Thesis Work: Ergotropy and Quantum Phase Transitions

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Analitical Calculations

4.1 The XY Model ground state

Correlation Matrix Derivation

4.1.1 One Site

There are only two Majorana fermions: $\breve{a}_1$ and $\breve{a}_2$.
The one-site Hamiltonian is $-\frac{\lambda}{2}\sigma^z$
We write all the correlators in the form $\delta_{mn} + i\Gamma_{mn}$:

$$\langle \breve{a}_m \breve{a}_n \rangle = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \begin{bmatrix} 0 & g_0 \\ -g_0 & 0 \end{bmatrix} \tag{4.1}$$

Γ is already in the block diagonal form.
The density matrix ρ_1 has eigenvalues:

$$p_1 = (1 + g_0)/2 \quad p_2 = (1 - g_0)/2 \tag{4.2}$$

With g_0:

$$g_0 = \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{\lambda - \cos\phi + i \sin\phi}{|\lambda - \cos\phi + i\sin\phi|} = \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{\lambda - \cos\phi}{\sqrt{(\lambda - \cos\phi)^2 + \sin^2\phi}} \tag{4.3}$$

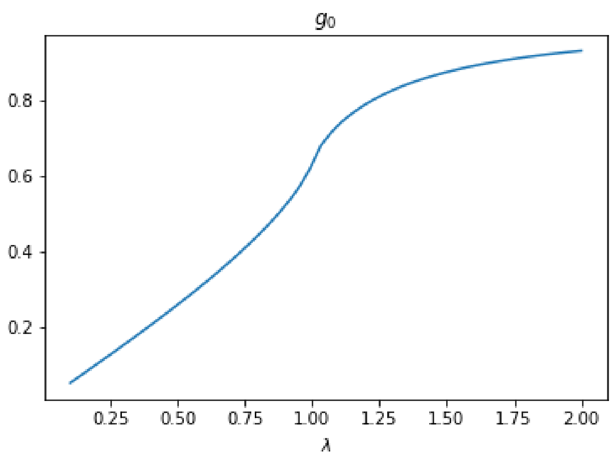

Figure 4.1

From the eigenvalues we can already calculate something:

- Purity:

$$\mathfrak{P}(1) = \sum_i (p_i)^2 = \frac{1 + g_0^2}{2} \tag{4.4}$$

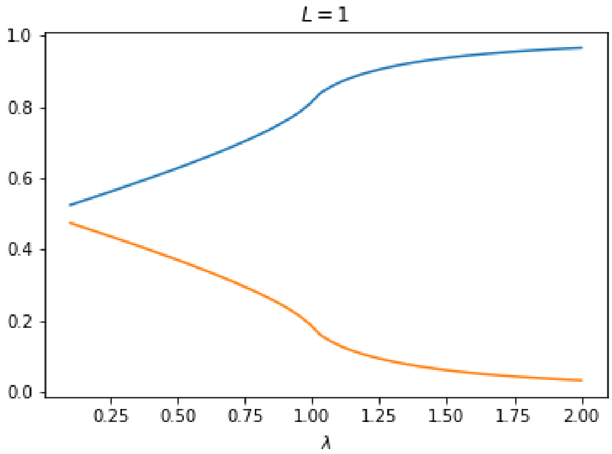

Figure 4.2: Eigenvalues of one-site density matrix

- Max-Ergo:

$$\mathcal{M}(1) = 2\sum_{i=1}^{D/2}\left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right)\left|\epsilon_i^{(\uparrow)}\right| = 2(p_1 - p_2)|e_1| = 2g_0\left|\frac{\lambda}{2}\right| \tag{4.5}$$

- Rescaled-Max-Ergo

$$\mathfrak{M}(\mathcal{I}) = g_0 \tag{4.6}$$

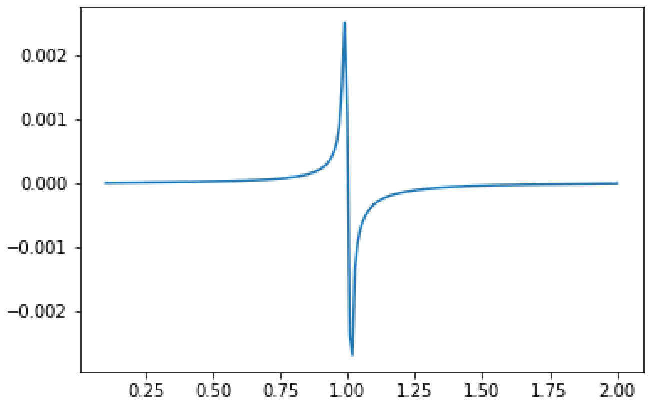

Figure 4.3: Second Derivative Ergotropy (g_0)

