Topology of mixed states

Michael Fleischhauer
University of Kaiserslautern

QM³ - Quantum Matter meets Math, Lissabon, 07.06.2021
Phases of matter

Landau-Ginzburg

Phases of matter differ by the way they break symmetries

\[ H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \]

\[ T > T_c \]

paramagnet

\[ T < T_c \]

ferromagnet
Phases of matter

- **Quantum Hall effect**
  
  Thouless, Kohmoto, Nightingale, denNijs, (TKNN) PRL 1982:
  
  topology of the wavefunction, characterized by integer quantum numbers!

v. Klitzing, PRL 1980

no broken symmetries!
Topological quantum systems

- Topological protection
- Quantized bulk transport
- Exotic quantum states

Protected edge states & edge transport
Hall conductivity & resistance normal
Abelian & non-Abelian anyons
mixed states?

- topology at finite $T$: what is left??

- topology in non-equilibrium driven, open systems??
mixed states?

topology at finite $T$: what is left??

topology in non-equilibrium driven, open systems??
mixed states?

steady state of open systems is an attractor of the dynamics:
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $\mathbb{Z}$ index

Time-reversal symmetric systems: $\mathbb{Z}_2$ index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $\mathbb{Z}$ index

Time-reversal symmetric systems: $\mathbb{Z}_2$ index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $\mathbb{Z}$ index

Time-reversal symmetric systems: $\mathbb{Z}_2$ index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: \( Z \) index

Time-reversal symmetric systems: \( Z_2 \) index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $\mathbb{Z}$ index

Time-reversal symmetric systems: $\mathbb{Z}_2$ index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $Z$ index

Time-reversal symmetric systems: $Z_2$ index

Interactions

Measurable consequences
Outline

Topological classification by symmetries of Hamiltonians

Gaussian mixed states and fictitious Hamiltonian

Topological invariants: Geometric Phases

Broken time-reversal symmetry: $Z$ index

Time-reversal symmetric systems: $Z_2$ index

Interactions

Measurable consequences
Classification of topological systems
### Symmetry operations in Fock space

#### Fermions on a lattice

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symbol</th>
<th>Equation</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unitary</strong></td>
<td>$\hat{U}$</td>
<td>$\hat{U} \hat{a}<em>i \hat{U}^{-1} = u</em>{ij} \hat{a}_j$</td>
<td>$\hat{U} i \hat{U}^{-1} = i$</td>
</tr>
<tr>
<td><strong>Time-reversal</strong></td>
<td>$\hat{T}$</td>
<td>$\hat{T} \hat{a}<em>i \hat{T}^{-1} = u</em>{ij}^t \hat{a}_j$</td>
<td>$\hat{T} i \hat{T}^{-1} = -i$</td>
</tr>
<tr>
<td><strong>Charge conjugation</strong></td>
<td>$\hat{C}$</td>
<td>$\hat{C} \hat{a}<em>i \hat{C}^{-1} = u</em>{ij}^c \hat{a}_j^\dagger$</td>
<td>$\hat{C} i \hat{C}^{-1} = i$</td>
</tr>
<tr>
<td><strong>Chiral transform</strong></td>
<td>$\hat{S} = \hat{T} \circ \hat{C}$</td>
<td>$\hat{S} \hat{a}<em>i \hat{S}^{-1} = u</em>{ij}^s \hat{a}_j^\dagger$</td>
<td>$\hat{S} i \hat{S}^{-1} = -i$</td>
</tr>
</tbody>
</table>

This is an exhaustive list !!!
Ten-fold way

There are only 10 different classes under Fock-space transformations!

- not invariant under trafo: "0"
- invariant and \( \hat{G}^2 = +1 \) "+1"
- Invariant and \( \hat{G}^2 = -1 \) "-1"

\[
\hat{G} = \hat{T}, \hat{C}, \hat{S}
\]

<table>
<thead>
<tr>
<th></th>
<th>T</th>
<th>C</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>+1</td>
<td>+1</td>
<td>+1</td>
<td></td>
</tr>
<tr>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
</tbody>
</table>

\( 3 \times 3 = 9 \) cases

only nontrivial if \( T = 0 \) and \( C = 0 \)

