Quantum phase transition in a far from equilibrium steady state of XY spin chain

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Using quantization in the Fock space of operators we compute the non-equilibrium steady state in an open Heisenberg XY spin 1/2 chain of finite but large size coupled to Markovian baths at its ends. Numerical and theoretical evidence is given for a far from equilibrium quantum phase transition with spontaneous emergence of long-range order in spin-spin correlation functions, characterized by a transition from saturation to linear growth with the size of the entanglement entropy in operator space.

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Non-perturbative physics of many-body open quantum systems far from equilibrium is largely an unexplored field. In one-dimensional locally interacting quantum systems equilibrium phase transitions—quantum phase transitions (QPT)—can occur at zero temperature only and are by now well understood [1]. QPT are typically characterized by vanishing of the Hamiltonian’s spectral gap in the thermodynamic limit at the critical point, and (logarithmic) enhancement of the entanglement entropy and other measures of quantum correlations in the ground state [2]. Much less is known about the physics of QPT out of equilibrium, studies of which have been usually limited to near equilibrium regimes or using involved and approximate analytical techniques (e.g. [3, 4]).

There exist two general theoretical approaches to a description of non-equilibrium open quantum systems, namely the non-equilibrium Green’s function method [5], and the quantum master equation [6, 7]. In this Letter we adopt the latter and present a quasi-exactly solvable example of an open Heisenberg XY spin 1/2 chain exhibiting a novel type of phase transition far from equilibrium; characterized by a sudden appearance of long-range magnetic order in non-equilibrium steady state (NESS) as the magnetic field is reduced, and the transition from saturation to linear growth with size of the operator space entanglement entropy (OSEE) of NESS.

The Hamiltonian of the quantum XY chain reads

\[ H = \sum_{m=1}^{n-1} \left( \frac{1 - \gamma}{2} \sigma^x_m \sigma^x_{m+1} + \frac{1 - \gamma}{2} \sigma^y_m \sigma^y_{m+1} \right) + \sum_{m=1}^{n} h \sigma^+_m \]  

(1)

where \( \sigma^x, \sigma^y, \sigma^z \) are Pauli operators acting on a string of n spins. We may assume that parameters \( \gamma \) (anisotropy) and \( h \) (magnetic field) are non-negative. It is known that XY model [1] exhibits (equilibrium) critical behavior in the thermodynamic limit \( n \rightarrow \infty \) along the lines: \( \gamma = 0, h \leq 1 \), and \( h = 1 \). Here we consider an open XY chain whose density matrix evolution \( \rho(t) \) is governed by the Lindblad master equation [8] (we set \( h = 1 \))

\[ \frac{d \rho}{dt} = \mathcal{L} \rho := -i[H, \rho] + \sum_{\mu=1}^{M} \left( 2L_\mu \rho L^\dagger_\mu - \{ L^\dagger_\mu L_\mu, \rho \} \right) \]  

(2)

and study a phase transition in NESS. The simplest non-trivial bath (Lindblad) operators acting only on the first and the last spin are chosen \( (M = 4) \)

\[ L_{1,2} = \sqrt{\Gamma^+_2} \sigma^+_1, \quad L_{3,4} = \sqrt{\Gamma^+_4} \sigma^+_3, \]  

(3)

where \( \sigma^+_m = (\sigma^x_m + i \sigma^y_m) / 2 \) [3]. For \( h \gg 1 \), the ratios \( \Gamma^+_2 / \Gamma^+_4 = \exp(-2h/T_L) \) are simply related to canonical temperatures of the end spins \( T_L = \lambda, L, R \).

