QMC Part I

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2 Simple power method

2.1 2x2 Matrix

Consider a Hamiltonian whose matrix form is shown in Eq:1. This Hamiltonian has two eigenvectors and two eigenvalues. Let the two eigenvectors be $\mathbf{u_0}$ and $\mathbf{u_1}$. Then consider ν any arbitrary trial vector which is not an eigenvector of Eq:1 but belongs to the 2x2 space. Any such trial vector can always be written in the form shown in Eq:2.

$$\begin{bmatrix} v_0 & -t \\ -t & v_1 \end{bmatrix} \tag{1}$$

$$\nu = c_0\mathbf{u_0} + c_1\mathbf{u_1} \tag{2}$$

The key idea is the realization that the ground state of the Hamiltonian 1 given by $\mathbf{u_0}$ can be extracted from ν by the repeated application of a filter $G(H)$. This filter systematically purifies ν to obtain the ground state $\mathbf{u_0}$ provided $c_0 > 0$, i.e. the trial vector ν has a non-zero projection on the ground state.

The form of the filter is inspired from the power method where a successive application of the Hamiltonian followed by the substraction of the residual leads to a convergent series of vectors. The limiting value of this convergent series is one of the extremal eigenvectors of the Hamiltonian. Following this, our filter $G(H)$ can be written as 3

$$\hat{G}(H) = \Big(\mathbf{1} - \tau(\hat{H} - E_T\mathbf{1})\Big) \tag{3}$$

The convergent series of vectors is then $\left\{\nu^{(0)}, \nu^{(1)},\ \nu^{(2)}, \ldots, \nu^{(n)}\right\}$ where $\nu^{(k)}$ is given by 4

$$\nu^{(k+1)} = \hat{G}(H)\nu^{(k)} \tag{4}$$

Using Eq:2, Eq:4 can be written as 5

$$\nu^{(k+1)} = c_0(1 - \tau(E_0 - E_T))^{(k)}\mathbf{u_0} + c_1(1 - \tau(E_1 - E_T))^{(k)}\mathbf{u_1} \tag{5}$$

From Eq:5, we can see that a repeated application of the filter Eq:3 with a trial guess energy E_T will result in the series converging geometrically to either E_0 or E_1 depending on the choice of E_T.

Here we shall show an example using the Hamiltonian given in Eq:1. In the case of a 2x2 Hamiltonian, and any general trial vector $[c_0, c_1]$, the recursion relations for the calculation of $c_0^{(k)}$ and $c_1^{(k)}$ are straight forward and given by Eq:6,7.

$$c_0^{(k+1)} = \left(\mathbf{1} - \tau\left(\nu_0 - E_T\right)\right)c_0^{(k)} + \tau t c_1^{(k)} \tag{6}$$

$$c_1^{(k+1)} = \tau t c_0^{(k)} + \left(\mathbf{1} - \tau\left(\nu_1 - E_T\right)\right)c_1^{(k)} \tag{7}$$

These are the working equations. As an example, we begin with the initial set of values given as follows:

```
\nu_0=1
\nu_1=2
t=1
\tau=0.1
E_T=3
c_0=0.31622776601683794
c_1=0.9486832980505138
nsteps=1024
```

The iteration can begin with these as starting values. The output is given in shown in the Figure:1.