1 additional case
Non-interacting fermions

<table>
<thead>
<tr>
<th>Class</th>
<th>T</th>
<th>C</th>
<th>S</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
</tr>
<tr>
<td>AIII</td>
<td>0</td>
<td>0</td>
<td>+</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
</tr>
<tr>
<td>AI</td>
<td>+</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>Z</td>
<td></td>
</tr>
<tr>
<td>BDI</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>Z</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>+</td>
<td>0</td>
<td>Z_2</td>
<td>Z_2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DIII</td>
<td>-</td>
<td>+</td>
<td>+</td>
<td>Z_2</td>
<td>Z_2</td>
<td>Z_2</td>
<td>0</td>
</tr>
<tr>
<td>AII</td>
<td>-</td>
<td>0</td>
<td>0</td>
<td>Z_2</td>
<td>Z_2</td>
<td>Z_2</td>
<td>Z</td>
</tr>
<tr>
<td>CII</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>Z</td>
<td>0</td>
<td>Z_2</td>
<td>Z_2</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>-</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z_2</td>
<td>Z_2</td>
</tr>
<tr>
<td>CI</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
</tr>
</tbody>
</table>

→ Intrinsic topology

symmetry-protected
Gaussian open systems
Gaussian mixed states

determined by single-particle correlations:  fictitious Hamiltonian

\[ \hat{\rho} \sim \exp\left\{ -\frac{1}{2} \hat{\mathbf{c}}^{\dagger T} \mathbf{G} \hat{\mathbf{c}} \right\} \]

\[ \langle \hat{c}_i^{\dagger} \hat{c}_j \rangle = \frac{1}{2} \left[ 1 - \tanh \left( \frac{\mathbf{G}}{2} \right) \right]_{ij} \]

- Gaussian states in **thermal equilibrium** require quadratic Hamiltonian

\[ \mathbf{G} = \beta \left( \mathbf{H} - \mu \right) \]

\[ \beta = 1/k_B T \]

- Gaussian **non-equilibrium steady state** (NESS) require linear Lindblad generators

\[ \frac{d \rho}{dt} = -i \left[ \hat{H}, \rho \right] + \frac{1}{2} \sum_{\mu} \left( 2L_\mu \rho L_\mu^{\dagger} - \left\{ L_\mu^{\dagger} L_\mu, \rho \right\} \right) = 0 \]

\[ L_j \sim \alpha \hat{c}_j^{\dagger} + \beta \hat{c}_j \]
Topological invariants: Geometric phases
Topological invariants

**Chern insulators**
- TR broken
- Quantum Hall (1980)
- $\mathbb{Z}$

**Topol. insulators**
- TR symmetric
- Quantum Spin Hall (2007)
- $\mathbb{Z}_2$

Quantum Hall

Quantum spin Hall

Science 340, 153 (2013)
locally indistinguishable
differ by global properties!
Geometric phase

Zak (Berry) phase

\[ \phi_{Zak} = \int_{-\pi/a}^{\pi/a} dk \langle u_k | i \partial_k | u_k \rangle \]

→ density matrix?
**Berry parallel transport**

\[ U(1) e^{i\phi} |\psi\rangle \]

\[ \| |\psi(\lambda)\rangle - |\psi(\lambda + d\lambda)\rangle \| = \text{min} \]

\[ \rho = |\psi\rangle \langle \psi| \]

**Berry (Zak) phase**: picked up at parallel transport cycle

\[ \phi_{\text{Zak}} = \int_{-\pi/a}^{\pi/a} dk \langle u_k | i\partial_k | u_k \rangle \]
Uhlmann parallel transport

\[ U(n) \]

\[ wU \]

\[ \left| \left| w(\lambda) - w(\lambda + d\lambda) \right| \right| = \min \]

\[ U(n) \text{ gauge freedom} \]

\[ w \rightarrow wU \]

\[ w^\dagger \rightarrow U^\dagger w^\dagger \]

\[ \rho = ww^\dagger \]

\[ U(1) \text{ Uhlmann phase} \]

\[ e^{i\phi} = \int d\lambda \ Tr [w\partial_\lambda w^\dagger] \]
Chern number

TR-broken
1+1 and 2-dimensional systems

1D: winding number

\[ \hat{H} = \hat{H}(\lambda) \]

\[ \nu = \frac{1}{2\pi} \int d\lambda \frac{\partial \phi_{Zak}}{\partial \lambda} \]

