ON THE APPROACH TO EQUILIBRIUM OF AN ISOLATED QUANTUM SYSTEM

THERMODYNAMIC NORMALITY AND RELATED ISSUES

HAL TASAKI, YUKAWA INSTITUTE, AUG. 2011

Related talks: P-17 Monnai, P-38 Ikeda, P-82 Deguchi

WE STUDY THE APPROACH TO EQUILIBRIUM IN AN ISOLATED MACROSCOPIC QUANTUM SYSTEM

THE PROBLEM MAY BE RELEVANT TO

- FOUNDATION OF STATISTICAL MECHANICS
- DYNAMICS OF COLD TRAPPED ATOMS

ALTHOUGH THERE ARE MANY IMPORTANT WORKS, WE HERE CONCENTRATE ON A CONCEPTUAL ISSUE ON THE SELECTION OF INITIAL STATE

OUR APPROACH IS BASED ON A DEEP WORK BY von Neumann (1929), AND A RELATED WORK BY Goldstein, Lebowitz, Mastrodonanto, Tumulka, Zanghi (2009)

arxiv:1003.5424

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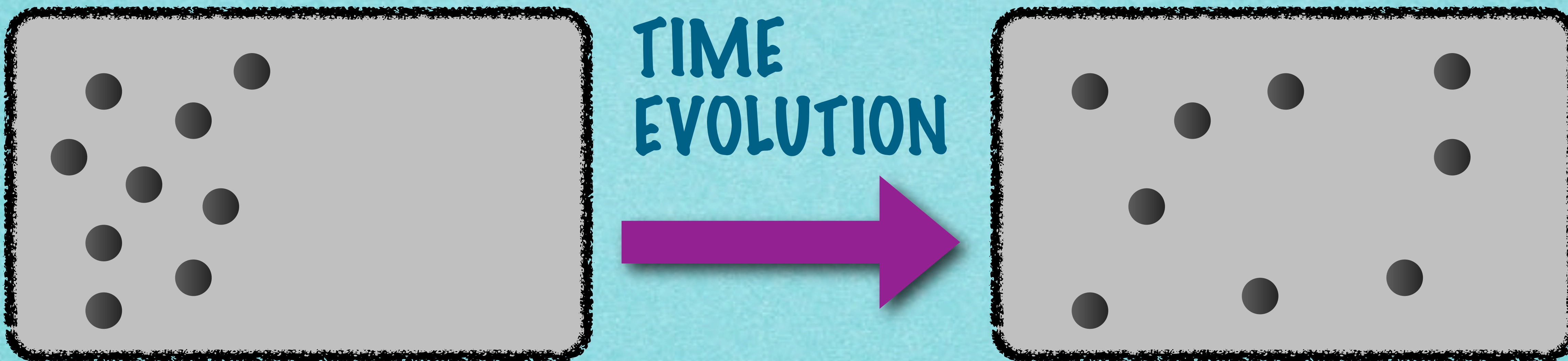
BASIC MOTIVATION

THE APPROACH TO EQUILIBRIUM

ISOLATED CLASSICAL MACROSCOPIC SYSTEM



NONEQUILIBRIUM INITIAL STATE

EQUILIBRIUM STATE

BASIS OF (CLASSICAL) STATISTICAL MECHANICS

EMPIRICAL FACT?

THE APPROACH TO EQUILIBRIUM

GENERAL BELIEF:
IF A CLASSICAL DYNAMICAL SYSTEM IS SUFFICIENTLY "CHAOTIC", IT WILL EVENTUALLY SPEND MOST OF THE TIME IN THE EQUILIBRIUM, PROVIDED THAT IT STARTS FROM A TYPICAL INITIAL STATE

THERE ARE ALWAYS **EXCEPTIONAL** INITIAL STATES

THE APPROACH TO EQUILIBRIUM

Q: WHY DON'T WE SEE SUCH EXCEPTIONAL STATES?

A: BECAUSE THEY ARE RARE

Q: IN WHAT SENSE ARE THEY RARE?

A: THE MEASURE OF SUCH STATES IS ZERO

Q: WITH RESPECT TO WHICH MEASURE?

A: LEBESGUE MEASURE OR MICROCANONICAL MEASURE

Q: WHY LEBESUGE MEASURE?

