The Kitaev-Hubbard chain (and a parafermion generalization)

Eddy Ardonne Stockholm University

Iman Mahyaeh

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Outline

- Kitaev chain and zero modes
- Kitaev-Hubbard chain
- Overview of the phase diagram
- Strong zero mode?
- Diagnosis using analytic argument and finite temperature edge magnetization
- Parafermion generalization: frustration free line

The Kitaev chain: prototypical model with Majorana zero-modes:

$$H_{\text{Kit}} = -J \sum_{j=1}^{L-1} \left(c_j^{\dagger} c_{j+1}^{\dagger} + c_j^{\dagger} c_{j+1} + \text{h.c.} \right) - h \sum_{j=1}^{L} \left(1 - 2c_j^{\dagger} c_j \right)$$

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In terms of Pauli matrices (after Jordan-Wigner):

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 $H_{\rm Kit}$ is a free-fermion model, solvable by a canonical transformation on the fermion operators:

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Operator connecting the pairs: σ_1^x

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More non-trivial example: XYZ chain (Fendley) Question: is the strong zero mode due to integrability or can non-integrable models have a strong zero mode?

Kitaev - Hubbard chain

A natural interaction term for the Kitaev chain is of Hubbard type

$$H_{\text{KH}} = -J \sum_{j=1}^{L-1} \left(c_j^{\dagger} c_{j+1}^{\dagger} + c_j^{\dagger} c_{j+1} + \text{h.c.} \right) - h \sum_{j=1}^{L} \left(1 - 2c_j^{\dagger} c_j \right) + U \sum_{j=1}^{L-1} \left(1 - 2c_j^{\dagger} c_j \right) \left(1 - 2c_{j+1}^{\dagger} c_{j+1} \right)$$

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Parity is a good quantum number:

$$P = \prod_{j=1}^{L} \sigma_{j}^{z} = \prod_{j=1}^{L} (1 - 2c_{j}^{\dagger}c_{j}) = \pm 1$$

Phase diagram, U < 0 (DMRG)



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There is a direct transition to the topological phase, described by Ising CFT (h > 0)

Phase diagram, U > 0 (DMRG)



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Topological & CDW phases separated by a gapless incommensurate phase and a 'exited state CDW' phase (ground state resembles an exited state of the CDW phase)

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Other observables used: entanglement entropy, site occupation, scaling of the gap.

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Performing the rotation $\sigma_j^x \to (-1)^j \sigma_j^x \quad \sigma_j^z \to -\sigma_j^z$ gives -H(h, U) = H(h, -U)

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Ground state in the trivial phase is non-degenerate, so we can exclude a strong zero mode above the dashed line.

In the remainder, we study the strong zero mode via the edge-magnetization (Fendley et al.)

Spin-auto correlation function is defined as $A_{j}(t) = \langle j | \sigma_{1}^{x}(t)\sigma_{1}^{x}(0) | j \rangle$

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Pairing due to a strong zero mode gives $\lim_{t\to\infty} \lim_{L\to\infty} A_j(t) \neq 0 \text{ for arbitrary state } j:$

$$A_{j}(t) = \sum_{j_{1}} e^{i(E_{j_{1}} - E_{j})t} |\langle j_{1} | \sigma_{1}^{x} | j \rangle|^{2}$$

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States with $E_{j_1} \approx E_{j_2}$, $\langle j_2 | \sigma_1^x | j_1 \rangle \neq 0$ give finite contribution to edge magnetization at large times. When $E_{j_1} \neq E_{j_2}$ one gets a sum of incoherent oscillations.

We will consider the edge magnetization at T > 0:

$$A(t,T) = \frac{1}{Z} \sum_{j_1} e^{-\epsilon_{j_1}/(kT)} A_{j_1}(t) = \frac{1}{Z} \sum_{j_1,j_2} e^{-\epsilon_{j_1}/(kT)} e^{i(\epsilon_{j_1}-\epsilon_{j_2})t} |\langle j_2 | \sigma_1^x | j_1 \rangle|^2$$

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We use exact diagonalization, to obtain *all* the eigenstates, for L up to 16.