4.2 Two sites

Eigenvalues of the correlation matrix

$$\nu_{\pm} = \sqrt{\left(\frac{g_1 - g_{-1}}{2}\right)^2 + g_0^2} \pm \left|\frac{g_1 + g_{-1}}{2}\right| \tag{4.7}$$

$\nu_- < \nu_+$

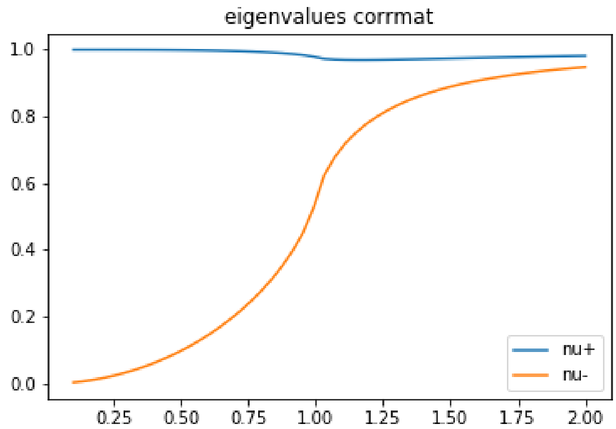

Figure 4.4

$$\langle \hat{c}_m \hat{c}_n \rangle = 0, \quad \langle \hat{c}_m^\dagger \hat{c}_n \rangle = \delta_{mn} \frac{1 + \nu_m}{2} \tag{4.8}$$

$$\left\langle g \left| c_j^\dagger c_j \right| g \right\rangle = \frac{1 + \nu_j}{2} \tag{4.9}$$

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.10}$$

Eigenvalues of 2 site Hamiltonian:

$$H = -\frac{1}{2}\left(\sigma^x \sigma^x + \lambda \sigma^z \sigma^0 + \lambda \sigma^0 \sigma^z\right) = \begin{pmatrix} -\lambda & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & \lambda \end{pmatrix} \tag{4.11}$$

$$\left\{-\frac{1}{2}\sqrt{1 + 4\lambda^2}, -\frac{1}{2}, \frac{1}{2}, , \frac{1}{2}\sqrt{1 + 4\lambda^2}\right\} \tag{4.12}$$

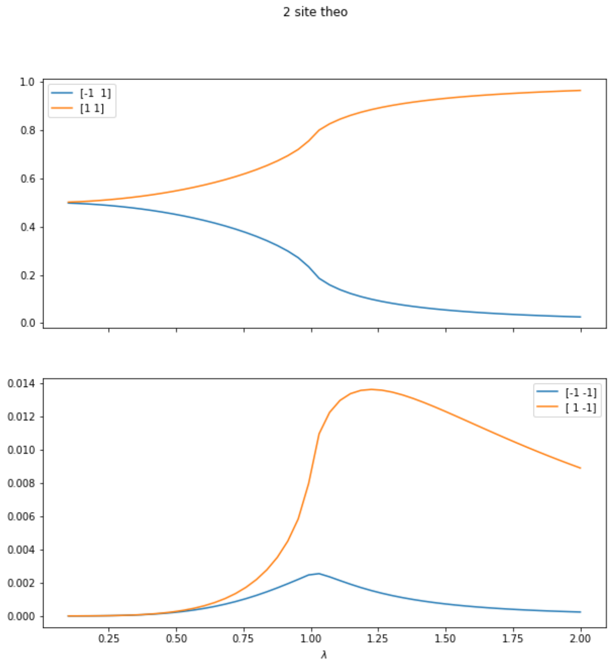

Figure 4.5: Eigenvalues of the 2-site density matrix

$$
\begin{aligned}
&\mathcal{M}(\mathcal{I}) = 2\sum_{i=1}^{2}\left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right)\left|\epsilon_i^{(\uparrow)}\right| \\
&\left(p_1^{(\downarrow)} - p_4^{(\downarrow)}\right)\left|\epsilon_1^{(\uparrow)}\right| + \left(p_2^{(\downarrow)} - p_3^{(\downarrow)}\right)\left|\epsilon_2^{(\uparrow)}\right| = \\
&(1/4)\left[(1+\nu_-)(1+\nu_+) - (1-\nu_-)(1-\nu_+)\right]\left(\sqrt{1+4\lambda^2}\right) + \\
&(1/4)\left[(1-\nu_-)(1+\nu_+) - (1+\nu_-)(1-\nu_+)\right] = \\
&\frac{(\nu_+ + \nu_-)}{2}\left(\sqrt{1+4\lambda^2}\right) + \frac{\nu_+ - \nu_-}{2}
\end{aligned}
\tag{4.13}
$$

