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

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

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.

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

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

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
```

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

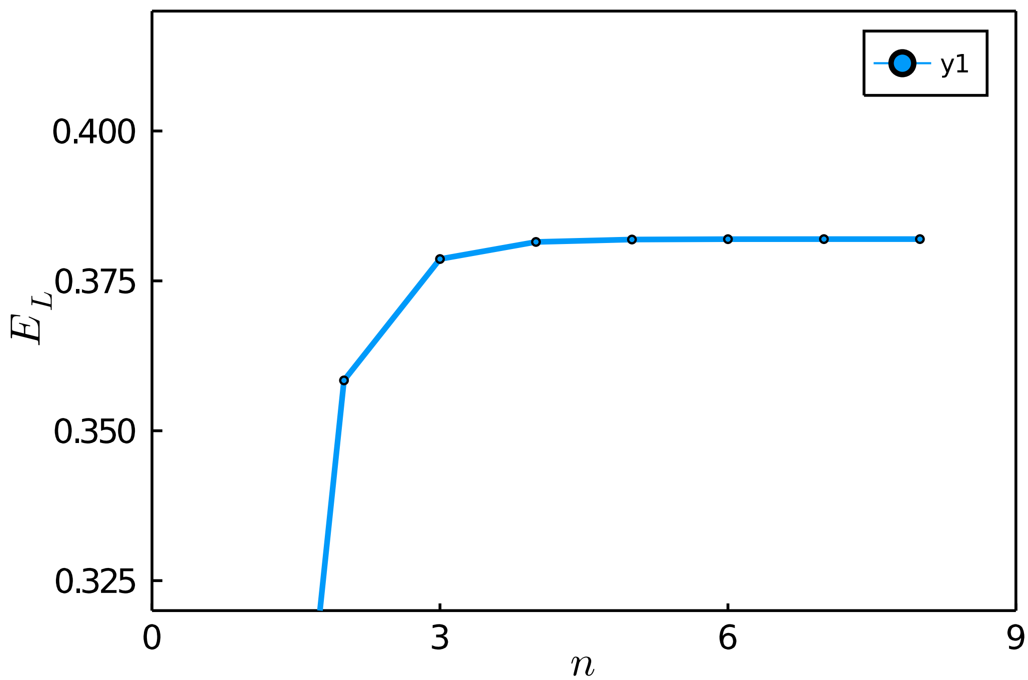

Figure 1: Convergence of the Local energy as a function of iterations.