Second law of thermodynamics in closed quantum many-body systems

YC, Y. Yoneta, R. Hamazaki, A. Shimizu, arXiv:2602.06657.

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Second law of thermodynamics for adiabatic operations

Second law of thermodynamics: Divide possible/impossible state transitions.

State transitions in thermodynamics:

- Transitions in isolated systems $\leftarrow$ energy conservation, scope of thermalization studies
- Adiabatic thermodynamic operations $\leftarrow$ energy exchange as work
- Isothermal thermodynamic operations $\leftarrow$ in contact with a heat bath

Second law for adiabatic operation

- Planck's principle: $(U_0, V_0, N) \xrightarrow{\mathrm{a}} (U_1, V_0, N)$ is possible $\Rightarrow U_0 \leq U_1$.
- Law of increasing entropy: possible only when $\Delta S \geq 0$

Can we derive it from quantum mechanics?

Difficulties in derivation from quantum mechanics

Lenard (1978): passive state $\simeq$ state satisfying Planck's principle

- Operation: arbitrary unitary
- Passive state: the canonical Gibbs and similar states $\leftarrow$ pure states are excluded

Every pure state violates Planck's principle if an arbitrary unitary is allowed.

Previous results on the law of increasing entropy [Neumann (1929), Meier, et al. (2025),...]

- Operation: generated by a time-independent Hamiltonian $\leftarrow$ isolated system
- Entropy: Boltzmann entropy, diagonal entropy, observable entropy,...
  $\uparrow$ do not necessarily agree with thermodynamic entropy
- Not applicable to energy eigenstates

Q. How can we reconcile thermal equilibrium represented by a pure state with the second law for adiabatic operations?

Short summary

Q. How can we reconcile thermal equilibrium represented by a pure state with the second law for adiabatic operations?

Definitions

- New notion of thermal equilibrium, which includes pure states
- Macroscopic operation, corresponding to adiabatic thermodynamic operations

Results

- Planck's principle
- New entropy formula
- Law of increasing entropy

Simplification in this talk

Our general results: YC, Y. Yoneta, R. Hamazaki, A. Shimizu, arXiv:2602.06657.

- Deal with states that may be non-uniform even macroscopically;
  $\Rightarrow$ Applicable to local equilibrium states, general nonequilibrium states ...

Simplified results: Present talk, based on Sec. II of arXiv:2602.06657.

- Deal with only macroscopically uniform states;
- Omit details about the thermodynamic limit $L \to \infty$.

Contents

Thermodynamic concepts by quantum mechanics

Here, we give quantum mechanical representations of the following:

Concepts in thermodynamics

- Additive quantities
- Thermal equilibrium states
- Adiabatic thermodynamic operations

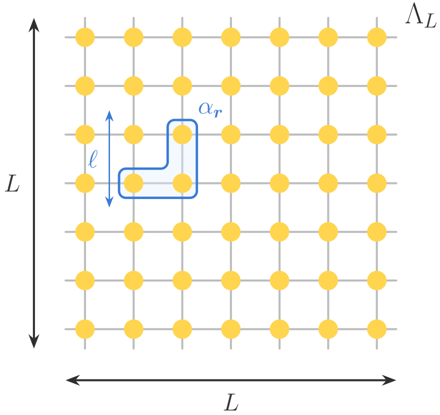
Local observable

Quantum systems on a d-dimensional hypercubic lattice Λ_L with $N = L^d$ sites.

Def. Local observable

An observable $\alpha_{\boldsymbol{r}}$ is called an ℓ-local observable if its support is contained in the d-dimensional hypercube of side length ℓ (near site $\boldsymbol{r}$).

Ex. $Z_{\boldsymbol{r}}$: 1-local obs., $X_{\boldsymbol{r}} Y_{\boldsymbol{r}+\boldsymbol{1}}$: 2-local obs.



Using this, we introduce additive observables.

Additive observable

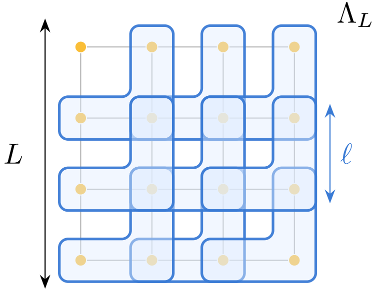
Def. Additive observable

For $\ell = O(L^0)$,

$$A_L = \sum_{\boldsymbol{r} \in \Lambda_L} \alpha_{\boldsymbol{r}}$$

is called an additive observable composed of ℓ-local observables.

