Quantum Phase Transitions and Heat Capacity in a two-atoms Bose-Hubbard Model

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We show that a two-atoms Bose-Hubbard model exhibits three different phases in the behavior of thermal entanglement in its parameter space. These phases are demonstrated to be traceable back to the existence of quantum phase transitions in the same system. Significant similarities between the behaviors of thermal entanglement and heat capacity in the parameter space are brought to light thus allowing to interpret the occurrence and the meaning of all these three phases.

PACS numbers:

Overview

- Connection between quantum phase transitions, entanglement and specific heat in a simple model.
- Two qutrits governed via bilinear-biquadtratic Hamiltonian
- The system is in a thermal state $\Rightarrow$ thermal entanglement

The Negativity - Entanglement Measure for Mixed States

Separable bipartite mixed states can always be written as

$$\rho = \sum_n w_n \; \rho'_n \otimes \rho''_n$$

If you take the transpose of only one subsystem, the resulting matrix is still a density matrix:

$$\sigma = \sum_n w_n \left(\rho'_n\right)^T \otimes \rho''_n$$

$\Rightarrow$ σ has only positive eigenvalues.

$\Rightarrow$ Construct σ, if you find negative eigenvalues, the state is entangled.

Entanglement measure negativity:

$$\mathcal{N}(\rho) := \frac{\sum_i |\lambda| - \lambda_i}{2} = \frac{\|\rho^{\Gamma_A}\|_1 - 1}{2}$$

C_V - Sometimes an Entanglement Witness

Link between the entanglement of a thermal system and its thermodynamic properties?

For certain systems there exists a value of C_V which is a separable bound: When you measure a smaller value of C_V, the system is entangled.

E.g.:

$$H = \sum_i^N \sigma_i^z \sigma_{i+1}^z + B \sum_i^N \sigma_i^x$$

Here the eigenstates are all entangled $\Rightarrow$ ground state is entangled

Heat capacity as an indicator of entanglement, M.Wiśniak, V. Vedral and Č. Brukner, Phys. Rev. B **78**, 064108 (2008)

The Hamiltonian

Two-site BHM for spin-1 bosons:

$$H = \frac{U_0}{2} \sum_{i=L,R} n_i(n_i - 1) - t \sum_{\sigma} (\hat{L}^{\dagger}_{\sigma} \hat{R}_{\sigma} + \hat{R}^{\dagger}_{\sigma} \hat{L}_{\sigma}) + \frac{U_2}{2} \sum_{i=L,R} \left(\vec{F}^2_i - 2n_i \right)$$

Effective Hamiltonian for low tunneling ($U_0 \gg t$):

$$H^{eff} = \omega \vec{J}_z \; + \; r \; + \tau \left(\vec{S}_L \cdot \vec{S}_R \right) \; + \; \gamma \left(\vec{S}_L \cdot \vec{S}_R \right)^2$$

where $r = \tau - \gamma$

The Toy Model

Put one spin-1 boson in each site.

The Hamiltonian is diagonal in the basis $|J, J_z\rangle$:

$$E(|J, J_z\rangle) = \omega J_z + \frac{\tau}{2}(J(J+1) - 2) + \frac{\gamma}{4}\left((J(J+1) - 4)^2 - 4\right)$$

Assume the system is in a thermal state.

Use the basis

$$\{|11\rangle, |10\rangle, |1-1\rangle, |01\rangle, |00\rangle, |0-1\rangle, |-11\rangle, |-10\rangle, |-1-1\rangle\}$$

The Negativity

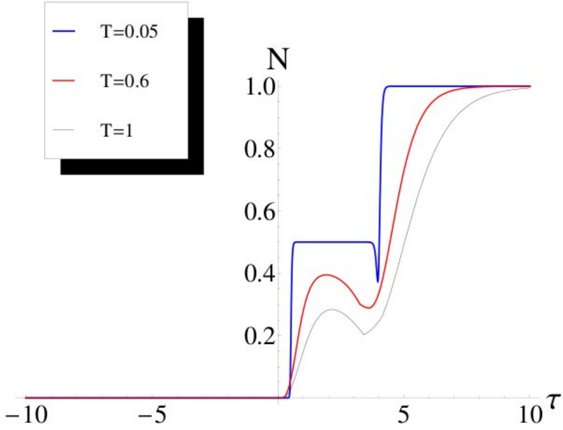
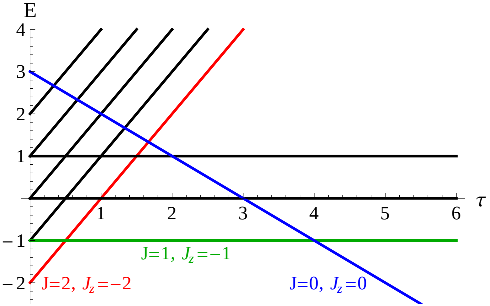