ENDLESS "METAPHYSICAL" DEBATE

THE APPROACH TO EQUILIBRIUM

Q: WHAT HAPPENS IN QUANTUM SYSTEMS?

Q: IS IT POSSIBLE THAT THE UNCERTAINTY PRINCIPLE WIPES OUT "EXCEPTIONAL INITIAL STATES"?

THERE IS A POSSIBILITY THAT **ANY** INITIAL STATE (WITH SUITABLE ENERGY) IS ALLOWED

von Neumann 1929, Goldstein et al. 2009

SETTING AND PRELIMINARIES

SETTING

A FINITE ISOLATED QUANTUM SYSTEM

$\mathcal{H}$ HILBERT SPACE $\hat{H}$ HAMILTONIAN

$\hat{H}\,\psi_\alpha = E_\alpha\,\psi_\alpha$ SUCH THAT $E_\alpha \neq E_\beta$ FOR $\alpha \neq \beta$

E MACROSCOPIC ENERGY

ΔE SMALL (BUT MACROSCOPIC) ENERGY INTERVAL

$\mathcal{H}_E$ ENERGY SHELL

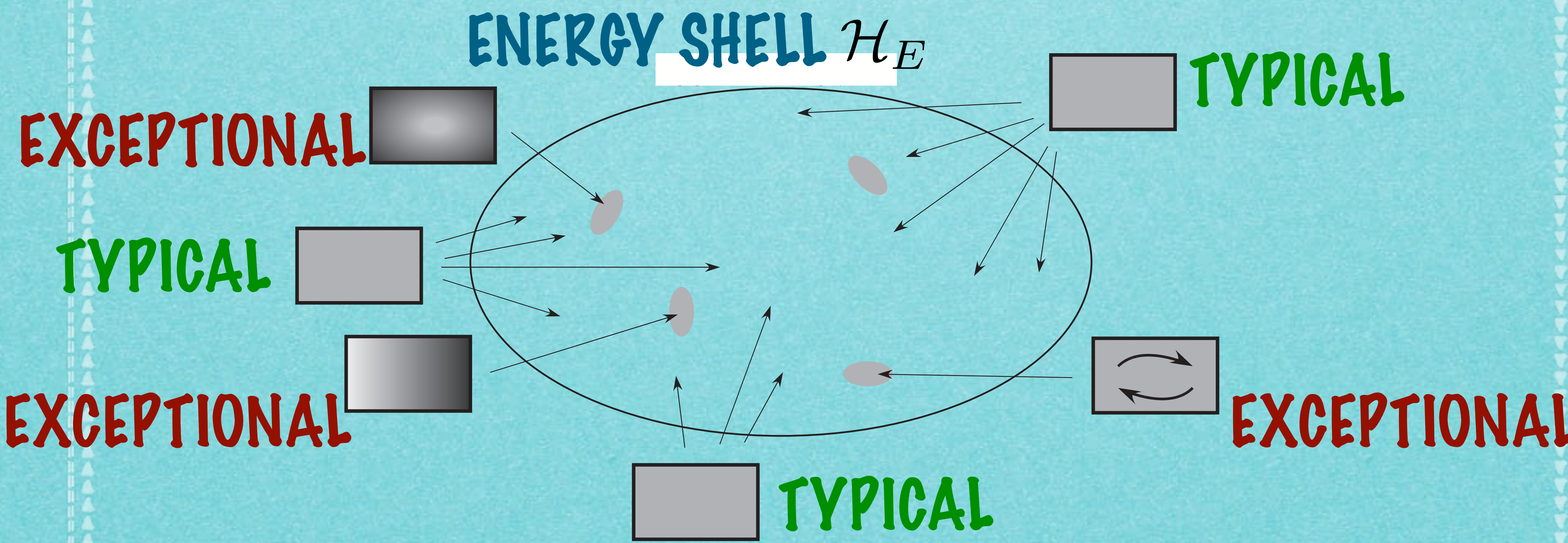
THE SUBSPACE SPANNED BY ALL ψ_α
SUCH TAHAT $E \leq E_\alpha \leq E + \Delta E$