Note that Lindblad equation [2] can be rigorously derived within the so-called Markov approximation [7] which is justified for macroscopic baths with fast internal relaxation times. As shown in [9], Eq. [2] with [13] can be solved exactly in terms of normal master modes (NMM) which are obtained from diagonalization of \( 4n \times 4n \) matrix \( A \) written in terms of \( 4 \times 4 \) blocks

\[ A_{l,m} = \delta_{l,m} \left( -2hR_0 + \delta_{l,1} B_{1L} + \delta_{l,3} B_{R} \right) \]  

(4)

\[ + \delta_{l+1,m} R_\gamma - \delta_{l-1,m} R^T_\gamma, \quad l, m = 1, \ldots, n, \]

where \( R_\gamma = 1_2 \otimes (i \sigma^y - \gamma \sigma^z) / 2 \) and \( B_\lambda = -\frac{1}{2} (\Gamma^+_2 + \Gamma^+_4) \sigma^y \otimes 1_2 + \frac{1}{2} (\Gamma^+_2 - \Gamma^+_4) (\sigma^z + i \sigma^x) \otimes \sigma^y \).

Following [9], the key concept is 4\textsuperscript{th} dimensional Fock space of operators \( \mathcal{K} \) spanned by an orthonormal basis \( \{ P_{a_1 a_2 \ldots a_{2n}} : w^{a_1} w^{a_2} \ldots w^{a_{2n}}, a_j \in \{0,1\} \} \) where \( w^{a_{2m-1}} = \sigma^z_m \prod_{m' < m} \sigma^z_{m'} \), \( w^{a_{2m}} = \sigma^y_m \prod_{m' < m} \sigma^y_{m'} \) are 2n anticommuting Majorana operators \( \{ w_j, w_k \} = 2 \delta_{j,k} \).

We introduce canonical adjoint Fermi maps over \( \mathcal{K} \), defined as \( \hat{c}_j | P_{2 \lambda} \rangle = \delta_{j\lambda} | w_j P_{2 \lambda} \rangle \), so the quantum Liouvillian [4] becomes bilinear \( \hat{\mathcal{L}} = \hat{A} \cdot \hat{A} + \text{const} \mathbb{I} \) in Hermitian maps \( \hat{a}_{2j-1} = \frac{1}{\sqrt{2}} (\hat{c}_j + \hat{c}^+_j), \hat{a}_{2j} = \frac{1}{\sqrt{2}} (\hat{c}_j - \hat{c}^+_j), \) satisfying \( \{ \hat{a}_p, \hat{a}_q \} = \delta_{pq} \hat{\rho} \).

Note that the eigenvalues of \( 4n \times 4n \) antisymmetric matrix \( A \) [4] called rapidities come in pairs \( \beta_j, -\beta_j, -\beta_{2n}, \ldots, -\beta_{2n-2}, -\beta_2, -\beta_1 \), \( \beta_j > 0 \). The corresponding eigenvectors \( v_p, p = 1, \ldots, 4n \), defined by \( A v_{2j-1} = \beta_j v_{2j-1}, A v_{2j} = -\beta_j v_{2j}, \) can always be normalized as \( \langle v_{2j-1} | v_{2j-1} \rangle = 1 \) and \( \langle v_{2j} | v_{2j} \rangle = 0 \) otherwise.

Writing NMM maps as \( \beta_j = \sum_{p=1}^{2n} \hat{v}_j v_p \hat{b}^*_p \), \( \hat{b}_j = \hat{b}^*_j \hat{\rho} \langle \hat{b}_j \hat{\rho} | \hat{b}^*_j \hat{\rho} \rangle = \delta_{j,k} \), the Liouvillian [4] takes the normal form, \( \hat{\mathcal{L}} = -\sum_{j=1}^{2n} \beta_j \hat{b}_j \hat{b}^*_j \). Thus a complete set of 4\textsuperscript{th} eigenvalues of \( \hat{\mathcal{L}} \) (real parts being the relaxation rates) can be constructed as \( -2 \sum_{j=1}^{2n} v_j \beta_j \) where \( v_j \in \{0,1\} \) are eigenvalues of \( 2n \) mutually commuting, non-hermitian number operators \( \hat{b}_j \hat{b}^*_j \).
Let $\rho_{\text{NESS}}$ be the element of $K$ corresponding to the stationary solution $\rho_{\text{NESS}}$ (NESS) of Eq. (2), i.e., zero eigenvalue of $\hat{\mathcal{L}}$, $\nu_j \equiv 0$. The main result of [9] (Th. 3) takes into account the fact that $\rho_{\text{NESS}}$ is a right-vacuum of $\hat{\mathcal{L}}$ – the left-vacuum being the trivial identity-state $|1\rangle$ – and asserts that any quadratic physical observable can be explicitly computed in terms of eigenvectors $\nu_{\rho}$, 