Ex. $M_z = \sum_{\boldsymbol{r}} Z_{\boldsymbol{r}}, \quad H = \sum_{\boldsymbol{r}} X_{\boldsymbol{r}} Y_{\boldsymbol{r}+1}$



$$A_L = \sum_{\boldsymbol{r}} \alpha_{\boldsymbol{r}}$$

Their density A_L/N represents spatial average of $\alpha_{\boldsymbol{r}}$. $\rightarrow$ Spatial coarse-graining.

Macroscopic equivalence

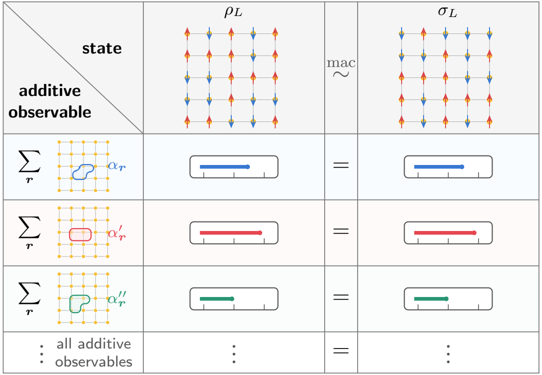
Def. Macroscopic equivalence $\overset{\text{mac}}{\sim}$

States ρ_L and σ_L are macroscopically equivalent,

$$\rho_L \overset{\text{mac}}{\sim} \sigma_L,$$

$$\overset{\text{def}}{\Leftrightarrow} \lim_{L\to\infty} \mathrm{Tr}\left[\rho_L \frac{A_L}{N}\right] = \lim_{L\to\infty} \mathrm{Tr}\left[\sigma_L \frac{A_L}{N}\right]$$

for every additive A_L composed of ℓ-local observables, for any $\ell = O(L^0)$.



Remark: Precisely, consider a sequence $(\rho_L)_{L\in\mathbb{N}}$ instead of ρ_L. See our paper for details.

$\overset{\text{mac}}{\sim}$ is crucial for our analysis!

Thermal equilibrium in this work — iMATE

Now, we consider thermal equilibrium

- In a simple system (described by an additive Hamiltonian H_L);
- Outside the first-order phase transition point;
- Specified by (β, N).

Def. Infinite observable macroscopic thermal equilibrium (iMATE)

ρ_L represents an iMATE of the system described by $H_L \overset{\text{def}}{\Leftrightarrow}$ there is $\beta \in \mathbb{R}$ s.t.

$$\rho_L \overset{\text{mac}}{\sim} \rho_L^\beta := e^{-\beta H_L}/Z.$$

This means that ρ_L and ρ_L^β have the same expectation values of A_L/N for all additive A_L.

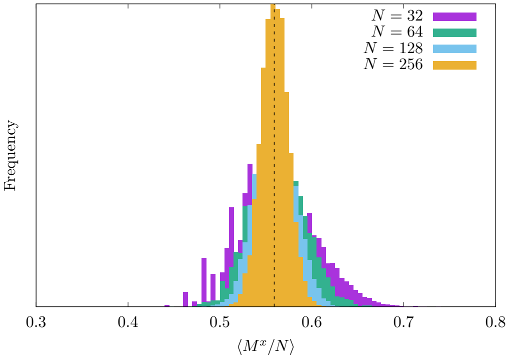
Comparison to previous notions of thermal equilibrium

Notion	Characterization	Examples
Ensemble	-	Gibbs states
MITE	All local observables	Typicality, TPQ states
iMATE	All additive observables	METTS
MATE	Finite macro-observables	-

-Lower notions contain more states than upper ones.

Example: Typical METTS represent iMATE

Minimally entangled typical thermal states (METTS): $|\phi(i)\rangle$'s defined below.



Let $\{|i\rangle\}_{i=1}^{D^N}$ be the computational basis on Λ_L.

$$\mathrm{Tr}\left[\rho_L^\beta A\right] = \sum_i \frac{P_i}{Z} \langle\phi(i)| A |\phi(i)\rangle$$

holds identically, where

$$P_i = \langle i| e^{-\beta H_L} |i\rangle ,$$

$$|\phi(i)\rangle = e^{-\beta H_L/2} |i\rangle / \sqrt{P_i}.$$

For most of i, $|\phi(i)\rangle$ represents iMATE, while it is not in MITE for any i.

