QMC Part I

Vijay Gopal Chilkuri

December 25, 2020

Contents

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 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.

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

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

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=0.7071067811865475
c_1=0.7071067811865475
```

The iteration can begin with these as starting values. The output is given in the table below.

```
10 0.8325345415688012 0.5539731375209688 0.384482692919926
20 0.8481318105729733 0.5297852696085559 0.3820169520382197
30 0.8502938016675892 0.5263083229872757 0.38196704124139036
40 0.8506000682828394 0.5258132024181487 0.38196603207543756
50 0.8506435939378749 0.5257427851073715 0.3819660116711711
60 0.8506497825205341 0.5257327719457557 0.3819660112586187
70 0.8506506624858821 0.5257313481354616 0.3819660112502773
80 0.8506507876108551 0.5257311456790742 0.38196601125010865
```