Geometric Phases for Quasi-Free Fermions at Finite Temperature

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School of Theoretical Physics - Seminar - DIAS (23.02.2023)

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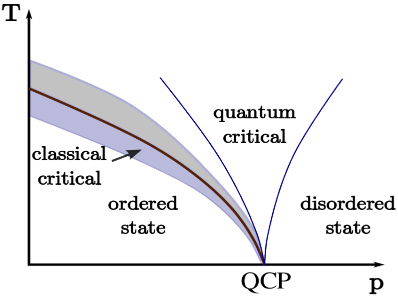
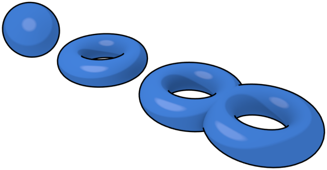
- Topological insulators
- Quantum phases of matter
- Relevance of geometry and topology (geometric phases, K-theory, operator algebras, NCG,..)
- The use of topological indices to label phases of matter predates many of the recent developments (Araki, Carey, Evans, Lewis, Matsui, Sisson, during the 1970's and 1980's)
- $\mathbb{Z}_2$-index:
$$\sigma(E_1, E_2) = (-1)^{\dim E_1 \wedge (1-E_2)}$$

Universality, criticality $\overset{?}{\longleftrightarrow}$ Topology





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Definition 1 (Self-dual CAR algebra)

Let $\mathcal{H}$ be a (sep.) Hilbert space and $\Gamma : \mathcal{H} \to \mathcal{H}$ a *conjugation* (antiunitary involution).
The self-dual CAR algebra $\mathrm{sCAR}(\mathcal{H}, \Gamma)$ is a C^*-algebra generated by a unit $\mathbb{1}$ and a family $\{B(\varphi)\}_{\varphi \in \mathcal{H}}$ of elements satisfying:

1. The map $\varphi \mapsto B(\varphi)^*$ is complex linear.
2. $B(\varphi)^* = B(\Gamma(\varphi)) \qquad \forall \varphi \in \mathcal{H}.$
3. (self-dual) CAR relations:

$$\{B(\varphi_1), B(\varphi_2)^*\} = \langle \varphi_1, \varphi_2 \rangle \mathbb{1}.$$

Definition 2 (Basis projection)

A basis projection associated with $(\mathcal{H}, \Gamma)$ is an orthogonal projection $P \in \mathcal{B}(\mathcal{H})$ satisfying $\Gamma P \Gamma = P^{\perp} \equiv \mathbb{1} - P$.
$\mathfrak{h}_P := \mathrm{ran}(P)$. The set of all basis projections associated with $(\mathcal{H}, \Gamma)$ will be denoted by $\mathfrak{p}(\mathcal{H}, \Gamma)$.

Remark

$\mathfrak{h}_P$ must satisfy the conditions

$$\Gamma(\mathfrak{h}_P) = \mathfrak{h}_P^{\perp} \qquad \text{and} \qquad \Gamma(\mathfrak{h}_P^{\perp}) = \mathfrak{h}_P.$$

Notice also that $\varphi \mapsto (\Gamma\varphi)^*$ is a unitary map from $\mathfrak{h}_P^{\perp}$ to the dual space $\mathfrak{h}_P^*$. In this case we can identify $\mathcal{H}$ with the "Nambu space"

$$\mathcal{H} \equiv \mathfrak{h}_P \oplus \mathfrak{h}_P^*.$$

Hence, P induces a decomposition

$$B(\varphi) \equiv B_P(\varphi) := B(P\varphi) + B\left(\Gamma P^{\perp}\varphi\right)^* .$$

- A unitary operator $U \in \mathcal{B}(\mathcal{H})$ s.t. $\Gamma U = U\Gamma$ is called Bogoliubov transformation.

- Such an operator induces a $*$-automorphism χ_U of $\mathrm{sCAR}(\mathcal{H},\Gamma)$ given on generators by

$$\chi_U(B(\varphi)) = B(U\varphi), \qquad \varphi \in \mathcal{H}.$$

- If $\mathbb{1} - U$ is trace class, then one can show that

$$\det(U) = \pm 1.$$

Definition 3 (Bilinear elements of self–dual CAR algebra)

Given an orthonormal basis $\{\psi_i\}_{i\in I}$ of $\mathcal{H}$, we define the bilinear element associated with $H \in \mathcal{B}(\mathcal{H})$ to be

$$\langle B, \ HB\rangle := \sum_{i,j\in I} \left\langle \psi_i, H\psi_j \right\rangle_{\mathcal{H}} B\left(\psi_j\right) B\left(\psi_i\right)^* .$$

- $\langle B, \ HB\rangle$ *does not depend* on the particular choice of orthonormal basis.
- Bilinear elements of sCAR have "adjoints" equal to

$$\langle B, \ HB\rangle^* = \langle B, H^* B\rangle, \qquad H \in \mathcal{B}(\mathcal{H}).$$

- *Bilinear Hamiltonians* are then defined as bilinear elements associated with *self–adjoint* operators $H = H^* \in \mathcal{B}(\mathcal{H})$.