THE DIMENSION IS HUGE

THE APPROACH TO EQUILIBRIUM

BASIC PICTURE: MOST OF THE STATES IN $\mathcal{H}_E$ ARE SIMILAR FROM MACROSCOPIC POINT OF VIEW

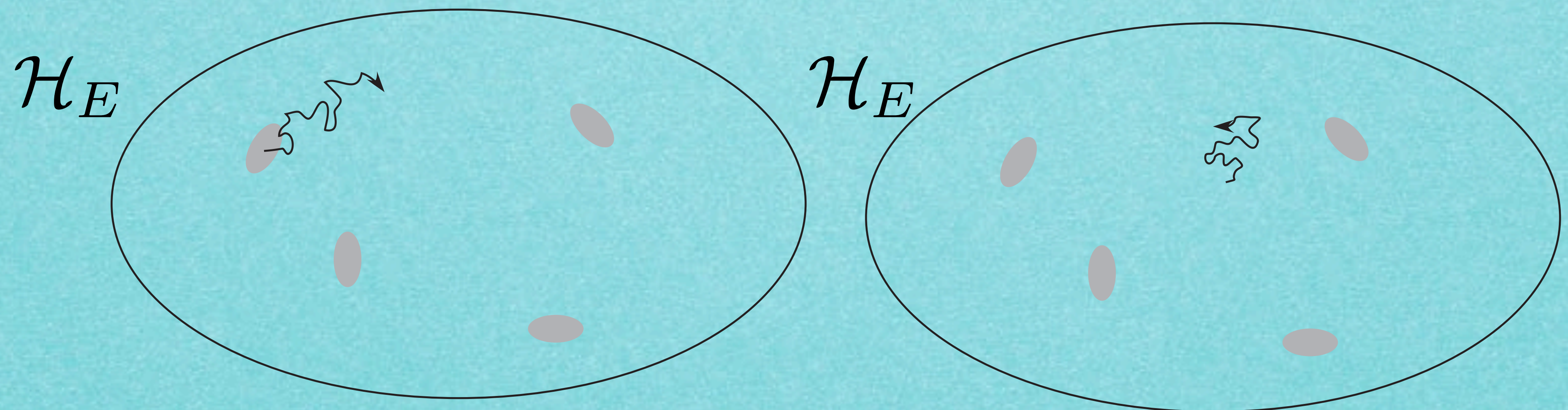
THESE TYPICAL STATES REPRESENT EQUILIBRIUM STATE



THE APPROACH TO EQUILIBRIUM

AN EXCEPTIONAL STATE WILL EVENTUALLY EVOLVE INTO A TYPICAL SATE

A TYPICAL STATE WILL REMAIN TYPICAL (FOR MOST OF THE TIME)



THIS ROUGHLY EXPLAINS THE APPROACH TO EQUILIBRIUM

BASIC ASSUMPTION ABOUT MACROSCOPIC OBSERVABLE

$\hat{A}$ MACROSCOPIC OBSERVABLE

THROUGHOUT THE PRESENTATION, WE ASSUME TAHT

$$\left\langle \left(\hat{A} - \langle \hat{A} \rangle_{\mathrm{mc}}\right)^2 \right\rangle_{\mathrm{mc}} = \mathrm{small}$$

WHERE MICROCANONICAL AVERAGE IS

$$\langle \cdots \rangle_{\mathrm{mc}} = \frac{\mathrm{Tr}_{\mathcal{H}_E}[\cdots]}{\mathrm{Tr}_{\mathcal{H}_E}[1]}$$

WE CONCENTRATE ON A SINGLE QUANTITY $\hat{A}$
THIS LIMITATION SIMPLIFIES THE CONSIDERATION

MICROCANONICAL TYPICALITY

MOST $\varphi \in \mathcal{H}_E$ IS ESSENTIALLY "EQUILIBRIUM" IN THE SENSE THAT $\langle\varphi|\left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi\rangle = \text{small}$

MORE PRECISELY,

THERE EXIST SMALL $\varepsilon > 0$ AND $\eta > 0$

$\mathcal{U}_E$ THE UNIT SPHERE IN $\mathcal{H}_E$

THERE IS A SUBSET $\tilde{\mathcal{U}} \subset \mathcal{U}_E$ WITH $\dfrac{\text{Volume}[\tilde{\mathcal{U}}]}{\text{Volume}[\mathcal{U}_E]} \geq 1 - \eta$

AND ONE HAS $\langle\varphi|\left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi\rangle \leq \varepsilon$ FOR ANY $\varphi \in \tilde{\mathcal{U}}$

VARIATION OF THE RESULTS BY Goldstein et al.