$$\text{tr}(w_j w_k \rho_{\text{NESS}}) = \delta_{j,k} + \langle 1 | \epsilon_j \epsilon_k | \text{NESS} \rangle,$$

Higher order observables can be computed using the Wick theorem. For example, noting $\sigma_n^2 = -iw_{2m-1}w_{2m}$, spin-spin correlator which we shall study later reads

$$C_{l,m} = \text{tr}(\sigma_l \sigma_m \rho_{\text{NESS}}) - \text{tr}(\sigma_l \rho_{\text{NESS}}) \text{tr}(\sigma_m \rho_{\text{NESS}}) \quad (6)$$

As proven in [9], NESS is unique if rapidity spectrum is non-degenerate, $\beta_j \neq 0$ for all $j$, and (almost) any initial state approaches NESS asymptotically exponentially with the rate $\Delta = 2 \text{ min} \Re \beta_j$ if $\Delta > 0$.

Let us now proceed to detailed analytical and numerical investigation of the structure of NESS in XY chain. The bulk spectrum of rapidities for $n \to \infty$ is insensitive to the coupling to the baths and is given by $\beta = \pm i \epsilon(\phi)$, $\phi \in (-\pi, \pi]$ where

$$\epsilon(\phi) = \sqrt{(\cos \phi - h)^2 + \gamma^2 \sin^2 \phi}$$

is the quasi-particle dispersion relation in an infinite XY chain (see e.g., [10]). For a finite chain [11] with the bath coupling on the edges [3] we find that the bulk (nearly continuous) rapidity spectrum gains a small never-vanishing real part $\Re \beta(\phi) = O(n^{-1})$. At the spectral edges $\beta^*, \beta^* \epsilon(\phi^*)$, with $\phi^*$ defined by $d\epsilon(\phi^*)/d\phi = 0$, the gap is actually much smaller $\Re \beta^* = O(n^{-3})$ (analytical result, generalizing [9]). Thus, the asymptotic relaxation time to NESS $1/\Delta = O(n^3)$ diverges in the thermodynamic limit $n \to \infty$.

We note, however, that the structure of the quasi-particle spectrum $\epsilon(\phi)$ qualitatively changes as the magnetic field crosses a critical value

$$h_c(\gamma) = 1 - \gamma^2,$$

namely for $h < h_c$ the minimal quasi-particle energy exists for a nontrivial value of quasi-momentum $\phi^* = \arccos[h/h_c(\gamma)]$ yielding a new, non-trivial band edge $\beta^*$, whereas for $h > h_c$ the band edges can exist only at points $\phi^* = 0, \pi$ (see Fig. 1). Consequently, complex rapidities of an open XY chain shape up a third condensation point near the imaginary axis for $h < h_c$ which is composed of NMMs (eigenvectors of $A$) with pseudo-momenta near $\phi^* \neq 0, \pi$ and has a dramatic effect on the structure of NESS as we demonstrate below.

Indeed, as $h < h_c$, we find the emergence of long range magnetic correlations (LRMC) characterized by non-decaying structures in the correlation matrix $C_{l,m}$ [10]. Typical size $\ell$ of the correlation patches is of the or-
der $\ell \sim 1/\phi^*$ (Fig. 2). For $h \approx h_c$ one finds critical scaling $\phi^* \approx 2(1-h_c/h_c)^{-1/2}$ which agrees with the data.

