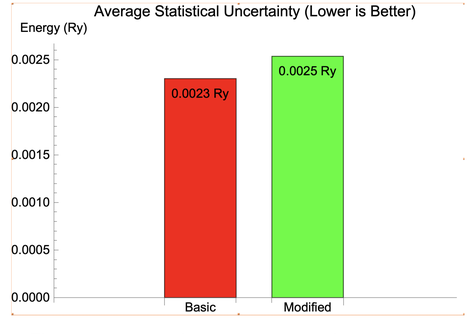

Figure 3: The average statistical uncertainty remained approximately the same.

Results

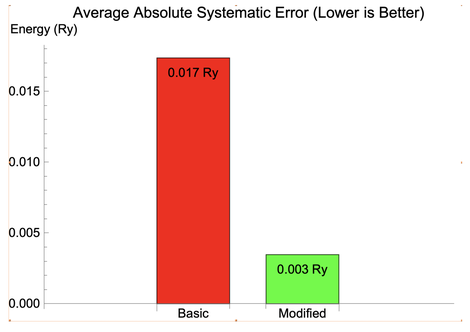

Figure 4: The modified algorithm has significantly lower systematic error than does the unmodified one.

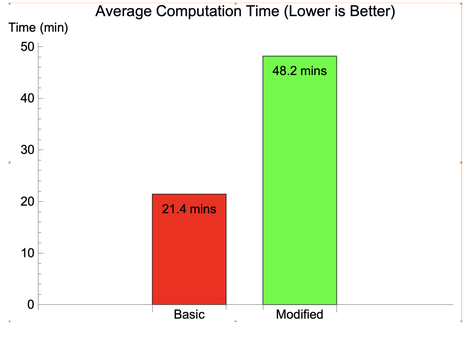

Figure 5: The modified algorithm takes over twice as long to run on average.

Conclusion

The modified algorithm yielded an average ground state energy of $-5.810Ry$, which is lower than the numerically exact value of $-5.807Ry$. For this reason, the algorithm did not provide a upper bound on the ground state energy, as expected. However, this energy is closer to the numerically exact value than is the energy from the unmodified algorithm ($-5.790Ry$). The similation overall shows that the modification is a definitive improvement over the original.

References

[1] Tao Pang.
Diffusion monte carlo: A powerful tool for studying quantum many-body systems.
2014.

[2] Jan Tobochnik Peter J. Reynolds and Harvey Gould.
Diffusion quantum monte carlo.
1990.

[3] Roland Assaraf Julien Toulouse and C. J. Umrigar.
Introduction to the variational and diffusion monte carlo methods.
2015.

[4] Berni J. Alder Peter J. Reynolds, David M. Ceperley and William A. Lester.
Fixed-node quantum monte carlo for molecules.
1982.

Acknowledgements

I give all of my gratitude to Darrell Schroeter for his help and unending patience in office hours while debugging Mathematica code.

REED COLLEGE