Notes on:
Alfredo Bartiromo Thesis work

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Comment October 7: a possible now measure

Let us start by setting the problem. We consider a many-body system of N sites coupled by an Hamiltonian H that includes both local and two-particle interactions (more specifically in what follows we shall focus on translationally invariant linear chain couplings with first-neighbouring interactions, even more specifically we shall consider a linear Ising Model Hamiltonian (IMH) coupling). Suppose that H depends upon a parameter λ which identifies different phases of the model (in the case of the IMH, for instance λ is associated with the intensity of an external, uniform magnetic field). Our goal is to try to characterize the different phases (and in particular the possible arising of Quantum Phase Transitions) via the study of Ergotropy functional of subpart of the system.

Accordingly given $|\Psi_g\rangle$ the ground state of the H (which for the moment we assume to be not degenerate) we consider the reduced density matrix $\rho_{\mathcal{I}}$ of a subset $\mathcal{I}$ of the sites the model – typically $\mathcal{I}$ will contain L neighbouring sites, but in general we can assume it to be formed by an arbitrary collection of particles which are not necessarily directly connected. Indicating with $\bar{\mathcal{I}}$ the sites of the model which do not belong to $\mathcal{I}$, we can decompose the total Hamiltonian H as

$$H = H_{\mathcal{I}} + H_{\bar{\mathcal{I}}} + H_{int} \; , \tag{1}$$

where $H_{\mathcal{I}}$ and $H_{\bar{\mathcal{I}}}$ include respectively all the Hamiltonian terms which only involves elements of $\mathcal{I}$ and $\bar{\mathcal{I}}$ respectively and with H_{int} the coupling among the two sets. Introduce now the spectral decompositions of $\rho_{\mathcal{I}}$ and $H_{\mathcal{I}}$, i.e.

$$\rho_{\mathcal{I}} = \sum_i p_i^{(\downarrow)} |i\rangle\langle i| \;, \qquad H_{\mathcal{I}} = \sum_i \epsilon_i^{(\uparrow)} |e_i\rangle\langle e_i| \;, \tag{2}$$

with $\{|i\rangle\}$ and $\{|e_i\rangle\}$ the eigenvectors of $\rho_{\mathcal{I}}$ and $H_{\mathcal{I}}$, and with $\{p_i^{(\downarrow)}\}$ $\{\epsilon_i^{(\uparrow)}\}$ the associated eigenvalues listed in decreasing and increasing order respectively, i.e.

$$p_i^{(\downarrow)} \geq p_{i+1}^{(\downarrow)} \;, \qquad \epsilon_i^{(\uparrow)} \leq \epsilon_{i+1}^{(\uparrow)} \;. \tag{3}$$

We hence define the passive $\rho_{\mathcal{I}}^{(pass)}$ and the anti-passive $\rho_{\mathcal{I}}^{(a-pass)}$ counterparts of $\rho_{\mathcal{I}}$ as the density matrices

$$\rho_{\mathcal{I}}^{(pass)} = \sum_i p_i^{(\downarrow)} |e_i\rangle\langle e_i| \;, \qquad \rho_{\mathcal{I}}^{(a-pass)} = \sum_i p_i^{(\uparrow)} |e_i\rangle\langle e_i| \;, \tag{4}$$

with $p_i^{(\uparrow)}$ a re-organization of the elements of $p_i^{(\downarrow)}$ in increasing order, i.e.[1]

$$p_i^{(\uparrow)} \leq p_{i+1}^{(\uparrow)} \;. \tag{5}$$

The associated energy expectation values are then

$$\begin{aligned} E(\rho_{\mathcal{I}}) &= \mathrm{Tr}[H_{\mathcal{I}}\rho] = \sum_{i,j} p_i^{(\downarrow)} \epsilon_j^{(\uparrow)} |\langle i|e_j\rangle|^2 \;, && (6)\\ E(\rho_{\mathcal{I}}^{(pass)}) &= \mathrm{Tr}[H_{\mathcal{I}}\rho_{\mathcal{I}}^{(pass)}] = \sum_i p_i^{(\downarrow)} \epsilon_i^{(\uparrow)} \;, && (7)\\ E(\rho_{\mathcal{I}}^{(a-pass)}) &= \mathrm{Tr}[H_{\mathcal{I}}\rho_{\mathcal{I}}^{(a-pass)}] = \sum_i p_i^{(\uparrow)} \epsilon_i^{(\uparrow)} \;, && (8) \end{aligned}$$

which fulfil the following trivial inequalities

$$E(\rho_{\mathcal{I}}^{(pass)}) \leq E(\rho_{\mathcal{I}}) \leq E(\rho_{\mathcal{I}}^{(a-pass)}) \;. \tag{9}$$