FIG. 1: System negativity plotted against τ when $\gamma = \omega = 1$. Energy is measured in units of t and $k_B = 1$

"This first Order QPT is a consequence a level crossing in the ground state energy ..."



At $\tau = \omega/2$ and $\tau = \omega + 3\gamma$ the ground state changes.

$$|2,-2\rangle = |\downarrow\downarrow\rangle \qquad \Rightarrow \; EOF(|2,-2\rangle) = 0$$

$$|1,-1\rangle = \sqrt{1/2}\,(|\downarrow 0\rangle - |0\downarrow\rangle) \qquad \Rightarrow \; EOF(|1,-1\rangle) = 1$$

$$|0,0\rangle = \sqrt{1/3}\,(|\downarrow\uparrow\rangle - |00\rangle + |\uparrow\downarrow\rangle) \qquad \Rightarrow \; EOF(|0,0\rangle) = \log_2 3 = 1.584$$

The Heat Capacity

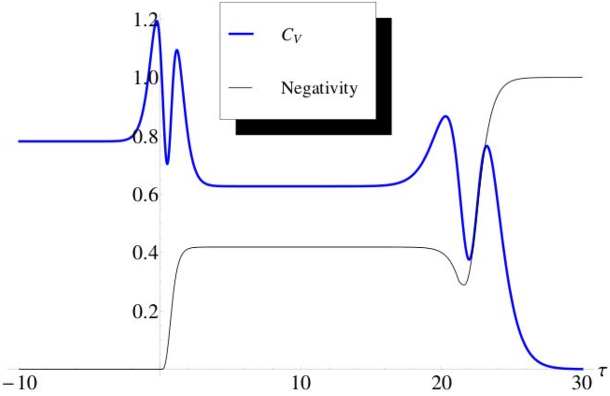


FIG. 2: Heat capacity and system negativity plotted against τ when $T = 0.6$, $\gamma = 7$ and $\omega = 1$

Energy Eigenvalues

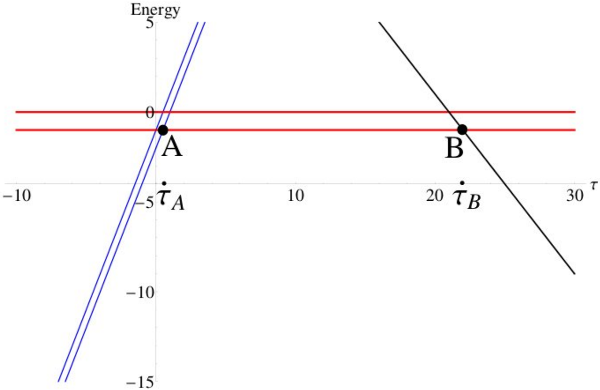
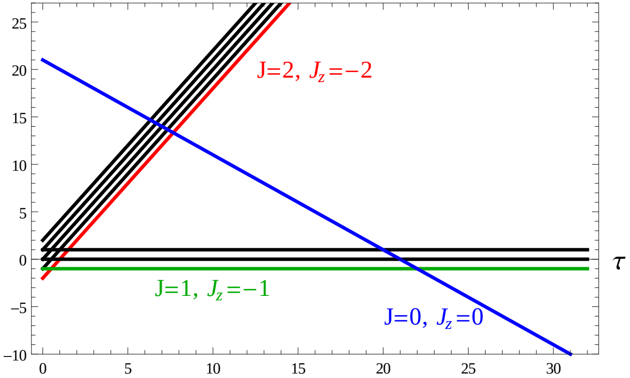


FIG. 3: Low-lying energy levels of H (in units of t) versus τ when $\gamma = 7$ and $\omega = 1$. Two crossing points, **A** and **B** in the plot, are clearly visible in correspondence to the values $\tau_A = \frac{1}{2}$ and $\tau_B = 22$

Energy Eigenvalues



- Less states close to the ground state $\Rightarrow$ smaller $\Delta E = T^2 C_V$
- High $\Delta E = T^2 C_V \Rightarrow$ entanglement is not possible

Conclusions

- "We establish a link between negativity and heat capacity."
- "...the first time thermodynamical signatures of the thermal entanglement in a two-atom BHM ..."
- "systematic correspondence at the critical points between quantum phase transitions and a peculiar oscillating behavior of the heat capacity."