2D: Chern number

\[ C = \frac{i}{2\pi} \int \int_{BZ} d^2k \sum_\alpha \left\{ \langle \partial_{k_y} u_\alpha^* | \partial_{k_x} u_\alpha \rangle - \langle \partial_{k_x} u_\alpha^* | \partial_{k_y} u_\alpha \rangle \right\} \]

\[ = \frac{1}{2\pi} \int_{BZ} dk_y \frac{\partial \phi_{Zak}^x}{\partial k_y} = -\frac{1}{2\pi} \int_{BZ} dk_x \frac{\partial \phi_{Zak}^y}{\partial k_x} \]
Failure of the Uhlmann phase

- SSH model at finite T (1D)  (class BDI)
  Viyuela, Rivas, Martin-Delgado PRL (2014)
  Huang, Arovas PRL (2014)

- asymmetric Qi-Wu-Zhang model at finite T (2D)  (class A)

\[ H(k) = \sum_{j} d^j(k) \hat{\sigma}_j \quad d^1 = \sin(k_x) \quad d^2 = 3 \sin(k_y) \quad d^3 = 1 - \cos(k_x) - \cos(k_y) \]

\[ C = \frac{1}{2\pi} \int dk_y \left( \frac{\partial \phi(k_y)}{\partial k_y} \right) \neq C' = \frac{1}{2\pi} \int dk_x \left( \frac{\partial \phi(k_x)}{\partial k_x} \right) \]

Invariants & quantized bulk transport

Thouless, Kohmoto, Nightingale, den Nijs (TKNN) PRL (1982)

\[ \Delta n = \frac{1}{2\pi} \int d\lambda \frac{\partial \phi_{Zak}}{\partial \lambda} \]
Charge pumps (Thouless)

- **Rice-Melev model (1+1 D)**

\[
\hat{H}_{RM} = -t_1 \sum_{j: \text{even}} c_\dagger_{j+1} c_j - t_2 \sum_{j: \text{odd}} c_\dagger_{j+1} c_j + h.a. + \Delta \sum_{j} (-1)^j c_\dagger_{j} c_j
\]

Charge pumps (Thouless)
Charge pumps (Thouless)
Charge pumps (Thouless)
Charge pumps (Thouless)
Charge pumps (Thouless)
Charge pumps (Thouless)

Geometric phase: \( \Delta \Omega_{\text{Zak}} \)

Topological pumps: \( \Delta n \)

Mixed states
Charge pumps (Thouless)

Wang, Troyer, Dai, PRL (2013)

particle transport no longer quantized
Charge pumps (Thouless)

Wang, Troyer, Dai, PRL (2013)
Charge pumps (Thouless)

geometric phase

\[ \Delta \phi_{ak} \]

mixixed states

\[ \Delta n \]

topological pumps
Polarisation

\[ \Delta \phi_{Zak} \leftrightarrow \Delta \phi \]

\[ \Delta P \]

King-Smith, Vanderbildt PRB (1983)

\[ \Delta \phi_{Zak} = \frac{2\pi}{\alpha} \Delta P \]
Many-body polarization

\[ P = \int dx \, w^*(x) \, x \, w(x) \]


\[ P = \frac{1}{2\pi} \text{Im} \ln \left\langle \exp \left\{ i \frac{2\pi}{L} \hat{X} \right\} \right\rangle \]

\[ \hat{X} = \sum_j j \, \hat{c}_j^\dagger \hat{c}_j \quad (a = 1) \]
Ensemble Geometric Phase

\[ \varphi_{Zak} = \text{Im} \ln \langle \psi_0 | \hat{T} | \psi_0 \rangle \]

\[ \hat{T} = e^{i \frac{2\pi}{L} \hat{X}} \]

momentum-shift operator in x

\[ \varphi_E = \text{Im} \ln \text{Tr}(\rho \hat{T}) \]

D. Linzner et al. PRB (2016); Ch. Bardyn et al. PRX (2018)
Finite-T Rice-Mele model

\( \phi_E / 2\pi \)

\[ T = 0 \]

\[ T = 100 \]
Finite-T SSH model

\[ \frac{\varphi_E}{2\pi} \]

\[ T = 0 \]

\[ T = 100 \]
Finite-T Qi-Wu-Zhang model

\[ C_x = \int_{BZ} dk_y \frac{\partial P_x(k_y)}{\partial k_y} \]

or

\[ C_y = -\int_{BZ} dk_x \frac{\partial P_y(k_x)}{\partial k_x} \]

or

\[ P_x(k_y) \]

or

\[ P_y(k_x) \]

\[ C_x = C_y \]
EGP and fictitious Hamiltonian

finite-T Rice Mele model (Thouless charge pump)