[1]The notion of passive and anti-passive state are well defined only when $H_{\mathcal{I}}$ has spectrum which is not degenerate: this however does not affect the value of $\mathcal{E}(\mathcal{I})$, $E(\rho^{(pass)})$, and $E(\rho^{(pass)})$ which are always well behaved.

The ergotropy is the (positive) gap between the first two

$$\begin{aligned}\mathcal{E}(\mathcal{I}) &\equiv E(\rho_{\mathcal{I}}) - E(\rho^{(pass)}) = \sum_{i,j} p_i^{(\downarrow)} \epsilon_j^{(\uparrow)} |\langle i|e_j\rangle|^2 - \sum_i p_i^{(\downarrow)} \epsilon_i^{(\uparrow)} \\ &= \sum_{i,j} p_i^{(\downarrow)} \epsilon_j^{(\uparrow)} (|\langle i|e_j\rangle|^2 - \delta_{ij}) \;, \end{aligned} \tag{10}$$

the anti-ergotropy the (positive) gap between the last two

$$\mathcal{A}(\mathcal{I}) \equiv E(\rho_{\mathcal{I}}^{(a-pass)}) - E(\rho_{\mathcal{I}}) = \sum_i p_i^{(\uparrow)} \epsilon_i^{(\uparrow)} - \sum_{i,j} p_i^{(\downarrow)} \epsilon_j^{(\uparrow)} |\langle i|e_j\rangle|^2 \;, \tag{11}$$

while finally the max-ergo is the (positive) gap between the last and the first term, i.e. the quantity

$$\begin{aligned}\mathcal{M}(\mathcal{I}) &\equiv E(\rho_{\mathcal{I}}^{(a-pass)}) - E(\rho_{\mathcal{I}}^{(pass)}) = \mathcal{E}(\mathcal{I}) + \mathcal{A}(\mathcal{I}) \\ &= \sum_i (p_i^{(\uparrow)} - p_i^{(\downarrow)}) \epsilon_i^{(\uparrow)} \;. \end{aligned} \tag{12}$$

Some observations: in case the dimension D of the Hilbert space of $\mathcal{I}$ is even then we can express $\mathcal{M}(\mathcal{I})$ as follows

$$\mathcal{M}(\mathcal{I}) = \sum_{i=1}^{D/2} (p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)})(\epsilon_{D-i+1}^{(\uparrow)} - \epsilon_i^{(\uparrow)}) \;, \tag{13}$$

if instead D is odd we have

$$\mathcal{M}(\mathcal{I}) = \sum_{i=1}^{(D-1)/2} (p_i^{(\downarrow)} - p_{D-i+1}^{(\downarrow)})(\epsilon_{D-i+1}^{(\uparrow)} - \epsilon_i^{(\uparrow)}) \;. \tag{14}$$

From the above identities it hence follows that $\mathcal{M}(\mathcal{I})$ is always upper bounded by the maximum gap in the spectrum of $H_{\mathcal{I}}$ and lower bounded by 0,

$$0 \leq \mathcal{M}(\mathcal{I}) \leq \epsilon_D^{(\uparrow)} - \epsilon_1^{(\uparrow)} \;, \tag{15}$$

the first inequality been saturated when $\rho_{\mathcal{I}}$ is the completely mixed density operator, and the second one when $\rho_{\mathcal{I}}$ instead is a pure state. This quantity is hence very sensitive to the degree of mix-ness of the state $\rho_{\mathcal{I}}$ and motivates us to introduce the following rescaled measure

$$\mathfrak{M}(\mathcal{I}) \equiv \frac{\mathcal{M}(\mathcal{I})}{\epsilon_D^{(\uparrow)} - \epsilon_1^{(\uparrow)}} \in [0,1] \;. \tag{16}$$

To do list:

1. since the computation of $\mathcal{E}(\mathcal{I})$, $\mathcal{A}(\mathcal{I})$, and $\mathfrak{M}(\mathcal{I})$ strongly depends upon the spectrum of $H_{\mathcal{I}}$, it would be helpful to compute it for the cases we are considering (i.e. for $L = 2$, $L = 3$, etc).

