Systematic improvement of neural network quantum states using Lanczos(Supplementary Material)

Hongwei Chen[1,2,3] **Douglas Hendry**[1] **Phillip Weinberg**[1] **Adrian E. Feiguin**[1]
[1]Department of Physics, Northeastern University, Boston, USA
[2]Stanford Institute for Materials and Energy Sciences, Stanford University, Stanford, USA
[3]Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, USA
{chen.hongw, hendry.d, p.weinberg, a.feiguin}@northeastern.edu

A Accuracy of ground state energy

To show the energy improvements from restoring different kinds of symmetry, we tried several variational wave functions ψ_s, $\psi_{\mathbf{K}}$, and $\psi_{\mathbf{K}\mathcal{L}}$. Their variational energies are shown in the table 1.

Table 1: The ground state energy per site for the 2D Heisenberg model($J_2 = 0$) on a 6×6, 8×8, and 10×10 square lattice obtained from the RBM wave function with different kinds of symmetries restored.

Lattice Size	6×6	8×8	10×10
ψ_s: Spin flip symmetry(SFS)	-0.67762	-0.67154	-0.66737
$\psi_{\mathbf{K}}$: SFS + Translational symmetry(TS)	-0.678844	-0.673425	-0.671288
$\psi_{\mathbf{K}\mathcal{L}}$ SFS + TS + Lattice point symmetry	-0.678868	-0.673482	-0.671519

B Derivation of the Lanczos recursion

Using ψ_0 and ψ_1 as new basis, the Hamiltonian will be a 2×2 symmetric matrix.

$$\begin{pmatrix} \langle H \rangle & (\langle H^2 \rangle - \langle H \rangle^2)^{1/2} \\ (\langle H^2 \rangle - \langle H \rangle^2)^{1/2} & \frac{\langle H^3 \rangle - 2\langle H^2 \rangle \langle H \rangle + \langle H \rangle^3}{\langle H^2 \rangle - \langle H \rangle^2}. \end{pmatrix} \tag{1}$$

Considering the most generic 2×2 symmetric matrix $\begin{pmatrix} a & c \\ c & b \end{pmatrix}$, the two eigenvalues of this matrix can be written as :

$$\varepsilon_1 = \frac{1}{2}[a + b - ((b-a)^2 + 4c^2)^{1/2}] \quad \text{and} \quad \varepsilon_2 = \frac{1}{2}[a + b + ((b-a)^2 + 4c^2)^{1/2}]. \tag{2}$$

Plugging the expressions for a, b, c, we obtain Eq.(14):

$$\varepsilon_1 = \frac{1}{2} \left(\langle H \rangle + \frac{\langle H^3 \rangle - 2\langle H^2 \rangle \langle H \rangle + \langle H \rangle^3}{\langle H^2 \rangle - \langle H \rangle^2} - \left((\frac{\langle H^3 \rangle - 3\langle H^2 \rangle \langle H \rangle + 2\langle H \rangle^3}{\langle H^2 \rangle - \langle H \rangle^2})^2 + 4(\langle H^2 \rangle - \langle H \rangle^2) \right)^{1/2} \right) \tag{3}$$

$$= \langle H \rangle + \frac{\langle H^3 \rangle - 3\langle H^2 \rangle \langle H \rangle + 2\langle H \rangle^3}{2(\langle H^2 \rangle - \langle H \rangle^2)} - (\langle H^2 \rangle - \langle H \rangle^2)^{1/2} \left((\frac{\langle H^3 \rangle - 3\langle H^2 \rangle \langle H \rangle + 2\langle H \rangle^3}{2(\langle H^2 \rangle - \langle H \rangle^2)^{3/2}})^2 + 1 \right)^{1/2} \tag{4}$$

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$$= \langle H\rangle + (\langle H^2\rangle - \langle H\rangle^2)^{1/2}\left[\frac{\langle H^3\rangle - 3\langle H^2\rangle\langle H\rangle + 2\langle H\rangle^3}{2(\langle H^2\rangle - \langle H\rangle^2)^{3/2}} - \left((\frac{\langle H^3\rangle - 3\langle H^2\rangle\langle H\rangle + 2\langle H\rangle^3}{2(\langle H^2\rangle - \langle H\rangle^2)^{3/2}})^2 + 1\right)^{1/2}\right]. \quad (5)$$

The corresponding eigenvector is $\begin{pmatrix}\psi_0\\ \alpha\psi_1\end{pmatrix}$, with

$$\alpha = \frac{b-a-\sqrt{(b-a)^2+4c^2}}{2c} = \left[\frac{\langle H^3\rangle - 3\langle H^2\rangle\langle H\rangle + 2\langle H\rangle^3}{2(\langle H^2\rangle - \langle H\rangle^2)^{3/2}} - \left((\frac{\langle H^3\rangle - 3\langle H^2\rangle\langle H\rangle + 2\langle H\rangle^3}{2(\langle H^2\rangle - \langle H\rangle^2)^{3/2}})^2 + 1\right)^{1/2}\right], \quad (6)$$

which is the explicit form of α in Eq.(18). Hence, the new improved eigenvector becomes

$$\tilde{\psi}_0 = \psi_0 + \alpha\psi_1. \quad (7)$$

Notice that $\tilde{\psi}_0$ is not normalized. The normalized form of $\tilde{\psi}_0$ is given by Eq.(15):

$$\tilde{\psi}_0 = \frac{1}{(1+\alpha^2)^{1/2}}\psi_0 + \frac{\alpha}{(1+\alpha^2)^{1/2}}\psi_1, \quad (8)$$