Calculations

$$H_{BH} = -t\sum_{<ij>,\sigma}\left(a^\dagger_{i\sigma}a_{j\sigma} + a^\dagger_{j\sigma}a_{i\sigma}\right) + \epsilon\sum_i \hat{n}_i$$
$$+\frac{U_0}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i \frac{U_2}{2}\left((\mathbf{S}^i_{tot})^2 - 2\hat{n}_i\right)$$

$$H^{eff}_t = \widetilde{\omega}J_z + K_0 + K_1\sum_{<ij>}(\mathbf{S}_i\cdot\mathbf{S}_j) + K_2\sum_{<ij>}(\mathbf{S}_i\cdot\mathbf{S}_j)^2 \quad (2)$$

$$K_0 = \frac{4t^2}{3(U_0+U_2)} - \frac{4t^2}{3(U_0-2U_2)}$$
$$K_1 = \frac{2t^2}{U_0+U_2}$$
$$K_2 = \frac{2t^2}{3(U_0+U_2)} + \frac{4t^2}{3(U_0-2U_2)}$$

Calculations

$$\frac{H_t^{eff}}{t} \equiv H = \omega J_z + \tau(\mathbf{S}_1 \cdot \mathbf{S}_2) + \gamma(\mathbf{S}_1 \cdot \mathbf{S}_2)^2 + rI$$

where

$$\tau = K_1/t$$
$$\gamma = K_2/t$$
$$\omega = \widetilde{\omega}/t$$
$$r = \tau - \gamma$$

$$\begin{aligned} H \ &= \omega J_z + \tfrac{\tau}{2}(J^2 - S_1^2 - S_2^2) + \tfrac{\gamma}{4}(J^2 - S_1^2 - S_2^2)^2 + \\ &+ rI = \omega J_z + \tfrac{\tau}{2}(J^2 - 4I) + \tfrac{\gamma}{4}(J^2 - 4I)^2 + rI \end{aligned} \tag{8}$$

Calculations for the Heat Capacity

$$Z = e^{-\beta\tau}\Big[2\cosh\beta\tau\big(1 + 2\cosh\beta\omega\big) + $$
$$+2e^{-\beta\tau}\cosh 2\beta\omega + e^{-\beta(3\gamma-2\tau)}\Big]$$

$$C_V = \frac{\partial U}{\partial T} \qquad \text{and} \qquad U = T^2\frac{\partial \ln Z}{\partial T}$$

Calculations

$$\sigma = \begin{pmatrix} R_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & R_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & P_- & Q_- & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & Q_- & P_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & P_- & Q_- & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & Q_- & P_+ & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & L_- & M_- & R_- \\ 0 & 0 & 0 & 0 & 0 & 0 & M_- & Q_+ & M_+ \\ 0 & 0 & 0 & 0 & 0 & 0 & R_- & M_+ & L_+ \end{pmatrix}$$

where

$$L_\pm = \frac{1}{Z} e^{-2\beta(\tau \pm \omega)}$$
$$M_\pm = -\frac{1}{Z} e^{-\beta(\tau \pm \omega)} \sinh(\beta\tau)$$
$$P_\pm = \frac{1}{Z} e^{-\beta(\tau \pm \omega)} \cosh \beta\tau$$
$$R_\pm = \frac{1}{6Z} e^{-\beta\tau} \left(e^{-\beta\tau} \pm 3e^{\beta\tau} + 2e^{-\beta(3\gamma - 2\tau)}\right)$$
$$Q_\pm = \frac{1}{3Z} e^{-\beta\tau} \left(\frac{3 \pm 1}{2} e^{-\beta\tau} \pm e^{-\beta(3\gamma - 2\tau)}\right)$$