In the critical case $h = h_c$ (see Fig. 3) one finds power-law decay of the correlation matrix $C_{\ell,m} \sim |l-m|^{-\xi}$ if neglecting finite size/boundary effects. If we scale the distance we find numerically a finite size scaling $nC_{\ell,m} \sim |l-m|^{-\xi}$ if neglecting finite size/boundary effects. If we scale the distance we find numerically a finite size scaling $nC_{\ell,m} \sim |l-m|^{-\xi}$ if neglecting finite size/boundary effects.

For $h > h_c$, we have $\phi^* = 0$ and no LRMC in NESS. Then one finds an exponential decay of the correlation matrix $C_{\ell,m} \sim \exp(-|l-m|/\xi)$ with the localization length which can be estimated from a scattering problem defined by the matrix $\hat{H}$:

$$\xi^{-1} = 4 \cosh^{-1}(h/h_c) \approx 4[2(h-h_c)/|h_c|]^{1/2} \quad (9)$$

where factor 4 reflects the fact that $C_{\ell,m}$ is a 4-point function in NMM amplitudes $\xi_p$ (see Fig. 3).

The above results are summarized in a nonequilibrium phase diagram of XY chain (Fig. 8) showing the residual correlator $C_{\ell,m} = \sum_{l,m} |l-m| \cdot n^{2 \ell} / \sum_{l,m} |l-m|^{n^2/2} \pi$ (which is found to be always negative) in the $\gamma$-plane, with the critical curve $h_c(\gamma)$ separating the two phases. Note that the other boundary lines $\gamma = 0$ (XX chain) and $h = 0$ (XY with zero field) are not in LRMC phase.

In analogy to equilibrium QPTs \cite{11,12}, we wish to characterize the non-equilibrium transition in terms of quantum information theoretic concept, namely with the difficulty of classical simulation of $\rho_{\text{NESS}}$ which is described in terms of QSEE \cite{13} (or block-entropy in $K$), i.e. von Neumann entropy $S(n) = - \text{tr} \rho_{[n/2]} \log_2 \rho_{[n/2]}$ of the reduced density matrix of a half-chain $\rho_{[n/2]} = \text{tr}_{[n/2+1,n]}(\rho_{[n/2+1,n]}|\text{NESS})$. $\rho_{[n/2]}$ corresponds to a partial trace over the sublattice $[j,k]$. Straightforward calculation, combining Refs. \cite{11,12}, results in $S(n) = -\sum_{j=1}^{n} (\frac{2}{n} + \eta_j) \log_2 (\frac{2}{n} + \eta_j) + (\frac{2}{n} - \eta_j) \log_2 (\frac{2}{n} - \eta_j)$, where $\eta_j$ are $n$ positive eigenvalues of an upper-left (or lower-right) $2n \times 2n$ block of $4n \times 4n$ Hermitian correlation matrix $D_{p,q} = \langle \text{NESS}_{[p]} | \text{NESS}_{[q]} \rangle$. $\rho_{[n/2]}$ can be computed by expressing $\hat{a}_p$ in terms of NMM maps $\hat{b}_j$ and $\hat{b}_j^\dagger$ (not $\hat{b}_j^\dagger$), $\hat{a}_q = \hat{Q}^\dagger \hat{a}_q \hat{Q}^\dagger$, where $\hat{Q} = \prod_{p=1}^{n} (v_{2j-1,p}^2 v_{2k-1,p}^2)$ is $2n \times 2n$ matrix, and $Q = V_{[n]} K_{[1,2]}$ where $K_{[1,2]}$ designates upper-right $2n \times 2n$ quarter of $4n \times 4n$ matrix $K = -(\langle \text{NESS}_{[p]} | \text{NESS}_{[q]} \rangle)^{-1} (\langle \text{NESS}_{[p]} | \text{NESS}_{[q]} \rangle)$ and $\langle \text{NESS}_{[p]} | \text{NESS}_{[q]} \rangle = v_{2k-1,p} v_{2k-1,p}^*$ are $4n \times 2n$ matrices. $(\text{X|Y})$ denotes vertical concatenation of two $4n \times 2n$ matrices into a single $4n \times 4n$ matrix.