Definition 4 (Self–dual Hamiltonian)

A self–dual Hamiltonian on $(\mathcal{H}, \Gamma)$ is a self-adjoint operator $H \in \mathcal{B}(\mathcal{H})$ satisfying the equality $H = -\Gamma H \Gamma$.

We say that the basis projection P (block–) “diagonalizes” the self–dual Hamiltonian $H \in \mathcal{B}(\mathcal{H})$ whenever

$$PHP^{\perp} = 0 = P^{\perp}HP.$$

In this situation, we also say that the basis projection P diagonalizes $\langle B,\ HB\rangle$.

For any $H = H^* \in \mathcal{B}(\mathcal{H})$, define a continuous group $\{\tau_t\}_{t\in\mathbb{R}}$ of *–automorphisms of sCAR through

$$\tau_t(A) := e^{-it\langle B,\,HB\rangle} A e^{it\langle B,\,HB\rangle}\ , \quad A \in \mathrm{sCAR}(\mathcal{H},\Gamma),\ t \in \mathbb{R}.$$

Provided H is a self–dual Hamiltonian on $(\mathcal{H},\Gamma)$, this group is a *quasi–free dynamics*, that is, a strongly continuous group of Bogoliubov *–automorphisms.
It follows that

$$\exp\left(-\frac{it}{2}\langle B,\ HB\rangle\right) B(\varphi)^* \exp\left(\frac{it}{2}\langle B, HB\rangle\right) = B\left(e^{itH}\varphi\right)^*,$$

for any self–dual Hamiltonian H in $(\mathcal{H},\Gamma)$, $t \in \mathbb{R}$ and $\varphi \in \mathcal{H}$.

Definition 5 (Quasi-Free State)

A state ω in $\mathrm{sCAR}(\mathcal{H}, \Gamma)$ is said to be *quasi–free* when, for all $N \in \mathbb{N}$ and $\varphi_1, \ldots, \varphi_{2N+1} \in \mathcal{H}$,

$$\omega\left(B\left(\varphi_1\right) \cdots B\left(\varphi_{2N+1}\right)\right) = 0,$$

and

$$\omega\left(B\left(\varphi_1\right) \cdots B\left(\varphi_{2N}\right)\right) = \mathrm{Pf}\left[\omega\left(B(\varphi_i), B(\varphi_j)\right)\right].$$

Quasi–free states are particular states that are uniquely defined by their two–point correlation functions. In fact, a quasi–free state ω is uniquely defined by its so–called *symbol*, that is, a positive operator $S_\omega \in \mathcal{B}(\mathcal{H})$ such that

$$0 \le S_\omega \le \mathbb{1}_{\mathcal{H}} \qquad \text{and} \qquad S_\omega + \Gamma S_\omega \Gamma = \mathbb{1}_{\mathcal{H}},$$

through the identity

$$\omega\left(B(\varphi_1)B(\varphi_2)^*\right) = \langle \varphi_1, S_\omega \varphi_2 \rangle_{\mathcal{H}}, \qquad \varphi_1, \varphi_2 \in \mathcal{H}.$$

Definition 6 (Ground state)

A state ω on $\mathrm{sCAR}(\mathcal{H}, \Gamma)$ is a *ground state* for a self-dual Hamiltonian H on $(\mathcal{H}, \Gamma)$, if

$$i\omega(A^* \delta(A)) \geq 0,$$

for all $A \in \mathcal{D}(\delta)$.

- Let $A \in \mathcal{B}(\mathcal{H})$ be a bounded self–dual operator on $(\mathcal{H}, \Gamma)$, such that $E_\Sigma(A) := \chi_\Sigma(A)$ defines the *spectral projection* of A on the Borel set $\Sigma \subset \mathbb{R}$.
- For H a self–adjoint Hamiltonian on $(\mathcal{H}, \Gamma)$, i.e., $H = -\Gamma H \Gamma$, we denote by E_0, E_- and E_+, the restrictions of the spectral projections of H on $\{0\}$, $\mathbb{R}_-$ and $\mathbb{R}_+$, respectively. We have

$$H = \int_{\mathrm{spec}(H)} \lambda dE_\lambda = \int_{\mathbb{R}} \lambda dE_\lambda .$$