MICROCANONICAL TYPICALITY

MOST $\varphi \in \mathcal{H}_E$ IS ESSENTIALLY "EQUILIBRIUM" IN THE SENSE THAT $\langle\varphi|\left(\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi\rangle = \text{small}$

SKETCH OF THE PROOF: $\hat{s} = (\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}})^2$

$$\int_{\varphi\in\mathcal{H}_E,\ \|\varphi\|=1} \mathcal{D}\varphi\,\langle\varphi|\hat{s}|\varphi\rangle = \int_{\sum|c_\alpha|^2=1} \prod_\alpha dc_\alpha \sum_{\alpha,\beta} c_\alpha^*\,c_\beta\,\langle\psi_\alpha|\hat{s}|\psi_\beta\rangle$$

$$= \langle\hat{s}\rangle_{\mathrm{mc}} = \text{small}$$

SINCE $\langle\varphi|\hat{s}|\varphi\rangle \geq 0$, $\langle\varphi|\hat{s}|\varphi\rangle$ **ITSELF MUST BE SMALL FOR MOST** φ

MICROCANONICAL TYPICALITY

MOST $\varphi \in \mathcal{H}_E$ IS ESSENTIALLY "EQUILIBRIUM" IN THE SENSE THAT $\langle\varphi|\left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi\rangle = \text{small}$

BUT THERE IS NO INFORMATION ABOUT TIME-EVOLUTION

THERMODYNAMIC NORMALITY

THERMODYNAMIC NORMALITY

GENERAL CONSIDERATION

THERMODYNAMIC NORMALITY

DEFINITION:
$\hat{A}$ IS THERMODYNAMICALLY NORMAL IF

$$\langle\psi_\alpha|\left(\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\psi_\alpha\rangle = \text{small}$$

FOR ANY α SUCH THAT $E \leq E_\alpha \leq E + \Delta E$

EACH ENERGY EIGENSTATE IS "EQUILIBRIUM"
(VERY STRONG ASSUMPTION)

"ENERGY EIGENSTATE THERMALIZATION"

BUT THERE CAN BE MANY $\varphi \in \mathcal{H}_E$ SUCH THAT
$\langle\varphi|\left(\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi\rangle$ IS NOT SMALL

MAIN (BUT TRIVIAL) THOREM

THEOREM:

SUPPOSE THAT $\hat{A}$ IS THERMODYNAMICALLY NORMAL

THEN FOR **ANY** INITIAL STATE $\varphi(0) \in \mathcal{H}_E$,

ONE HAS $\langle\varphi(t)|\left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi(t)\rangle = \text{small}$

FOR SUFFICIENTLY LARGE AND TYPICAL t

WHERE $\varphi(t) = e^{-i\hat{H}t}\,\varphi(0)$

IF ONE MEASURES $\hat{A}$ AT SUCH t, THEN THE OUTCOME IS VERY CLOSE THE EQUILIBRIUM VALUE $\langle\hat{A}\rangle_{\mathrm{mc}}$ WITH A PROBABILITY CLOSE TO 1

$\varphi(0)$ CAN BE VERY FAR FROM EQUILIBRIUM!

ONE HAS $\langle\varphi(t)|\left(\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi(t)\rangle = \mathrm{small}$