2. As we discussed in the Skype conversation, if H admits a degenerate groundstate level, clearly there is a fundamental ambiguity in the our analysis (simply we do not know how to selected $|\psi_g\rangle$, and different choices of such vector could lead to different results). One way to address this issue is to remove the degeneracy by adding external perturbation which brake the symmetry of the problem. By the way: what it is known regarding the degeneracy of the IMH ground state? Do we have degeneracy at $\lambda = 0$ only or such effect persist also at higher values of the parameter λ? (It seems to me that only the $\lambda = 0$ case is explicitly degenerate – if this is the case however I do not understand why the discrepancy between the plots by Alfredo and Davide persists for all the region $\lambda < 1$ instead of being just confined around $\lambda \sim 0$ (any comment for this?).

   The other option would be to look for the best choice of $|\psi_g\rangle$ which yields the best signature of the phase transition point (but this I guess is rather combersome).

3. beside computing $\mathcal{E}(\mathcal{I})$, $\mathcal{A}(\mathcal{I})$, and $\mathfrak{M}(\mathcal{I})$ it would be interesting to compare the latter with the purity of $\rho_{\mathcal{I}}$, i.e. the quantity $\mathfrak{P}(\mathcal{I}) = \sum_i (p_i^{(\downarrow)})^2$ (which is an explicit measure of entanglement).

Comment October 8

About the symmetry of the spectrum of $H_{\mathcal{I}}$

Assume the spectrum of $H_{\mathcal{I}}$ is symmetric under sign inversion (a case which I think applies for the IMH model, isn't it?), so that

$$\epsilon_{D-i+1}^{(\uparrow)} = -\epsilon_i^{(\uparrow)} \quad \forall i = 1, \cdots, D/2 , \tag{17}$$

when D even, and

$$\begin{aligned} \epsilon^{(\uparrow)}_{D-i+1} &= -\epsilon^{(\uparrow)}_i \quad \forall i = 1, \cdots, (D-1)/2 && (18) \\ \epsilon^{(\uparrow)}_{(D+1)/2} &= 0 \,, && (19) \end{aligned}$$

when D odd. Under this circumstance Eqs. (13) and (14) get simplified as

$$\begin{aligned} \mathcal{M}(\mathcal{I}) &= 2\sum_{i=1}^{D/2}(p^{(\downarrow)}_i - p^{(\downarrow)}_{D-i+1})|\epsilon^{(\uparrow)}_i| \,, \qquad \text{(for } D \text{ even)} && (20) \\ \mathcal{M}(\mathcal{I}) &= 2\sum_{i=1}^{(D-1)/2}(p^{(\downarrow)}_i - p^{(\downarrow)}_{D-i+1})|\epsilon^{(\uparrow)}_i| \,, \qquad \text{(for } D \text{ odd)} && (21) \end{aligned}$$

while Eq. (16) becomes

$$\mathfrak{M}(\mathcal{I}) \equiv \frac{\mathcal{M}(\mathcal{I})}{2|\epsilon^{(\uparrow)}_1|} \in [0,1] \,. \tag{22}$$

0.1 Some considerations regarding the choice of $\mathcal{I}$.

We said that $\mathcal{I}$ contains L sites. Till now we have implicitly assumed that such sites will form a cluster of connected elements. Of course this is not strictly mandatory and we should try to see what happens under this assumption.

1. First of all, even though we do not expect this case to be particularly interesting for our purposes let's also include the trivial case where $L = 1$ and the the Hamiltonian $H_{\mathcal{I}}$ becomes $-\frac{\lambda}{2}\sigma^z$. Here everything should be easily computable, so let try it.

2. For $L = 2$, besides the case where the two sites are first neighbours let's also discuss the scenario where their distance is $k \geq 2$ for all possible values of k. Once more $H_{\mathcal{I}}$ will only contains local terms of the form $-\frac{\lambda}{2}\sigma^z$, but of course $\rho_{\mathcal{I}}$ will depends upon k do to the correlations in the ground state $|\psi_g\rangle$. Let's see if our functionals can still keep track of the quantum phase transition. I expect the calculation to be fully analytical in this case.

3. For $L = 3$ the scenario becomes slightly more complex as now we have two distance parameter to account for k_1, and k_2.