- Thus, one verifies that

$$\Gamma E_\lambda \Gamma = E_{-\lambda} \quad \text{for all} \quad \lambda \in \mathbb{R} \quad \text{and} \quad E_0 + E_- + E_+ = \mathbb{1}_{\mathcal{H}} .$$

We will make the following assumptions ($\mathcal{C} \equiv [0,1]$):

(a) $\mathbf{H} := \{H_s\}_{s\in\mathcal{C}} \subset \mathcal{B}(\mathcal{H})$ is a differentiable family of self–dual gapped Hamiltonians such that $\partial\mathbf{H} := \{\partial_s H_s\}_{s\in\mathcal{C}} \subset \mathcal{B}(\mathcal{H})$.

(b) For the infinite volume case we assume that the sequences of self–dual Hamiltonians $H_{s,\,L} : \mathcal{C} \to \mathcal{B}(\mathcal{H}_\infty)$ and $\partial_s H_{s,\,L} : \mathcal{C} \to \mathcal{B}(\mathcal{H}_\infty)$ converge in norm and pointwise, that is, $\lim_{L\to\infty} H_{s,L} = H_{s,\infty}$ and $\lim_{L\to\infty} \partial_s H_{s,L} = \partial_s H_{s,\infty}$ in the norm sense.

Now, for any self–dual Hilbert space $(\mathcal{H}, \Gamma)$, take 2 basis projections $P_1, P_2 \in \mathfrak{p}(\mathcal{H}, \Gamma)$. If $P_1 - P_2$ is H.S., define the "$\mathbb{Z}_2$–index"

$$\sigma(P_1, P_2) := (-1)^{\dim(P_1 \wedge P_2^\perp)}.$$

Remark

This index was introduced by Araki and Evans (1983) and used to classify the thermodynamical phases of the (classical) 2D-Ising model.

Theorem*

Take $C \equiv [0,1]$ and let $\mathbf{H} := \{H_{s,\infty}\}_{s\in} \subset \mathcal{B}(\mathcal{H}_\infty)$ be a differentiable family of self–dual Hamiltonians on $(\mathcal{H}_\infty, \Gamma_\infty)$, with $\partial\mathbf{H} := \{\partial_s H_{s,\infty}\}_{s\in C} \subset \mathcal{B}(\mathcal{H}_\infty)$. For any $s \in C$, $E_{+,s,\infty}$ denotes the spectral projection associated to the positive part of $\mathrm{spec}(H_{s,\infty})$ and consider the $\mathbb{Z}_2$–index given by $\sigma(P_1, P_2)$. Then:

1. For any $s \in C$, $H_{0,\infty}$ is unitarily equivalent to $H_{s,\infty}$ via the unitary operator $V_s^{(\infty)} \in \mathcal{B}(\mathcal{H}_\infty)$ satisfying the differential equation (1) below.
2. The Bogoliubov *–automorphism $\chi_{V_s^{(\infty)}}$ is inner and maintains its parity, *even* $V_s^{(\infty)} \in \mathfrak{U}_+^\infty$ or *odd* $V_s^{(\infty)} \in \mathfrak{U}_-^\infty$, over the family $\mathbf{H}$, according to the value of $\det V_s^{(\infty)}$.
3. For $r, s \in C$, $\sigma(H_{r,\infty}, H_{s,\infty}) \equiv \sigma(E_{+,r,\infty}, E_{+,s,\infty})$ satisfies $\sigma(H_{r,\infty}, H_{s,\infty}) = 1$.

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*N.J.B. Aza, L. Sequera, A.R., Math. Phys. Anal. Geom. 25, 11 (2022)

Lemma

Take $\mathcal{C} \equiv [0, 1]$ and let $\mathbf{H}$ be a family of Hamiltonians as defined above. For any $s \in \mathcal{C}$, let $E_{+,s}$ be the spectral projection associated to the positive part of $\mathrm{spec}(H_s)$. Then, for the family of spectral projections $\{E_{+,s}\}_{s\in\mathcal{C}}$, there exists a family of automorphisms $\{\kappa_s\}_{s\in}$ on $\mathcal{B}(\mathcal{H})$ satisfying

$$\kappa_s\left(E_{+,s}\right) = E_{+,0}.$$

Idea of proof:

- Use the resolvent equation $R_\zeta(A) - R_\zeta(B) = R_\zeta(A)(B-A)R_\zeta(B)$, in order to establish existence of $\partial_s E_{+,s}$.
- Show that this derivative can be written in the form

$$\partial_s E_{+,s} = -i[\mathfrak{D}_{\mathfrak{g},s}, E_{+,s}],$$

  where $\mathfrak{D}_{\mathfrak{g},s}$ is a suitably defined self-adjoint bounded operator.
- Define $\kappa_s\left(E_{+,s}\right) := V_s^* E_{+,s} V_s$, where V_s is the solution to

$$\partial_s V_s = -i\mathfrak{D}_{,s} V_s. \tag{1}$$

- If $V_s \in \mathcal{B}(\mathcal{H})$ is a unitary operator such that $\Gamma V_s = V_s \Gamma$ and $1 - V_s$ is trace-class, then we have (Araki-Evans '83): $\sigma(E_{+,0}, V_s^* E_{+,0} V_s) = \det(V_s)$. We need to show that $1 - V_s$ is in fact trace-classs. This is done using Combes-Thomas estimates.