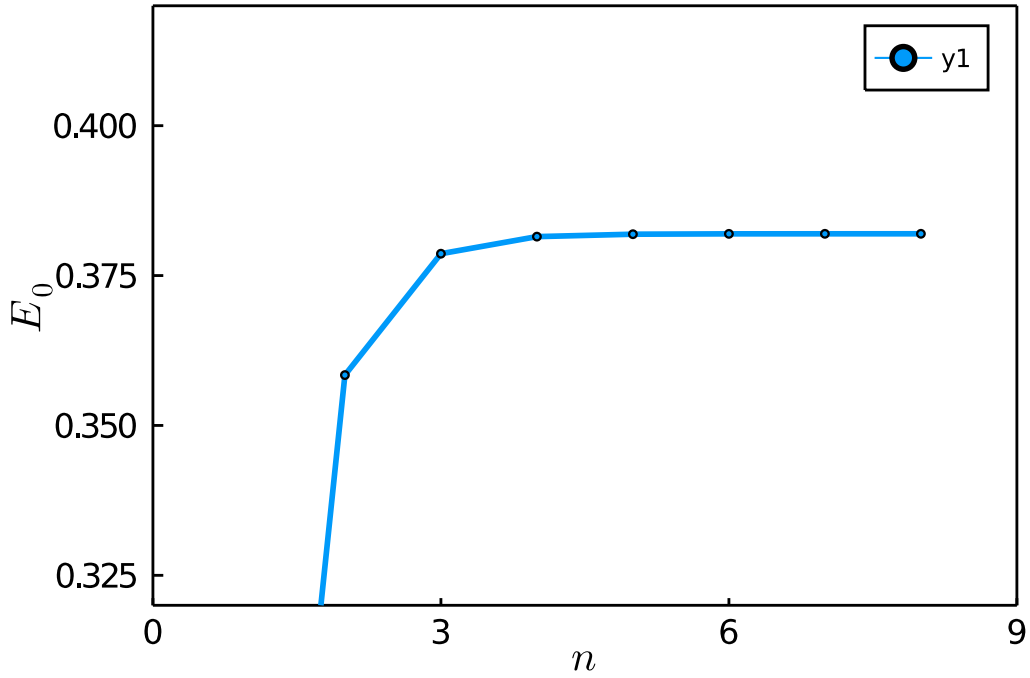

Figure 1: Convergence of the Local energy as a function of iterations.

2.2 3x3 Matrix

A demonstration of all the different variants of QMC requires more than two states. Here we show a Hamiltonian with 3 states. The matrix form of the

Hamiltonian is shown in Eq:8.

$$\begin{bmatrix} v_0 & -t & -t \\ -t & v_1 & -t \\ -t & -t & v_2 \end{bmatrix} \tag{8}$$

The trial vector can be written as shown in Eq:9.

$$\nu = c_0\mathbf{u}_0 + c_1\mathbf{u}_1 + c_2\mathbf{u}_2 \tag{9}$$

The three coefficients required are c_0, c_1, and c_2. The recurrence relations for the three coefficients shown in Eq:10, Eq:11, Eq:12, and Eq:13.

$$\nu^{(k+1)} = c_0(1-\tau(E_0-E_T))^{(k)}\mathbf{u_0} + c_1(1-\tau(E_1-E_T))^{(k)}\mathbf{u_1} \tag{10}$$

$$c_0^{(k+1)} = (\mathbf{1} - \tau\left(\nu_0 - E_T\right))\, c_0^{(k)} + \tau t c_1^{(k)} + \tau t c_2^{(k)} \tag{11}$$

$$c_1^{(k+1)} = \tau t c_0^{(k)} + (\mathbf{1} - \tau\left(\nu_1 - E_T\right))\, c_1^{(k)} + \tau t c_2^{(k)} \tag{12}$$

$$c_2^{(k+1)} = \tau t c_0^{(k)} + \tau t c_1^{(k)} + (\mathbf{1} - \tau\left(\nu_2 - E_T\right))\, c_2^{(k)} \tag{13}$$

```
\nu_0=1
\nu_1=2
\nu_2=3
t=1
\tau=0.05
E_T=3
c_0=0.4082482904638631
c_1=-0.8164965809277261
c_1=0.4082482904638631
nsteps=1024
```

The iteration can begin with these as starting values. The output is given in shown in the Figure:2.

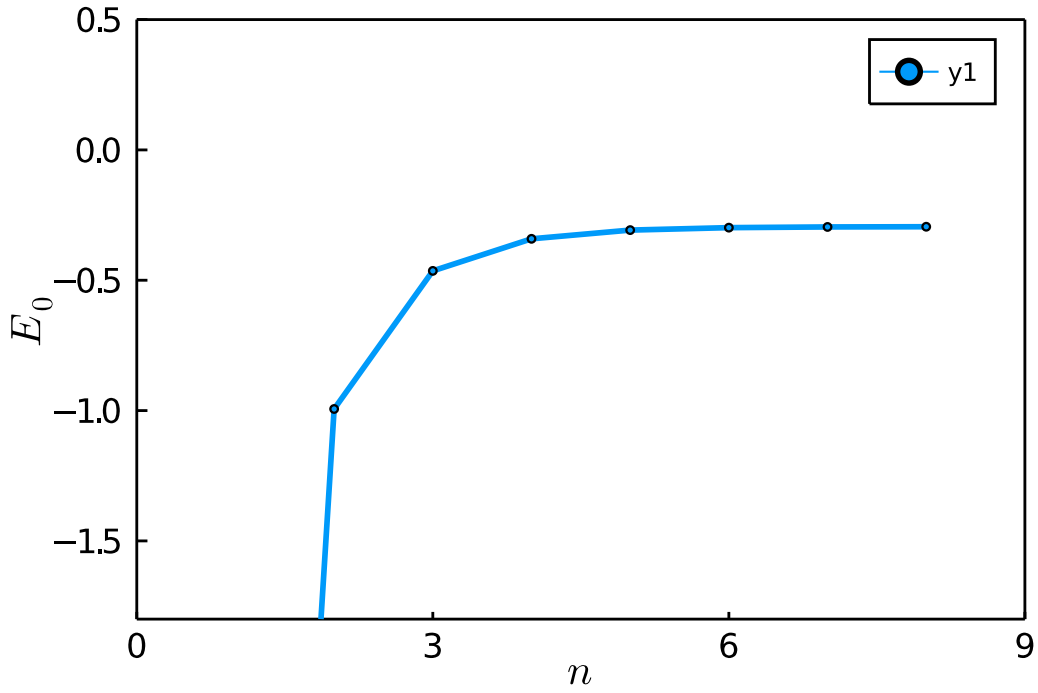

Figure 2: Convergence of the Local energy as a function of iterations.

