

# QMC Part I

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January 5, 2021

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## 1 Part I

## 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  $\nu$  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.

$$\begin{bmatrix} v_0 & -t \\ -t & v_1 \end{bmatrix} \quad (1)$$

$$\nu = c_0 \mathbf{u}_0 + c_1 \mathbf{u}_1 \quad (2)$$

The key idea is the realization that the ground state of the Hamiltonian 1 given by  $\mathbf{u}_0$  can be extracted from  $\nu$  by the repeated application of a filter  $G(H)$ . This filter systematically purifies  $\nu$  to obtain the ground state  $\mathbf{u}_0$  provided  $c_0 > 0$ , i.e. the trial vector  $\nu$  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 subtraction 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

$$\hat{G}(H) = \left( \mathbf{1} - \tau(\hat{H} - E_T \mathbf{1}) \right) \quad (3)$$

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

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

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

$$\nu^{(k+1)} = c_0(1 - \tau(E_0 - E_T))^{(k)} \mathbf{u}_0 + c_1(1 - \tau(E_1 - E_T))^{(k)} \mathbf{u}_1 \quad (5)$$

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.

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

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

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.

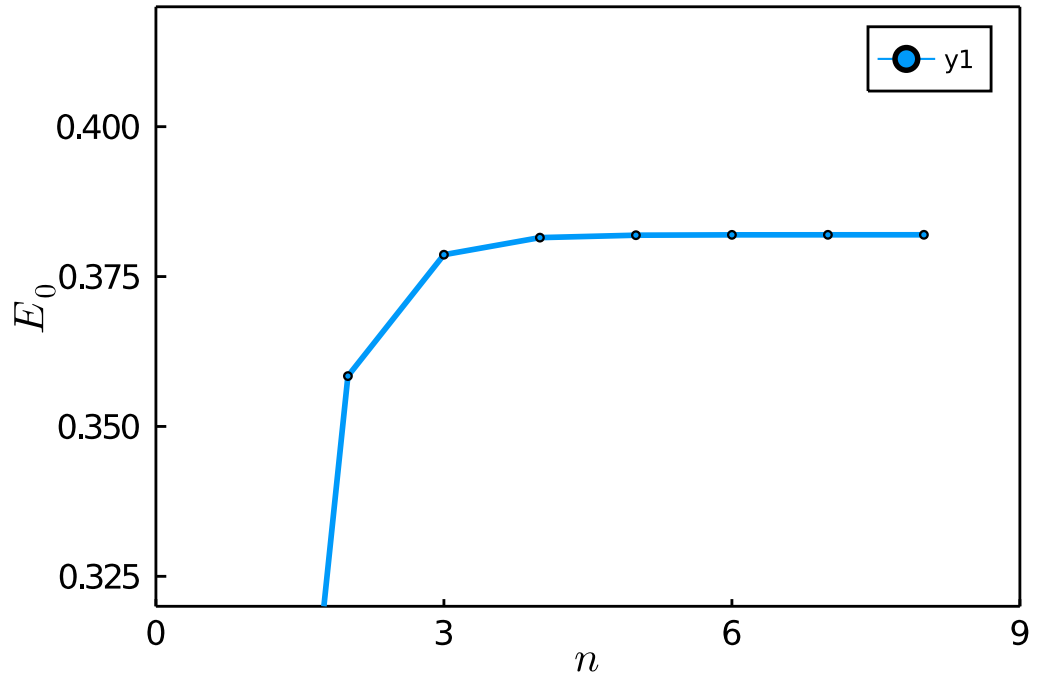


Figure 1: Convergence of the Local energy as a function of iterations.

## 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.

$$\begin{bmatrix} v_0 & -t & -t \\ -t & v_1 & -t \\ -t & -t & v_2 \end{bmatrix} \quad (8)$$

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

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

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.

$$\nu^{(k+1)} = c_0(1 - \tau(E_0 - E_T))^{(k)} \mathbf{u}_0 + c_1(1 - \tau(E_1 - E_T))^{(k)} \mathbf{u}_1 \quad (10)$$

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

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

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

```
\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_2=0.4082482904638631
nsteps=1024
```