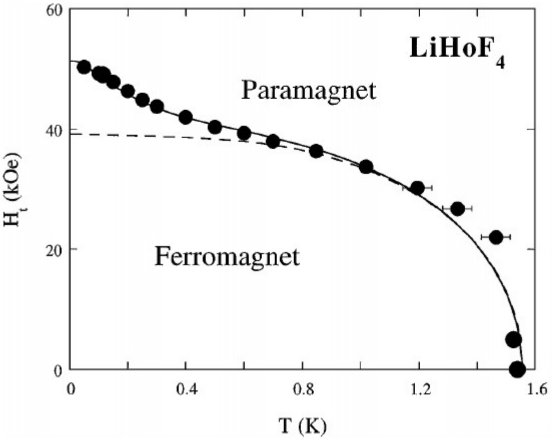
XY chain

$$
\begin{aligned}
H &= -\frac{1}{2}\sum_j \left(\frac{1+\gamma}{2}\sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2}\sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right) \\
&= -\frac{1}{2}\sum_j \left(a_j^* a_{j+1} + \gamma a_j^* a_{j+1}^* + (\lambda/2) a_j^* a_j + h.c. \right).
\end{aligned}
$$

Longitudinal magnetization$\longrightarrow$ $\mathrm{m}_x := \sqrt{\lim_{n\to\infty} \langle \sigma_j^x \sigma_{j+n}^x \rangle_\beta}$,

$$
\langle \sigma_j^x \sigma_{j+n}^x \rangle_\beta = \frac{1}{4} \det \begin{pmatrix} c(-1) & c(-2) & \cdots & c(-n) \\ c(0) & c(-1) & \cdots & c(-n+1) \\ \vdots & \vdots & \ddots & \vdots \\ c(n-2) & c(n-3) & \cdots & c(-1) \end{pmatrix},
$$

$$
c(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{\Lambda_k} \Big[\cos(nk)(\lambda - \cos k) + \gamma \sin(nk) \sin k \Big] \tanh\left(\frac{\beta \Lambda_k}{2}\right).
$$



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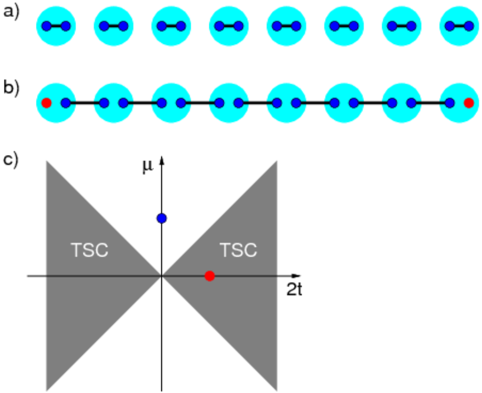
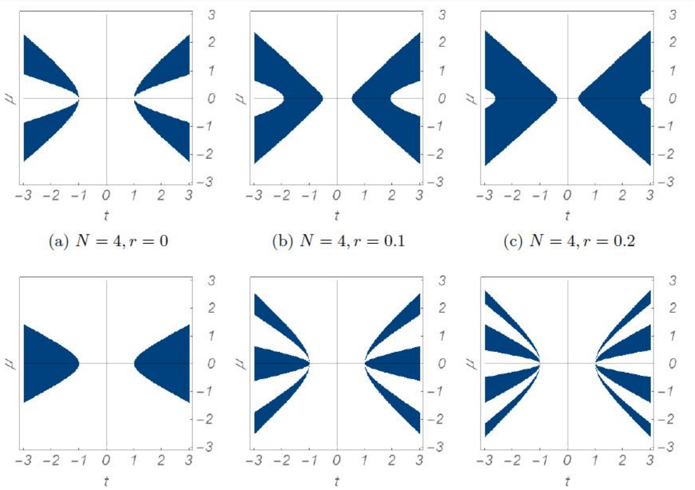
*D. Bitko, T.F. Rosenbaum, and G. Aeppli Phys. Rev. Lett. 77, 940 (1996)

$$H = \sum_{i=l}^{N} t(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + \Delta(a_i^\dagger a_{i+1}^\dagger - a_i a_{i+1}) - 2\mu a_i^\dagger a_i. \qquad (2)$$