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Compare different system sizes for h=0.1, U = 0.1, and T=1000



Correlation time increases exponentially with system size, consistent with a strong zero mode, but unclear if this persists to larger sizes.

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For U = 0.1, h=0.7, there is no strong zero mode

Emery-Peschel constructed a 'frustration free' line in the topological phase:

$$H = \sum_{j} h_{j,j+1}^{\text{PE}} \qquad U(l) = (\cosh(l) - 1)/2 \quad h(l) = \sinh(l)$$
$$h_{j,j+1}^{\text{PE}}(l) = -\sigma_{j}^{x}\sigma_{j+1}^{x} + \frac{h(l)}{2}(\sigma_{j}^{z} + \sigma_{j+1}^{z}) + U(l)\sigma_{j}^{z}\sigma_{j+1}^{z} + (U(l) + 1)$$

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Model has two *exactly degenerate ground states* (E=0): $|\psi_1(l)\rangle = (|\uparrow\rangle + e^{\frac{l}{2}}|\downarrow\rangle)^{\otimes L} \quad |\psi_2(l)\rangle = (|\uparrow\rangle - e^{\frac{l}{2}}|\downarrow\rangle)^{\otimes L}$

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Parity eigenstates are *not* product states:

 $|E = 0; \pm \rangle = \mathcal{N}_{\pm}(l)(|\psi_1(l)\rangle \pm |\psi_2(l)\rangle) \qquad \mathcal{N}_{\pm}(l) = \left[2(1+e^l)^L \pm 2(1-e^l)^L\right]^{-\frac{1}{2}}$

One can construct *edge-localized* Majorana operators that permutes the parity eigenstates

$$\Gamma_{\rm L} = \frac{1}{\sqrt{\sum_{j=0}^{L-1} q^{2j}}} \sum_{j=1}^{L} q^{(j-1)} \gamma_{A,j} \qquad \Gamma_{\rm R} = \frac{1}{\sqrt{\sum_{j=0}^{L-1} q^{2j}}} \sum_{j=1}^{L} q^{(L-j)} \gamma_{B,j} \qquad q = -\tanh(l/2)$$
$$\gamma_{A,j} = \left(\prod_{k < j} \sigma_k^z\right) \sigma_j^x \qquad \gamma_{B,j} = \left(\prod_{k < j} \sigma_k^z\right) \sigma_j^y$$

Generalization to parafermions

The frustration free line can be generalized to parafermions (as in Joffe's talk): X and Z satisfy

 $X^3 = Z^3 = \mathbf{1}$ $X^2 = X^{\dagger}$ $Z^2 = Z^{\dagger}$ $XZ = \omega ZX$ $\omega = e^{2\pi i/3}$

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Frustration free model can be constructed: $H = \sum_{j=1}^{L-1} h_{j,j+1}^{Z_3}(r)$ $h_{j,j+1}^{Z_3}(r) = \left[-X_j^{\dagger}X_{j+1} - f(r)(Z_j + Z_{j+1}) - g_1(r)Z_jZ_{j+1} - g_2(r)Z_jZ_{j+1}^{\dagger} + h \cdot c\right] + \epsilon(r)$ $f(r) = (1 + 2r)(1 - r^3)/(9r^2) \qquad g_1(r) = -2(1 - r)^2(1 + r + r^2)/(9r^2)$ $g_2(r) = (1 - r)^2(1 - 2r - 2r^2)/(9r^2) \qquad \epsilon(r) = 2(1 + r + r^2)^2/(9r^2)$

 $h_{j,j+1}^{Z_3}(r) = \left[-X_j^{\dagger}X_{j+1} - f(r)(Z_j + Z_{j+1}) - g_1(r)Z_jZ_{j+1} - g_2(r)Z_jZ_{j+1}^{\dagger} + h \cdot c\right] + \epsilon(r)$

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The E=0 ground states are product states:

 $|G_{0}(r)\rangle = \left(|0\rangle + r|1\rangle + r|2\rangle\right)^{\otimes L} \qquad |G_{1}(r)\rangle = \left(|0\rangle + r\omega|1\rangle + r\bar{\omega}|2\rangle\right)^{\otimes L} \qquad |G_{2}(r)\rangle = \left(|0\rangle + r\bar{\omega}|1\rangle + r\omega|2\rangle\right)^{\otimes L}$

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Use them to construct symmetry eigenstates

 $|E = 0; 1\rangle = \mathcal{N}_{1}(|G_{0}(r)\rangle + |G_{1}(r)\rangle + |G_{2}(r)\rangle)$ $|E = 0; \omega\rangle = \mathcal{N}_{\omega}(|G_{0}(r)\rangle + \bar{\omega} |G_{1}(r)\rangle + \omega |G_{2}(r)\rangle)$ $|E = 0; \bar{\omega}\rangle = \mathcal{N}_{\bar{\omega}}(|G_{0}(r)\rangle + \omega |G_{1}(r)\rangle + \bar{\omega} |G_{2}(r)\rangle)$

$$\mathcal{N}_{1} = \left[3(1+2r^{2})^{L} + 6(1-r^{2})^{L} \right]^{-\frac{1}{2}}$$
$$\mathcal{N}_{\omega,\bar{\omega}} = \left[3(1+2r^{2})^{L} - 3(1-r^{2})^{L} \right]^{-\frac{1}{2}}$$

 $h_{j,j+1}^{Z_3}(r) = \left[-X_j^{\dagger}X_{j+1} - f(r)(Z_j + Z_{j+1}) - g_1(r)Z_jZ_{j+1} - g_2(r)Z_jZ_{j+1}^{\dagger} + h \cdot c\right] + \epsilon(r)$

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$$\begin{split} |E = 0; 1\rangle &= \mathcal{N}_{1}(|G_{0}(r)\rangle + |G_{1}(r)\rangle + |G_{2}(r)\rangle) \\ |E = 0; \omega\rangle &= \mathcal{N}_{\omega}(|G_{0}(r)\rangle + \bar{\omega} |G_{1}(r)\rangle + \omega |G_{2}(r)\rangle) \\ |E = 0; \bar{\omega}\rangle &= \mathcal{N}_{\bar{\omega}}(|G_{0}(r)\rangle + \omega |G_{1}(r)\rangle + \bar{\omega} |G_{2}(r)\rangle) \\ \mathcal{N}_{\omega,\bar{\omega}} &= \left[3(1 + 2r^{2})^{L} - 3(1 - r^{2})^{L}\right]^{-\frac{1}{2}} \end{split}$$

Unfortunately, constructing an *edge-localized* parafermion operator that permutes the states is hard!

The most general 2-site operator is:

$$a_{1;1} = \frac{2r^3 + (cd + r^2)\cos(\phi_1) + (-d + cr^2)\sin(\phi_1)}{2cd}$$

$$a_{2;1} = \frac{2r^3 + (-cd + r^2)\cos(\phi_1) - (d + cr^2)\sin(\phi_1)}{2cd}$$

$$a_{3;1} = \frac{r(1 - r^3\cos(\phi_1) + dr\sin(\phi_1))}{cd}$$

$$b_{1;1} = \frac{2r^3 + (cd + r^2)\cos(\phi_2) + (d - cr^2)\sin(\phi_2)}{2cd}$$

$$b_{2;1} = \frac{2r^3 + (-cd + r^2)\cos(\phi_2) - (d + cr^2)\sin(\phi_2)}{2cd}$$

$$b_{3;1} = \frac{r(r^3 - \cos(\phi_2) + c\sin(\phi_2))}{cd}$$

$$c_{1;1} = \frac{r^2(1 + (1 + r^2)\cos(\phi_3))}{d^2}$$

$$c_{2;1} = -\frac{r^2(-1 + \cos(\phi_3) + d\sin(\phi_3))}{d^2}$$

$$c_{3;1} = \frac{r(r^2 - r^2\cos(\phi_3) + d\sin(\phi_3))}{d^2}$$

$$a_{1;2} = \frac{2r^3 + (-cd + r^2)\cos(\phi_1) + (d + cr^2)\sin(\phi_1)}{2cd}$$