Bardyn, Wawer, Altland, Fleischhauer, Diehl  (PRX 2018)
EGP and fictitious Hamiltonian

finite-T Rice Mele model (Thouless charge pump)

Bardyn, Wawer, Altland, Fleischhauer, Diehl  (PRX 2018)
EGP and fictitious Hamiltonian

- finite-T Rice Mele model (Thouless charge pump)

Bardyn, Wawer, Altland, Fleischhauer, Diehl  (PRX 2018)
EGP and fictitious Hamiltonian

- finite-T Rice Mele model (Thouless charge pump)

Bardyn, Wawer, Altland, Fleischhauer, Diehl  (PRX 2018)
EGP and fictitious Hamiltonian

\[ P(\rho_{ss}) = P(|\psi\rangle\langle\psi|) + \mathcal{O}(L^{-1}) \]

\[ |\psi\rangle \text{ ground state of } \mathcal{H}_{\text{fict}} = \sum_{ij} G_{ij} c_i^\dagger c_j \]

\[ \mathcal{\varphi}_{\text{EGP}} = \text{Zak phase of } |\psi\rangle \]

Bardyn, Wawer, Altland, Fleischhauer, Diehl (PRX 2018)
Topological classification

\[ \mathcal{H}_{\text{fict}} = \sum_{ij} G_{ij} c_i^\dagger c_j \]

- symmetries of fictitious Hamiltonian classify topology
- topological phase transitions
  
  (I) closing of the purity gap = gap of fictitious Hamiltonian

  \[ \underline{G} = \beta \left( \underline{H} - \mu \right) \]

  thermal equilibrium

  (II) closing of the damping gap (criticality)
$Z_2$ number

TR-symmetric
Kramers degeneracy

- Time-reversed Bloch eigenstate is again an eigenstate
  \[ |u_{\Pi}(-k)\rangle = e^{i\chi(k)} \mathcal{T} |u_{\Pi}(k)\rangle \]

- Total Chern number vanishes
  \[ C = \frac{1}{2\pi} \int_{BZ} d\kappa_y \frac{\partial P_{\text{tot}}(\kappa_y)}{\partial \kappa_y} = 0 \]

Energy bands come in pairs.
Continuous TR polarization

**Z\textsubscript{2} invariant:** winding of continuous TR polarization over half Brillouin zone

\[ \nu_2 = \int_0^\pi d\kappa_y \frac{\partial P_\theta(\kappa_y)}{\partial \kappa_y} \]

\[ P_\theta = P^I - P^{II} \]

\[ P^I(\kappa_y) \sim \text{arg} \prod_{\kappa_x = 0^+}^{0^-} \langle u^u(\kappa_x + \delta \kappa) | u^u(\kappa_x) \rangle \times \prod_{\kappa_x = -\pi}^{\pi} \langle u^l(\kappa_x + \delta \kappa) | u^l(\kappa_x) \rangle \]
Kane Mele model at finite $T$

**individual EGPs**

- I
- II

**time-reversal EGP**

- Winding as for $T=0$
Interacting systems
Extended superlattice Bose-Hubbard model

\[
H = -t_1 \sum_{\text{odd}} \hat{a}_i^\dagger \hat{a}_{i+1} - t_2 \sum_{\text{even}} \hat{a}_i^\dagger \hat{a}_{i+1} + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i + V \sum_{\langle i, j \rangle} \hat{a}_i^\dagger \hat{a}_i \hat{a}_j^\dagger \hat{a}_j
\]

insulating phase with fractional filling
fractional filling & topological order

atomic limit

\[ \rho = 1/4 \]

degenerate CDWs

\[ |\Phi_0^{(\pm)}\rangle = \text{CDW}_1 \pm \text{CDW}_2 \]
Degeneracy & Wilson loop

\[ \hat{T} = e^{i \frac{2\pi}{L} \hat{X}} \]

\[ U \hat{T} U^{-1} = \hat{T} e^{i \frac{2\pi N}{L}} \]

\[ \hat{x} = \sum_j \hat{n}_j \]

\[ \langle \hat{T} \rangle = 0 \]