FOR SUFFICIENTLY LARGE AND TYPICAL t

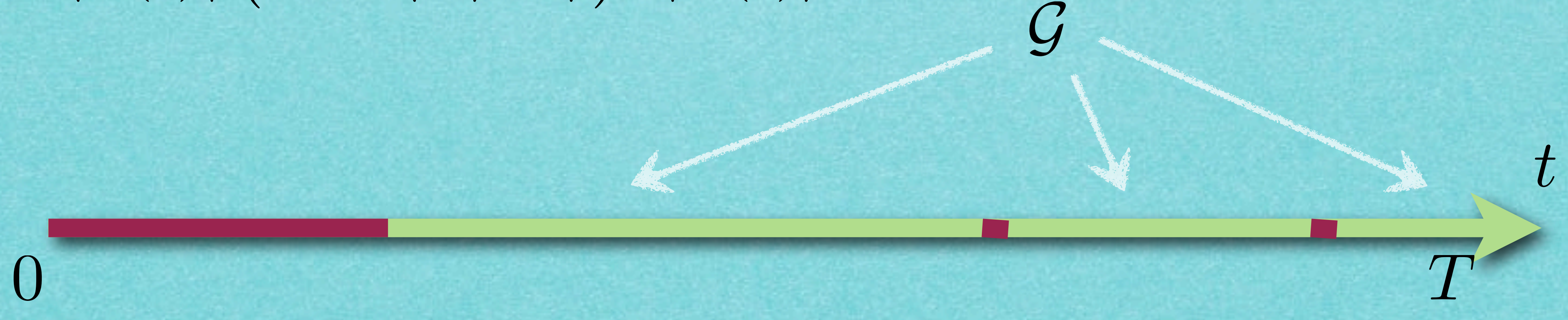
MORE PRECISELY,

THERE ARE SMALL $\varepsilon>0$, $\eta>0$, LARGE $T>0$

THERE IS A "GOOD" SUBSET $\mathcal{G}\subset[0,T]$ SUCH THAT

$\frac{|\mathcal{G}|}{T}\ge 1-\eta$ AND

$\langle\varphi(t)|\left(\hat{A}-\langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\varphi(t)\rangle\le\varepsilon$ FOR ANY $t\in\mathcal{G}$



PROOF (EASY)

INITIAL STATE $\varphi(0) = \sum_\alpha c_\alpha \, \psi_\alpha$

TIME EVOLUTION $\varphi(t) = \sum_\alpha c_\alpha \, e^{-iE_\alpha t} \, \psi_\alpha$

EXPECTATION VALUE

$$\langle \varphi(t) | \, \hat{s} \, | \varphi(t) \rangle = \sum_{\alpha,\beta} c_\alpha^* \, c_\beta \, e^{i(E_\alpha - E_\beta)t} \, \langle \psi_\alpha | \, \hat{s} \, | \psi_\beta \rangle$$

$$\hat{s} = (\hat{A} - \langle \hat{A} \rangle_{\mathrm{mc}})^2$$

LONG-TIME AVERAGE

$$\lim_{T\uparrow\infty} \frac{1}{T} \int_0^T dt \, \langle \varphi(t) | \, \hat{s} \, | \varphi(t) \rangle = \sum_\alpha |c_\alpha|^2 \, \langle \psi_\alpha | \, \hat{s} \, | \psi_\alpha \rangle$$

$$\lim_{T\uparrow\infty}\frac{1}{T}\int_0^T dt\,\langle\varphi(t)|\,\hat{s}\,|\varphi(t)\rangle = \sum_\alpha |c_\alpha|^2\,\langle\psi_\alpha|\,\hat{s}\,|\psi_\alpha\rangle$$

$$= \text{small}$$

ASSUMPTION

THEN

$$\frac{1}{T}\int_0^T dt\,\langle\varphi(t)|\,\hat{s}\,|\varphi(t)\rangle = \text{small}$$

FOR SUFFICIENTLY LARGE T

THIS MEANS (VIA CHEBISHEV-TYPE ESTIMATE)

$\langle\varphi(t)|\,\hat{s}\,|\varphi(t)\rangle$ ITSELF IS SMALL FOR MOST $t \in [0, T]$

$$\hat{s} = (\hat{A} - \langle\hat{A}\rangle_{\text{mc}})^2$$

SO FAR WE HAVE SEEN THAT

IF $\hat{A}$ IS THERMODYNAMICALLY NORMAL, THEN FOR ANY INITIAL STATE $\varphi(0) \in \mathcal{H}_E$ THE RESULT OF A MEASUREMENT OF $\hat{A}$ IS ESSENTIALLY EQUATL TO $\langle \hat{A} \rangle_{\rm mc}$ FOR SUFFICIENTLY LONG AND TYPICAL t

THE APPROACH TO EQUILIBRIUM!

WE DO NOT HAVE TO WORRY ABOUT THE "METAPHYSICAL" PROBLEM OF THE SELECTION OF INITIAL STATES

BUT, THE THERMODYNAMIC NORMALITY IS A VERY STRONG CONDITION

NEXT ISSUE

IS THERMODYNAMIC NORMALITY SATISFIED IN REALISTIC QUANTUM SYSTEMS?