Macroscopic operations

In thermodynamics, operations are limited to "macroscopic" ones.

Q. What does "macroscopic" mean quantum-mechanically?

Def. Macroscopic operation

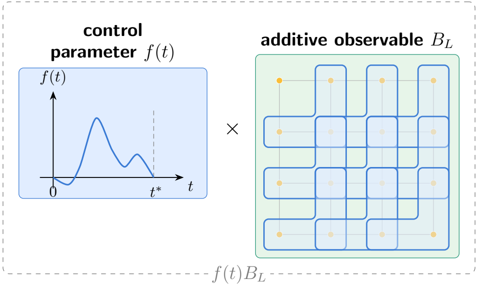
Unitary evolution by

$$H_L(t) = H_L - \sum_{\mu=1}^{m} f^\mu(t) B_L^\mu$$

is called a macroscopic operation.

Macroscopic operation: $i\partial_t \rho_t = [H_L(t), \rho_t]$

$H_L(t) = H_L -$



The system is closed and exchanges no heat.

⇒ Macroscopic operations will represent adiabatic operations in TD.

Contents

Main results

Main results

1. Macroscopic equivalence after macroscopic operations
2. Macroscopic passivity
3. Entropy formula
4. Law of increasing quantum macroscopic entropy

1. Macroscopic equivalence after macroscopic operations

Consider a time evolution $\rho_L(0) \to \rho_L(t)$ induced by a macroscopic operation.

Result 1: Macroscopic equivalence is preserved under macroscopic operations

Suppose that

$$\rho_L(0) \overset{\text{mac}}{\sim} \sigma_L(0).$$

Then, under any macroscopic operation,

$$\rho_L(t) \overset{\text{mac}}{\sim} \sigma_L(t) \quad \text{as long as } t = O(L^0).$$

responses in $\rho_L(t)$ = responses in $\sigma_L(t)$

for any macroscopic operation up to $t = O(L^0)$.

2. Macroscopic passivity

Result 1 + the passivity of the canonical Gibbs state ρ_L^β $(\beta \geq 0) \Rightarrow$ Result 2.

Result 2: Macroscopic passivity

Suppose that $\rho_L(0)$ represents iMATE described by H_L with $\beta \geq 0$. Then, any macroscopic operation does not decrease $\langle H_L \rangle$ extensively as long as $t = O(L^0)$:

$$\lim_{L\to\infty} \mathrm{Tr}\left[\rho_L(t)\frac{H_L}{N}\right] \geq \lim_{L\to\infty} \mathrm{Tr}\left[\rho_L(0)\frac{H_L}{N}\right].$$

In other words, an extensive work cannot be extracted from any iMATE by any macroscopic operation of operation time $= O(L^0)$.

$\rightarrow$ Correspond to Planck's principle

Trade-off between equilibrium and operations

Equilibrium	Operation	Planck's principle
Gibbs state	Arbitrary unitary	Original passivity (1978)
MITE	Local control	Hokkyo and Ueda (2025)
iMATE	Local control	× Inconsistent
iMATE	Macroscopic operation	Our macroscopic passivity
MATE	Macroscopic operation	× Inconsistent

-Lower rows contain more states than upper ones

-Lower rows contain fewer operations than upper ones

(Local control: unitary evolution generated by $H(t) = \sum_r$ local observables, without translation inv.)

3. Entropy formula (1/3)

Target : Thermodynamic entropy density

$$s_{\mathrm{TD}} := \lim_{L\to\infty} \frac{1}{N} S_{\mathrm{vN}}(\rho_L^\beta).$$

Problem: an iMATE does not always give s_{TD}:

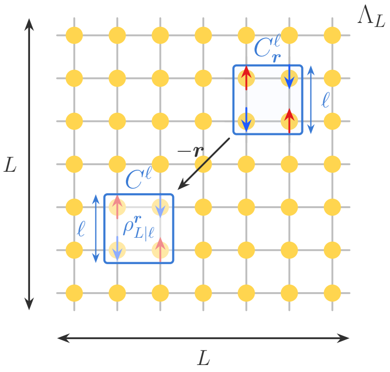
Ex. $s_{\mathrm{TD}} \neq \lim_{L\to\infty} \frac{1}{N} S_{\mathrm{vN}}(\,|\mathrm{METTS}\rangle\langle\mathrm{METTS}|) = 0.$

Def. Local density matrices

The reduced density matrix on $C_{\boldsymbol{r}}^\ell$ moved to $C^\ell := C_{\boldsymbol{0}}^\ell$,

$$\rho_{L|\ell}^{\boldsymbol{r}} := \mathop{\mathrm{Tr}}_{\Lambda_L \setminus C^\ell}[T_{\boldsymbol{r}}^\dagger \rho_L T_{\boldsymbol{r}}],$$

is called the ℓ-local density matrix around $\boldsymbol{r}$.