Explicit evaluation* of the $\mathbb{Z}_2$-index $(-1)^{\frac{1}{2}\dim\ker(J+J_h)}$:



(a) $N=4, r=0$ (b) $N=4, r=0.1$ (c) $N=4, r=0.2$

(d) $N=2, r=0$ (e) $N=6, r=0$ (f) $N=8, r=0$

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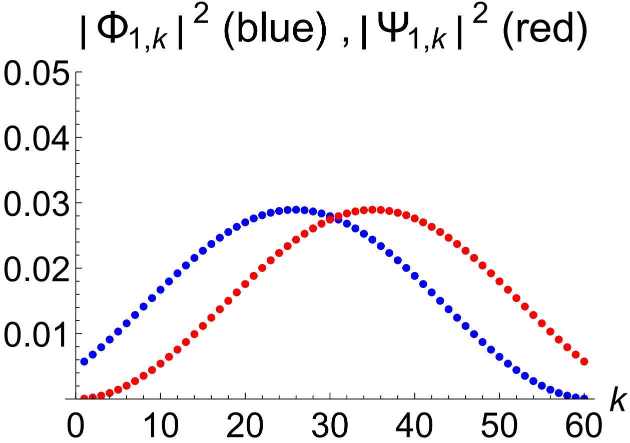
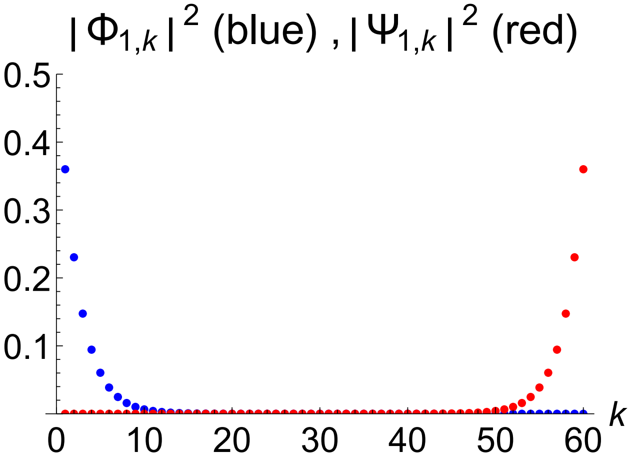
*Calderón-García, A.R., Mod.Phys.Lett. A 33 (14), 1840001 (2018)

- Majorana fermions: $a_k = \gamma_k^A + i\gamma_k^B$.
- $H = \sum_k \Lambda_k c_k^* c_k \longrightarrow c_k = \sum_l \Phi_{kl}\, \gamma_l^A + i\, \Psi_{kl}\, \gamma_l^A$.
- Fermion occupation numbers: $\langle c_1 a_k^* a_k c_1^* \rangle_\beta$
- Edge-to-edge correlation function: $\langle i\gamma_1^A \gamma_N^B \rangle_\beta$
- Majorana “wave function”: $\langle (a_k + a_k^*) c_1^* c_1 (a_k + a_k^*) \rangle_\beta$.

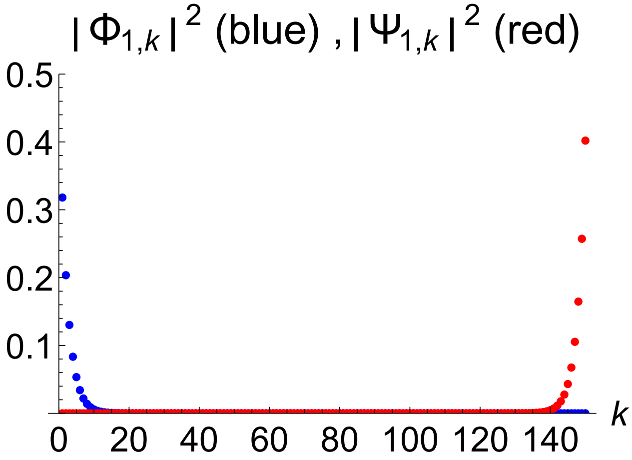
($\mu = 1.1, t = \Delta = 1 \rightsquigarrow \mathbb{Z}_2$-index equals +1)