3 Pure Diffusion Monte Carlo (PDMC)

The basic idea is the same, i.e. applying the power method to converge to the ground state. However, the integration over n is done stochastically as shown in Eq:16.

$$E_0 = \frac{E_L(i_0) + E_L(i_1) + E_L(i_2) + \dots}{1 + 1 + 1 + \dots} \tag{14}$$

$$E_1 = \frac{E_L(i_1)w_{i_0 i_1} + E_L(i_2)w_{i_1 i_2} + E_L(i_3)w_{i_2 i_3} + \dots}{w_{i_0 i_1} + w_{i_1 i_2} + w_{i_2 i_3} + \dots} \tag{15}$$

$$E_2 = \frac{E_L(i_2)w_{i_0 i_1}w_{i_1 i_2} + E_L(i_3)w_{i_1 i_2}w_{i_2 i_3} + E_L(i_4)w_{i_2 i_3}w_{i_3 i_4} + \dots}{w_{i_0 i_1}w_{i_1 i_2} + w_{i_1 i_2}w_{i_2 i_3} + w_{i_2 i_3}w_{i_3 i_4} + \dots} \tag{16}$$

3.1 A simple implementation of PDMC

3.1.1 Calculate Local Energy (E_L)

3.1.2 Calculate the probability ($P_{i \to j}$)

3.1.3 Calculate the weights ($w_{i_1 i_2}$)

3.1.4 Combine E_L and w_{ij} to do PDMC

The simulation requires the calculation of a markov chain $i_0, i_1, i_2, \dots$. This is generated by picking a random number ϵ and choosing $1, 2$, or 3 according to what 3ϵ is.

The iteration can begin with these as starting values. The output is given in shown in the Figure:3.

3.1.5 Conclusion

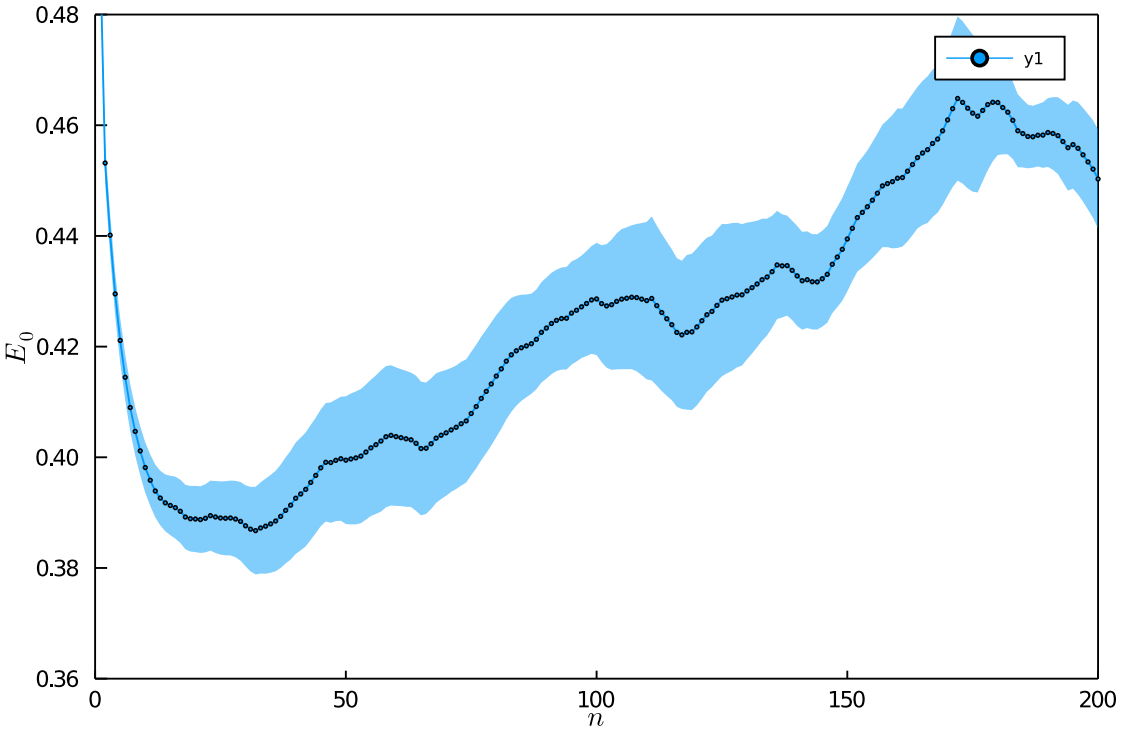

Figure 3: Convergence of the Local energy as a function of iterations(PDMC).