$$a_{2;2} = \frac{2r^3 + (cd + r^2)\cos(\phi_1) + (d - cr^2)\sin(\phi_1)}{2cd}$$

$$a_{3;2} = -\frac{r(-1 + r^3\cos(\phi_1) + dr\sin(\phi_1))}{cd}$$

$$b_{1;2} = \frac{2r^3 + (-cd + r^2)\cos(\phi_2) + (d + cr^2)\sin(\phi_2)}{2cd}$$

$$b_{2;2} = \frac{2r^3 + (cd + r^2)\cos(\phi_2) + (-d + cr^2)\sin(\phi_2)}{2cd}$$

$$b_{3;2} = -\frac{r(-r^3 + \cos(\phi_2) + c\sin(\phi_2))}{cd}$$

$$c_{1;2} = \frac{r^2(1 - \cos(\phi_3) + d\sin(\phi_3))}{d^2}$$

$$c_{2;2} = \frac{r^2(1 + (1 + r^2)\cos(\phi_3))}{d^2}$$

$$c_{3;2} = \frac{r(r^2 - r^2\cos(\phi_3) - d\sin(\phi_3))}{d^2}$$

$$o(r) = \begin{cases} 0 & b_{2,3} & 0 & b_{1,3} & 0 & 0 & 0 & 0 & b_{3,3} \\ 0 & 0 & c_{1,2} & 0 & c_{2,2} & 0 & a_{1,1} & 0 \\ a_{3,1} & 0 & 0 & 0 & 0 & a_{2,3} & 0 & a_{1,3} & 0 \\ 0 & b_{2,2} & 0 & b_{1,2} & 0 & 0 & 0 & b_{3,2} \\ a_{3,2} & 0 & 0 & 0 & 0 & a_{2,3} & 0 & a_{1,3} & 0 \\ 0 & b_{2,1} & 0 & b_{1,1} & 0 & 0 & 0 & b_{3,1} \\ 0 & 0 & c_{1,3} & 0 & c_{3,3} & 0 & c_{2,3} & 0 & 0 \\ 0 & b_{2,1} & 0 & b_{1,1} & 0 & 0 & 0 & b_{3,1} \\ 0 & 0 & c_{1,3} & 0 & c_{3,3} & 0 & c_{2,3} & 0 & 0 \\ 0 & b_{2,3} & = \frac{r(r^3 - \cos(\phi_1) + c\sin(\phi_1))}{cd} \\ a_{3,3} & = \frac{r^2(1 + 2r\cos(\phi_1))}{cd} \\ a_{3,3} & = \frac{r^2(1 + 2r\cos(\phi_1))}{cd} \\ b_{1,3} & = -\frac{r(-1 + r^3\cos(\phi_2) + dr\sin(\phi_2))}{cd} \\ b_{2,3} & = \frac{r(1 - r^3\cos(\phi_2) + dr\sin(\phi_2))}{cd} \\ b_{3,3} & = \frac{r^2(1 + 2r\cos(\phi_2))}{cd} \\ c_{1,3} & = \frac{r(r^2 - r^2\cos(\phi_3) - d\sin(\phi_3))}{d^2} \\ c_{2,3} & = \frac{r(r^2 - r^2\cos(\phi_3) + d\sin(\phi_3))}{d^2} \\ c_{3,3} & = \frac{r^2(r^2 + 2\cos(\phi_3))}{d^2} \end{cases}$$

$$c = \sqrt{1 + 2r^4}$$
 $d = \sqrt{2r^2 + r^4}$ $\phi_1 + \phi_2 + \phi_3 = 0$

Not easy to find localized operator for arbitrary system size

Summary

- Topological phase survives Hubbard interactions
- Interesting regime in phase diagram for repulsive interaction
- Can exclude strong zero mode for large part of the topological phase
- Finite temperature behaviour of edge magnetization not fully understood
- Generalization to parafermion case, phase diagram not studied in detail
- Frustration free line, but no localized operators (yet?)