$S_{\mathrm{vN}}(\rho_{L|\ell}^{\boldsymbol{r}})$: entanglement entropy. $\leftarrow$ Does it always give s_{TD}?

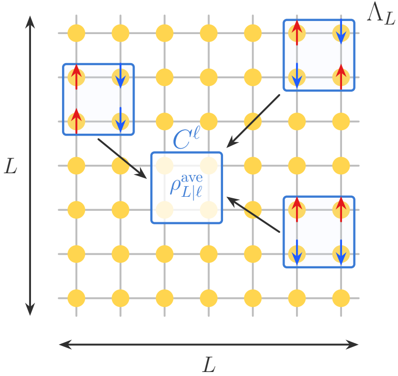
3. Entropy formula (2/3)

For METTS [Kusuki, *et al.*, PRB (2024)],

$$s_{\mathrm{TD}} \neq \lim_{L\to\infty} \frac{1}{\ell^d} S_{\mathrm{vN}}(\rho^{\boldsymbol{r}}_{L|\ell}) \quad \text{however large } \ell \text{ is.}$$

We can achieve "$=$" by taking

- spatial average: $\rho^{\mathrm{ave}}_{L|\ell} := \frac{1}{N}\sum_{\boldsymbol{r}} \rho^{\boldsymbol{r}}_{L|\ell}$
- iterated limits: $\lim_{\ell\to\infty}\lim_{L\to\infty}$

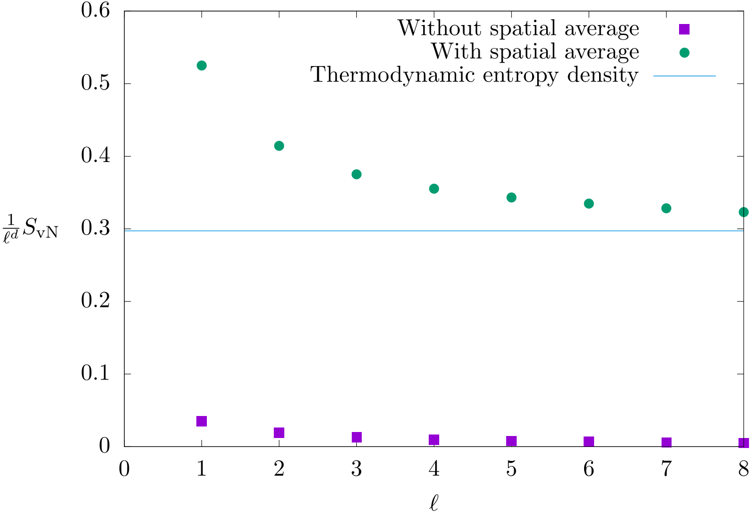


Result 3: Entropy formula for iMATE

When ρ_L represents iMATE, quantum macroscopic entropy density, the von Neumann entropy density of $\rho^{\mathrm{ave}}_{L|\ell}$, agrees with s_{TD}:

$$s_{\mathrm{TD}} = \lim_{\ell\to\infty}\lim_{L\to\infty} \frac{1}{\ell^d} S_{\mathrm{vN}}(\rho^{\mathrm{ave}}_{L|\ell}).$$

3. Entropy formula (3/3)



METTS of the transverse Ising model ($\beta = 1$). $L = 512$ using MPS.

Quantum macroscopic entropy density agrees with $s_{\rm TD}$, while entanglement entropy density does not.