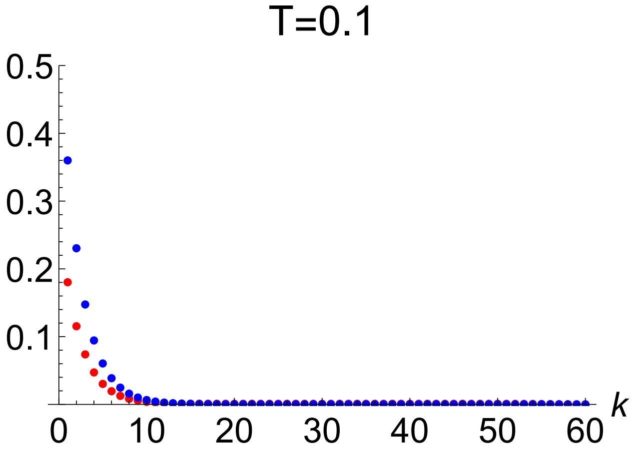
$(\mu = 0.8,\, t = \Delta = 1 \rightsquigarrow \mathbb{Z}_2\text{-index equals } -1)$



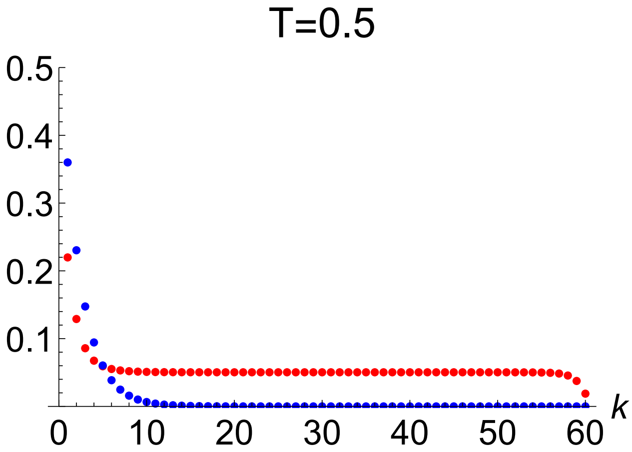
($\mu = 0.8$, $t = \Delta = 1 \rightsquigarrow \mathbb{Z}_2$-index equals -1)



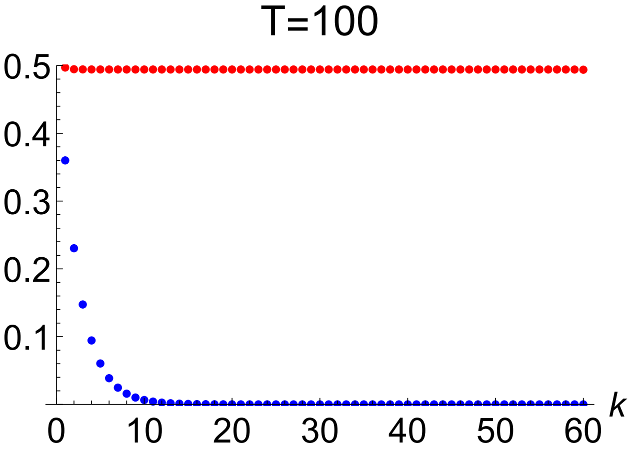
($\mu = 0.8, t = \Delta = 1$)



($\mu = 0.8$, $t = \Delta = 1$)



($\mu = 0.8, t = \Delta = 1$)



Quantum holonomy for mixed states

- $\mathcal{H}$: a finite dimensional Hilbert space ($n = \dim \mathcal{H} < \infty$).
- ρ: a density matrix.
  $\Rightarrow \ \exists$ ONB $\{|e_i\rangle\}_{1\le i\le n}$ and constants $\lambda_1, \dots, \lambda_n$ s.t.

$$\rho = \sum_{i=1}^{n} \lambda_i P_i, \quad \lambda_i \geq 0, \quad \sum_{i=1}^{n} \lambda_i = 1, \tag{3}$$

  where $P_i := |e_i\rangle\langle e_i|$.

Purification:

$$|\psi(\rho)\rangle := \sum_{i=1}^{n} \sqrt{\lambda_i}|e_i\rangle \otimes |e_i\rangle \in \mathcal{H} \otimes \mathcal{H}. \tag{4}$$

Let $\mathcal{M}$ be the space of positive, trace class operators. Define a projection $\pi : \mathcal{H} \otimes \mathcal{H} \longrightarrow \mathcal{M}, \ \psi \longmapsto \pi(\psi) \equiv \rho_\psi$, by requiring

$$\mathrm{Tr}(\rho_\psi L) = \langle \psi | L \otimes \mathbb{1} | \psi \rangle, \forall L \in \mathcal{B}(\mathcal{H}). \tag{5}$$

Ambiguity ⇝ if U is any unitary on $\mathcal{H}$, then

$$|\psi_U(\rho)\rangle := \sum_{i=1}^{n} \sqrt{\lambda_i}|e_i\rangle \otimes U^*|e_i\rangle \tag{6}$$

leads to the same density matrix ρ:

$$\pi(\psi_U(\rho)) = \rho.$$

Idea:

Think of the triple $(\mathcal{H} \otimes \mathcal{H}, \mathcal{M}, \pi)$ as a fibre bundle with gauge group $U(\mathcal{H})$.
Make use of $\mathcal{H} \otimes \mathcal{H}^* \cong \text{H.S.}(\mathcal{H})$ in order to define a connection.