The resulting behaviour of $S(n)$ in NESS of XY chain is striking (see Fig. 5): LRMC phase $h < h_c$ is characterized with a linear growth $S(n) = sn + \text{const}$, with some constant $s > 0$. This has to be contrasted with a long $n$ growth found for equilibrium critical models \cite{12}. As $h$ approaches $h_c$, the slope $s$ approaches $0$ as $s \propto (h_c-h)^{-\gamma}$, with numerically determined critical exponent $\gamma \approx 0.80$, and the fluctuations of $S(n)$ around the average linear growth increase. These fluctuations can be explained by sensitive dependence of NESS on boundary conditions (bath couplings or size changes) due to long range correlations, evident also in the structures of the correlation matrices (Fig. 2). Note also an interesting ‘quantization of bipartite entanglement’ which is observed for very small $h_c - h$ where $S(n)$ can take only approximately a discrete set of values $S(n) \approx S_0 + k, k \in \mathbb{Z}^+$ and which can be explained by the quasi-particle picture of NMM. At and above the critical field $h \sim h_c$, we find $S(n) = O(1)$, and vanishing fluctuations of $S(n)$ since there NESS becomes insensitive to boundary conditions due to fast decay of magnetic correlations. Only there can NESS be efficiently simulated, e.g. in terms
of matrix product states \[15\], by numerical methods like
density matrix renormalization group (DMRG) \[16\].

All the numerical results presented above have been
obtained for a fixed non-equilibrium bath couplings \(\Gamma_\mu^L = 0.5, \Gamma_2^L = 0.3, \Gamma_1^R = 0.5, \Gamma_2^R = 0.1\). However, the results did not change qualitatively, in particular the phase boundary, when we (i) varied the bath couplings \(\Gamma_\mu^\Lambda \\neq \emptyset\),
(ii) coupled several spins around each end to Lindbladian baths, or (iii) even set the bath couplings equal
\(\Gamma_\mu^L = \Gamma_\mu^R\). The latter case (iii) does not represent an equilibrium situation, i.e. \(\rho_{\text{NESS}}\) is not a thermal state \(\rho_T = Z^{-1}\exp(-H/T)\) as the XY chain is not ergodic.

For example, no discontinuity at \(h = h_c\) appears in the properties of \(\rho_T\) for any \(T\), and correlator \(C(r)\) essentially always decays with \(T\)-dependent rates \[10\], whereas in non-LRMC phase of NESS decay length \(\xi\) is asymptotically insensitive to bath parameters \(\Omega\). Furthermore, thermal states in one-dimension have always bounded (in \(n\)) OSEE \[17\], and related quantities like mutual information \[18\], hence the simulation complexity of NESS is qualitatively different.

In spite of demonstrated discontinuity in the spin-spin correlation function, the local observables such as energy or spin density in NESS are numerically found to be smooth functions of \(h\) at \(h_c\), so the non-equilibrium transition appears to be of high or infinite order (similar to Kosterlitz-Thouless transition). LRMC phase could perhaps be difficult to detect experimentally as the residual correlation \(C_{\text{res}}\) is not larger than few times \(10^{-3}\) (Fig. 1) even in the optimal case (w.r.t. varying \(\Gamma_\mu\)).

In conclusion, we report on the QPT in NESS of open quantum XY spin chain, whose theoretical and numerical description is formally analogous to equilibrium QPTs in spin chains at zero temperature inasmuch as NESS can formally be treated as a ‘ground state’ of the quantum Liouvillean. We show that the phase transition is of mean-field type as the quasi-particle picture gives a satisfactory theoretical description, in particular the phase boundary between long-range and exponentially decaying magnetic correlations. We have demonstrated that the two phases, respectively, correspond to linearly growing and saturating entanglement entropy of NESS in operator space as a function of the chain length. This behavior is drastically different than in equilibrium quantum XY chains. We thank M. Žnidarič for useful comments and independent verifications of the results on small systems with DMRG \[16\] codes. The work is supported by grants P1-0044 and J1-7347 of Slovenian Research Agency.

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