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

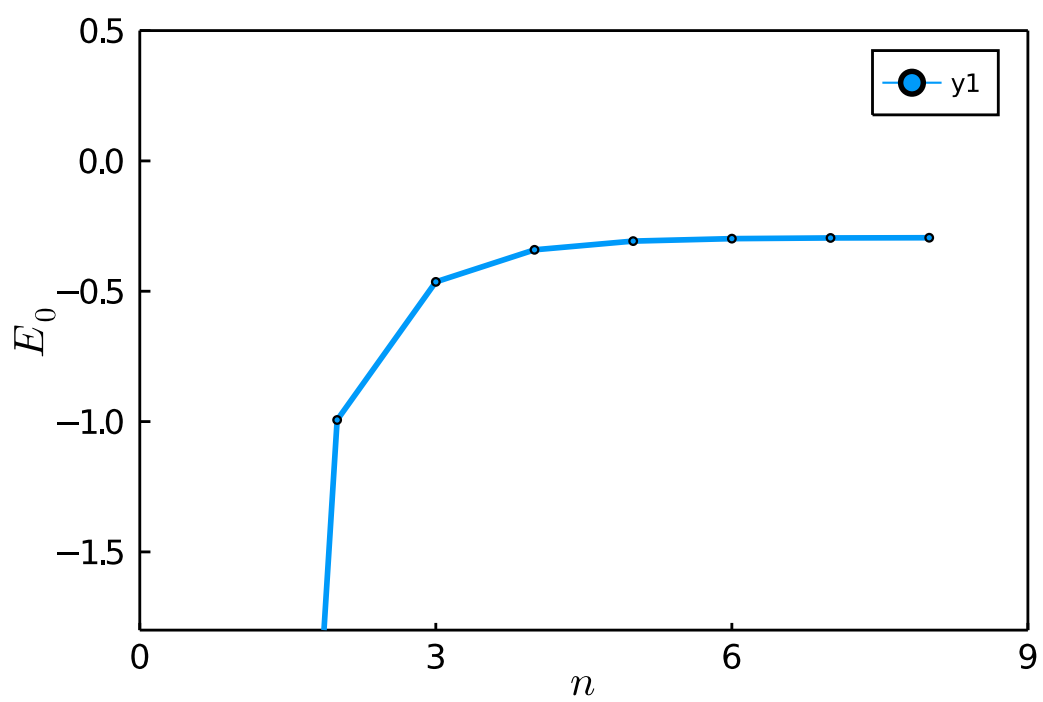


Figure 2: Convergence of the Local energy as a function of iterations.

### 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.

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

$$E_1 = \frac{E_L(i_1)w_{i_0i_1} + E_L(i_2)w_{i_1i_2} + E_L(i_3)w_{i_2i_3} + \dots}{w_{i_0i_1} + w_{i_1i_2} + w_{i_2i_3} + \dots} \quad (15)$$

$$E_2 = \frac{E_L(i_2)w_{i_0i_1}w_{i_1i_2} + E_L(i_3)w_{i_1i_2}w_{i_2i_3} + E_L(i_4)w_{i_2i_3}w_{i_3i_4} + \dots}{w_{i_0i_1}w_{i_1i_2} + w_{i_1i_2}w_{i_2i_3} + w_{i_2i_3}w_{i_3i_4} + \dots} \quad (16)$$

#### 3.1 A simple implementation of PDMC

##### 3.1.1 Calculate Local Energy ( $E_L$ )

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

##### 3.1.3 Calculate the weights ( $w_{i_1i_2}$ )

##### 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  $\epsilon$  and choosing 1, 2, or 3 according to what  $3\epsilon$  is.

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

##### 3.1.5 Conclusion

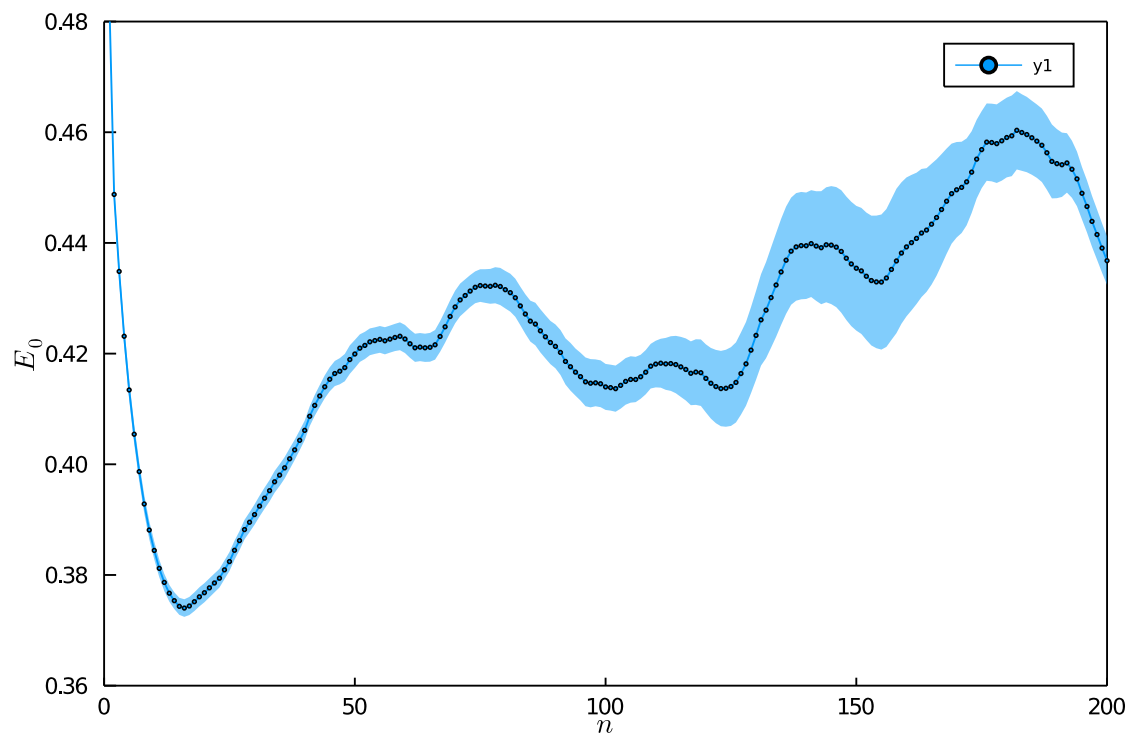


Figure 3: Convergence of the Local energy as a function of iterations(PDMC).