Macroscopic operation followed by relaxation process

Consider the following time evolution, with $t^* = O(L^0)$

$$H(t) = \begin{cases} H_0 & (t = 0) \quad : \text{ additive} \\ H(t) & (0 < t < t^*) \quad : \text{ macroscopic operation} \\ H_1 & (t \geq t^*) \quad : \text{ additive} \end{cases}$$

$t = 0$ The initial state ρ_L: iMATE described by H_0

$t > 0$ The state is denoted by $\rho_L(t)$

$t \to \infty$ The final state is evaluated by

$$\sigma_L := \lim_{\mathcal{T} \to \infty} \frac{1}{\mathcal{T}} \int_{t^*}^{t^*+\mathcal{T}} \rho_L(t) dt.$$

It models adiabatic operation followed by a waiting time for thermal relaxation.

4. Law of increasing quantum macroscopic entropy

$t = 0$ The initial state ρ_L: iMATE described by H_0

$t > 0$ The state is denoted by $\rho_L(t)$

$t \to \infty$ The final state is evaluated by

$$\sigma_L := \lim_{\mathcal{T}\to\infty} \frac{1}{\mathcal{T}} \int_{t^*}^{t^*+\mathcal{T}} \rho_L(t) dt.$$

Result 4: Law of increasing quantum macroscopic entropy

Under a mild assumption about the existence of the thermodynamic limit of σ_L, we have

$$\lim_{\ell\to\infty} \lim_{L\to\infty} \frac{1}{\ell^d} S_{\mathrm{vN}}\left(\rho_{L|\ell}\right) \leq \lim_{\ell\to\infty} \lim_{L\to\infty} \frac{1}{\ell^d} S_{\mathrm{vN}}\left(\sigma_{L|\ell}\right)$$

for any macroscopic operation with operation time $t^* = O(L^0)$.

Corollary: Law of increasing thermodynamic entropy

Result 4: Law of increasing quantum macroscopic entropy

Under a mild assumption about the existence of the thermodynamic limit of σ_L, we have

$$\lim_{\ell\to\infty}\lim_{L\to\infty}\frac{1}{\ell^d}S_{\mathrm{vN}}\left(\rho_{L|\ell}\right) \leq \lim_{\ell\to\infty}\lim_{L\to\infty}\frac{1}{\ell^d}S_{\mathrm{vN}}\left(\sigma_{L|\ell}\right)$$

for any macroscopic operation with operation time $t^* = O(L^0)$.

Corollary: Law of increasing thermodynamic entropy

If thermalization occurs, i.e., if the final state σ_L represents iMATE described by H_1, the mild assumption is satisfied, and we have

$$s_{\mathrm{TD}}^{\mathrm{initial}} \leq s_{\mathrm{TD}}^{\mathrm{final}}$$

for any macroscopic operation with operation time $t^* = O(L^0)$.

$\rightarrow$ Correspond to the law of increasing entropy in TD

Contents

Discussion on timescale

Q. Can the limitation on the operation time $t^* = O(L^0)$ be lifted?
A. No. A straightforward extension is impossible.

Proposition: Counterexamples exist

- Equilibrium: Not only in iMATE but also in MITE and MATE
- Operation: Macroscopic operation of timescale longer than $O(L^0)$
- $\langle H \rangle$, $S_{\mathrm{vN}}(\rho_{L|\ell}^{\mathrm{ave}})$, and s_{TD} decrease extensively.

We need the last piece to prove the perfect consistency!

Candidates

1. Initial states are not accurately known.
2. Macroscopic operations cannot be performed ideally with microscopic accuracy.

$\Rightarrow$ Subjects of future studies.

Summary

Definitions

- iMATE: state in which the expectation values of all additive observables agree with their equilibrium values
- Macroscopic operation: unitary operation generated by a time-dependent additive Hamiltonian

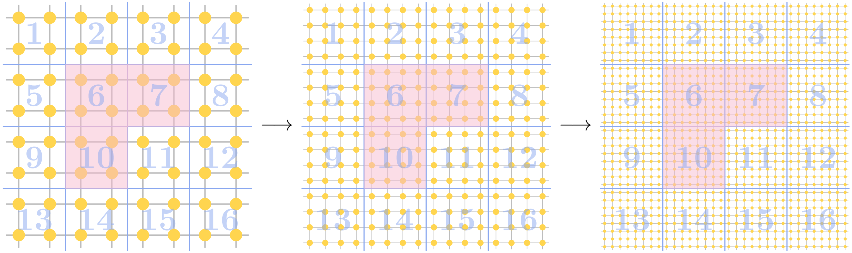
Results

- Macroscopic equivalence is preserved under macroscopic operations
- Macroscopic passivity: Extensive work cannot be extracted from iMATE through macroscopic operation of $t^* = O(L^0)$
- Quantum macroscopic entropy density $S_{\mathrm{vN}}\left(\rho_{L|\ell}\right)/\ell^d = s_{\mathrm{TD}}$
- Law of increasing quantum macroscopic entropy: $S_{\mathrm{vN}}\left(\rho_{L|\ell}\right)/\ell^d$ does not decrease through macroscopic operation of $t^* = O(L^0)$

Thermal equilibrium "characterized by..." vs. "specified by..."