▹ When suitably implemented, this idea leads to a generalization of Berry phase to mixed states[†].

[†] Uhlmann '86, Grosse & Dabrowski '89

- Restrict the base space to the subset $\mathcal{M}^{\times} \subset \mathcal{M}$ consisting of all *invertible* density operators.
- The (right) action of $U(\mathcal{H})$ on $\mathcal{H} \otimes \mathcal{H}$ preserves the scalar product: $\langle \psi_U, \psi'_U \rangle_{\mathcal{H}\otimes\mathcal{H}} = \langle \psi, \psi' \rangle_{\mathcal{H}\otimes\mathcal{H}}$.
- Identify $\sum_{i,j} A_{ij} |i\rangle \otimes |j\rangle \in \mathcal{H} \otimes \mathcal{H}$ with $\sum_{i,j} A_{ij} |i\rangle\langle j| \in \text{H.S.}(\mathcal{H})$.
- Put $\mathcal{P} := \pi^{-1}(\mathcal{M}^{+}) \subset \text{H.S.}(\mathcal{H})$.
- The (right) action of $G = U(\mathcal{H})$ on $\mathcal{P}$ is defined as follows:

$$
\begin{aligned}
R : \mathcal{P} \times G &\longrightarrow \quad \mathcal{P} \\
(A, U) &\longrightarrow R_U(A) := AU.
\end{aligned}
\tag{7}
$$

Vertical spaces

The vertical space at A, denoted V_A, can be described in terms of (equivalence classes of) paths of the form $\gamma_U(t) = AU(t)$, where $U(t)$ is a path in $G = U(\mathcal{H})$ with $U(0) = \mathbb{1}$. It follows that

$$V_A = \{AS \mid S : \mathcal{H} \to \mathcal{H}, S^* = -S\}. \tag{8}$$

Horizontal spaces

$\mathcal{P}$ inherits a Riemannian structure from $\langle \cdot, \cdot \rangle_{\mathrm{HS}(\mathcal{H})}$. It is given by

$$g(A, B) := \frac{1}{2}\left(\langle A, B\rangle_{\mathrm{HS}(\mathcal{H})} + \langle B, A\rangle_{\mathrm{HS}(\mathcal{H})}\right) \equiv \frac{1}{2}\,\mathrm{Tr}\left(A^* B + B^* A\right). \tag{9}$$

The horizontal space at A is defined as follows:

$$H_A := \{X \in T_A\mathcal{P} \mid g(X, Y) = 0 \text{ for all } Y \in V_A\}. \tag{10}$$

Let $\rho(t)$ denote a path in $\mathcal{M}^+$. It follows from the definition above that a curve $A(t)$ is a *horizontal* lift of $\rho(t)$ if and only it satisfies the following equations:

$$\dot{A}^* A - A^* \dot{A} = 0, \tag{11}$$

$$A \dot{A}^* + \dot{A} A^* = \dot{\rho}. \tag{12}$$

This can be simplified to

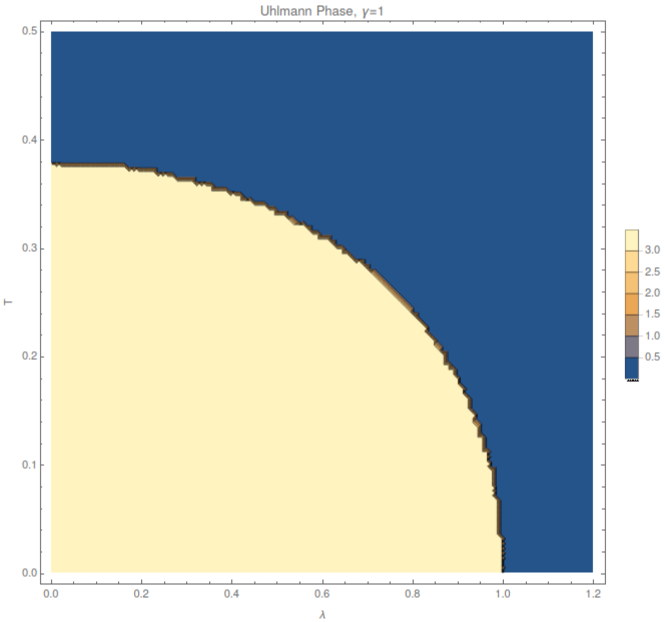
$$\dot{A} = TA, \tag{13}$$

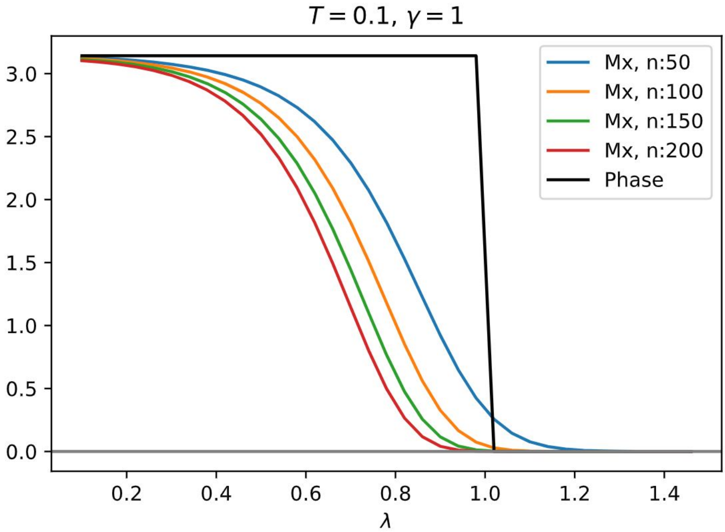
where T is given by

$$T = \sum_{i,j} P_i \, \dot{\rho} \, P_j \frac{1}{\lambda_i + \lambda_j} \tag{14}$$

(recall that $\rho = \sum_i \lambda_i P_i$).

Uhlmann phase




$T = 0.1$, $\gamma = 1$
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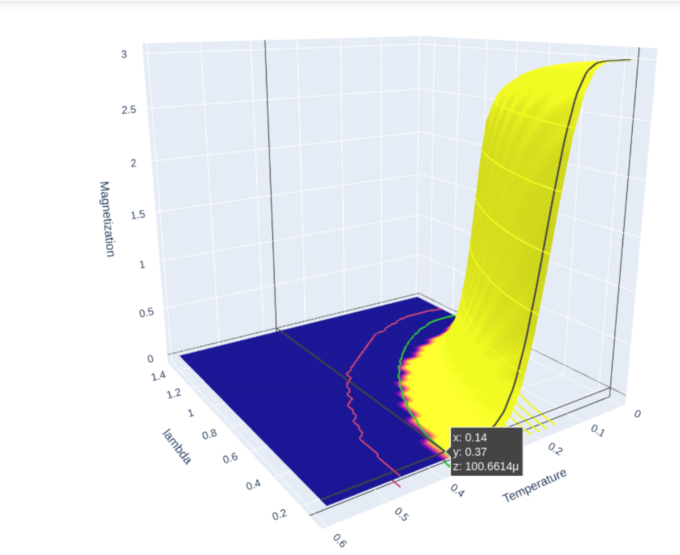
2.5
2.0
1.5
1.0
0.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
λ
Mx, n:50
Mx, n:100
Mx, n:150
Mx, n:200
Phase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2
1.5
1
0.5
0
Magnetization
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1.2
1
0.8
0.6
0.4
0.2
lambda
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0.4
0.2
0.1
0
Temperature
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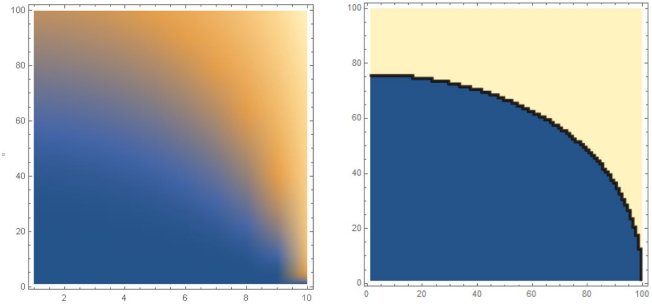
y: 0.37
z: 100.6614μ


100
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80
100

Thermal geometric phases in terms of projectors?

We have computed Uhlmann's phase for families of symbols $S_\beta = (1 + e^{-\beta H})^{-1}$ that define thermal states. But it is also possible to purify the state defined by S_β (through the GNS construction, for example) and then compute the usual geometric (Kato/Berry) phase in an enlarged Hilbert space. For the explicit examples we have studied, these two quantities coincide!

For us, this is a hint that it might be possible to label certain thermodynamical regimes using a generalization of the $\mathbb{Z}_2$ index!

Thanks for your attention!