Normalized:

$$
\mathfrak{M}(\mathcal{I}) = \frac{\mathcal{M}(\mathcal{I})}{2\left|\epsilon_1^{(\uparrow)}\right|} = \frac{(\nu_+ + \nu_-)}{2} + \frac{(\nu_+ - \nu_-)}{2\left(\sqrt{1+4\lambda^2}\right)} \tag{4.14}
$$

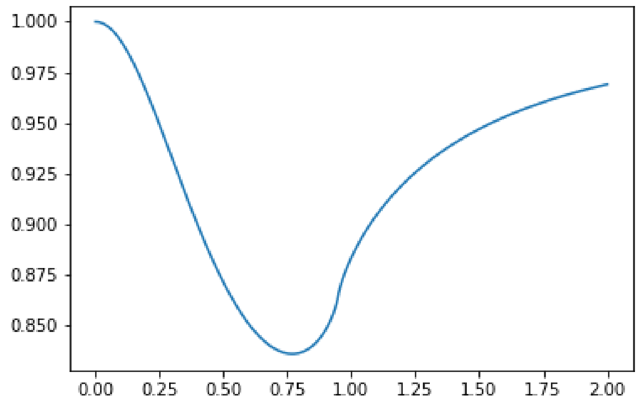

Figure 4.6: 2 Site Max-Ergotropy

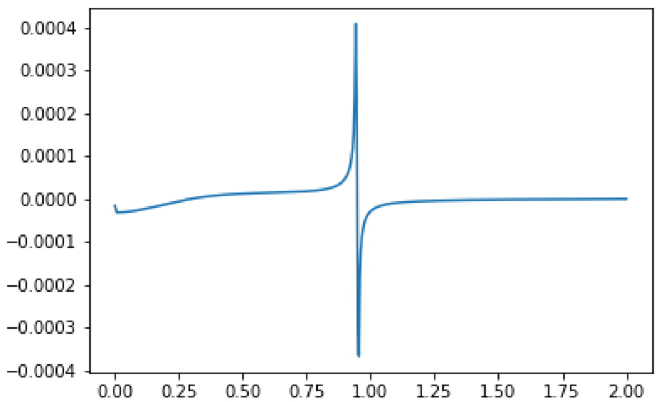

Figure 4.7: Second derivative 2 site Max-Ergotropy

4.2.1 Two distant sites

Let's try substituting g_1 with g_d with d distance between sites. Eigenvalues of the correlation matrix as in (PHYSICAL REVIEW A 78, 052302 2008)

$$\nu_\pm = \sqrt{\left(\frac{g_d - g_{-d}}{2}\right)^2 + g_0^2} \pm \left|\frac{g_d + g_{-d}}{2}\right| \tag{4.15}$$

Eigenvalues of the density matrix:

$$p_{\pm\pm} = (1 \pm \nu_-)(1 \pm \nu_+)/4 \tag{4.16}$$

Eigenvalues of distant Hamiltonian:

$$H_{dist} = -(\lambda/2)(\sigma_l^z \sigma_{l+d}^0 + \sigma_l^0 \sigma_{l+d}^z) \tag{4.17}$$

$$\text{eigs} = \{-\lambda, 0, 0, \lambda\} \tag{4.18}$$

Normalized-Max-Ergo: (the two eigenvalues of the Hamiltonian are the same, so we simplify)

$$\mathfrak{M}(\mathcal{I}) = \sum_{i=1}^{2} \left(p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)}\right) = \frac{(\nu_+ + \nu_-)}{2} + \frac{(\nu_+ - \nu_-)}{2} \tag{4.19}$$

Chapter 5

Numerical Simulations

5.1 Exact Diagonalization

5.2 DMRG

Chapter 6

Conclusions