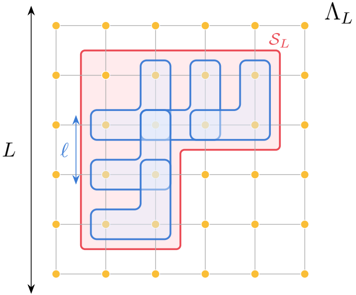
- Thermal equilibrium "characterized by" additive observables:
  Thermal equilibrium defined by focusing on additive observables.
- Systems in which thermal equilibrium is "specified by" $(U, \boldsymbol{M}, N)$: if two thermal equilibrium states have the same value of $(U, \boldsymbol{M}, N)$, then they also have the same values for other additive observables.

General results



macroscopic subsystem: $|\mathcal{S}_L| = \Theta(N)$
additive observable on $\mathcal{S}_L$

$$A_{\mathcal{S}_L}(\alpha) = \sum_{\boldsymbol{r}\in\mathcal{S}_L} \alpha_{\boldsymbol{r}}$$



$$A_{\mathcal{S}_L}(\alpha) = \sum_{\boldsymbol{r}:\,\mathrm{Supp}(\alpha_{\boldsymbol{r}})\subset\mathcal{S}_L} \alpha_{\boldsymbol{r}}$$

Example: MATE is insufficient

XY model on the square lattice ($d = 2$),

$$H = -\sum_{j,k=1}^{L}\left[J^x(\sigma^x_{j,k}\sigma^x_{j+1,k}+\sigma^x_{j,k}\sigma^x_{j,k+1})+J^y(\sigma^y_{j,k}\sigma^y_{j+1,k}+\sigma^y_{j,k}\sigma^y_{j,k+1})+h^x\sigma^x_{j,k}\right] \quad (J^x \neq J^y)$$

Its equilibrium state at hight T can be specified by (E, N) because

- H is the only local conserved quantity. [N. Shiraishi and H. Tasaki, 2025]
- Spin rotation symmetry is not broken at high T

If one looks only at three additive observables $\{M^x,\ M^y,\ H\}$, then

$$|\psi(0)\rangle \equiv |\uparrow\rangle^{\otimes L^2} \text{ is an MATE state with } \langle H\rangle = 0.$$

When you shine a $\pi/2$ pulse of h^x on this state,

$$\langle\psi(t)|H|\psi(t)\rangle \simeq -2J^yN < 0 \text{ in contradiction to passivity.}$$

Counterexample for longer operation time (1/2)

$$\text{spin chain: } H = \frac{\pi}{4}\sum_{j=1}^{L} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + \frac{\pi}{4}\sum_{j=1}^{L} \vec{\sigma}_j \cdot \vec{\sigma}_{j+3}$$

Take $T_L = O(L)$. Then

$$|\psi(0)\rangle = \bigotimes_{j=1}^{L/2} \frac{(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)_{2j-1-2\lfloor T_L \rfloor \bmod L,\ 2j+2\lfloor T_L \rfloor \bmod L}}{\sqrt{2}}$$

is MITE (and MATE and iMATE) with $\langle H \rangle = 0$. Do the macroscopic operation,

$$H(t) = \begin{cases} \frac{\pi}{2}\sum_{j=1}^{L/2} \vec{\sigma}_{2j-1} \cdot \vec{\sigma}_{2j} & (n \le t < n+1/2) \\ \frac{\pi}{2}\sum_{j=1}^{L/2} \vec{\sigma}_{2j} \cdot \vec{\sigma}_{2j+1} & (n+1/2 \le t < n+1) \end{cases} \qquad (n \in \mathbb{Z}_{\ge 0}).$$

Then

$$\langle \psi(T_L)|H|\psi(T_L)\rangle \lesssim -\frac{3\pi}{16}L < 0 \text{ in contradiction to passivity.}$$

Counterexample for longer operation time (2/2)