Wilson loop

\[ \nu_{\text{tot}} = \frac{1}{2\pi} \oint d\lambda \frac{\partial}{\partial \lambda} \text{Im} \ln \det W(\lambda) \]

\[ W(\lambda) = \mathcal{P} \exp \left\{ i \int_0^{2\pi} d\theta \ A(\theta) \right\} \]

\[ A_{\mu\nu}(\theta) = i \langle 0 | \partial_\lambda \Phi_0^\nu | \Phi_0^\mu \rangle \]
d-fold degeneracy

Niu, Thouless, Wu, PRB 1985

$$|\Phi_0^{(1)}\rangle \rightarrow |\Phi_0^{(2)}\rangle \rightarrow \cdots \rightarrow |\Phi_0^{(d)}\rangle \rightarrow |\Phi_0^{(1)}\rangle$$

$$\nu_{tot} = \frac{1}{2\pi} \int_0^{2\pi} d\lambda \int_0^{2\pi} d\theta \, \text{Im} \langle \Phi_0^\mu | \partial_\theta \Phi_0^\mu \rangle$$

$$\hat{T} \quad \rightarrow \quad \hat{T}^d$$
Extended SL-Bose-Hubbard model

\[ d = 2 \]

运输

\[\Delta n \]

时间（以 \( \mathcal{T} \) 为单位）

\[ P^{(2)} \]

time in units of \( \mathcal{T} \)

R. Unanyan et al. PRL (2020)
Measurable consequences?
Topology transfer

- coupling of open (finite-T) system to closed auxiliary fermion system at $T = 0$

$$H = -\eta \sum_{k, \alpha, \alpha'} c_{\alpha k}^\dagger c_{\alpha' k} a_{\alpha k}^\dagger a_{\alpha' k}$$
Topology transfer

- dynamics of auxiliary fermions in mean-field approximation

\[ H = -\eta \sum_{k,\alpha,\alpha'} c_{\alpha k}^\dagger c_{\alpha' k} a_{\alpha k}^\dagger a_{\alpha' k} \]

\[ a_n^\dagger a_m \rightarrow \langle a_n^\dagger a_m \rangle \sim G_{mn} \quad \text{fictitious Hamiltonian} \]

\[ H \sim -\eta \sum_{k,\alpha,\alpha'} \hat{c}_{\alpha k}^\dagger \hat{c}_{\alpha' k} G_{\alpha\alpha'}(k) \]

auxiliary system at T=0 \rightarrow quantized transport induced by topology transfer
Topology transfer at $T=0$

coupling of Ext. SL-BHM to auxiliary fermion chain

$L. Wawer et al. arxiv 2009.04149$
Topology transfer at $T=0$

charge transport in **boson** system

L. Wawer et al. arxiv 2009.04149
Topology transfer at $T=0$

- charge transport in auxiliary system

L. Wawer et al. arxiv 2009.04149
Topology transfer at $T > 0$

Rice Mele model at $T > 0$

$t = 0$

$t = \tau$

particle distribution after 1 cycle ($\eta \tau = 60$, $\eta / \Delta_{\text{gap}} = 0.01$, $L = 200$)

$T = 0.0 \Delta_{\text{gap}}$
$T = 0.1 \Delta_{\text{gap}}$
$T = 0.2 \Delta_{\text{gap}}$
$T = 0.3 \Delta_{\text{gap}}$
$T = 0.4 \Delta_{\text{gap}}$
$T = 0.5 \Delta_{\text{gap}}$
$T = 0.6 \Delta_{\text{gap}}$
$T = 0.7 \Delta_{\text{gap}}$
$T = 0.8 \Delta_{\text{gap}}$
$T = 0.9 \Delta_{\text{gap}}$
$T = 1.0 \Delta_{\text{gap}}$
$T = 1.5 \Delta_{\text{gap}}$
$T = 2.0 \Delta_{\text{gap}}$
Summary

- Topology of Gaussian mixed states of fermions governed by symmetries of fictitious Hamiltonian (single-particle correlations)

- $Z$ and $Z_2$ topological invariants in 1+1 and 2D: ensemble geometric phase = Zak phase of fictitious Hamiltonian

- Extension to interacting systems with fractional topological charges

- Measurable consequences: quantized transport through topology transfer
Thanks to

Max Kiefer
Lukas Wawer
Razmik Unanyan

Charles Bardyn
Sebastian Diehl
Alex Altland

(Domain) (Cologne) (Cologne)

Dominik Linzner
Rui Li
Christopher Mink
Thanks!