NOBODY KNOWS THE ANSWER

POSITIVE RESULTS

- TYPICALITY
- SIMPLE (AND ARTIFICIAL) EXAMPLES

THERMODYNAMIC NORMALITY

TYPICALITY AND EXAMPLES

TYPICALITY

A VARIATION OF THE RESULTS BY
von Neumann 1929, Goldstein et al. 2009

FIX $\mathcal{H}_E$ AND $\hat{A}$ SUCH THAT $\left\langle \left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2 \right\rangle_{\mathrm{mc}} = \text{small}$

$$\langle \cdots \rangle_{\mathrm{mc}} = \frac{\mathrm{Tr}_{\mathcal{H}_E}[\cdots]}{\mathrm{Tr}_{\mathcal{H}_E}[1]}$$

THEOREM:
CHOOSE THE HAMILTONIAN $\hat{H}$ RANDOMLY.
THEN WITH PROBABILITY CLOSE TO 1, $\hat{A}$ IS THERMODYNAMICALLY NORMAL

TYPICALITY

THEOREM:
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MORE PRECISELY,

THERE EXIST SMALL $\varepsilon > 0$ AND $\eta > 0$

CHOOSE AN ORTHONORMAL BASIS $\{\psi_\alpha\}$ OF $\mathcal{H}_E$ RANDOMLY

THEN WITH PROBABILITY LARGER THAN $1-\eta$, ONE HAS

$\langle\psi_\alpha|\left(\hat{A} - \langle\hat{A}\rangle_{\mathrm{mc}}\right)^2|\psi_\alpha\rangle \le \varepsilon$ FOR ANY α

MEANING OF TYPICALITY

THEOREM:
CHOOSE THE HAMILTONIAN $\hat{H}$ RANDOMLY.
THEN WITH PROBABILITY CLOSE TO 1, $\hat{A}$ IS THERMODYNAMICALLY NORMAL

WE DO NOT MEAN THAT THE HAMILTONIAN IS LITERALLY CHOSEN RANDOMLY

TYPICALITY GUARANTEES THAT THERE ARE A LOT OF HAMILTONIANS WITH WHICH $\hat{A}$ IS T.D. NORMAL

IT MAY NOT BE TOO STUPID TO THINK ABOUT THERMODYNAMIC NORMALITY

EXAMPLE 1 INDEPENDENT SPINS

TRIVIAL, BUT MAY BE USEFUL

INDEPENDENT $S = 1/2$ SPINS UNDER RANDOM MAGNETIC FIELD

$$\hat{H} = \sum_{j=1}^{N} h_j \, \hat{S}_j^{(z)}$$

RANDOM $h_j \in [-h, h]$

ENERGY EIGENSTATES AND EIGENVALUES

$$\psi_{\boldsymbol{\sigma}} = \bigotimes_{j=1}^{N} \psi_j^{\sigma_j} \qquad E_{\boldsymbol{\sigma}} = \sum_{j=1}^{N} \frac{h_j}{2} \, \sigma_j$$

NON-DEGENERATE WITH PROBABILITY ONE

WHERE $\hat{S}_j^{(z)} \, \psi_j^{\pm 1} = \pm \frac{1}{2} \, \psi_j^{\pm 1}$

$$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_N) \qquad \sigma_j = \pm 1$$

EXAMPLE 1
INDEPENDENT SPINS

THE MODEL IS TRIVIAL, BUT CHOOSE $\hat{A} = \frac{1}{N}\sum_{j=1}^{N} \hat{S}_j^{(x)}$

SINCE
$$\langle \psi_j^{\pm} | \hat{S}_j^{(x)} | \psi_j^{\pm} \rangle = 0 \quad \langle \psi_j^{\pm} | (\hat{S}_j^{(x)})^2 | \psi_j^{\pm} \rangle = \frac{1}{4}$$

WE HAVE
$$\langle \psi_{\boldsymbol{\sigma}} | \hat{A} | \psi_{\boldsymbol{\sigma}} \rangle = 0 \quad \langle \psi_{\boldsymbol{\sigma}} | \hat{A}^2 | \psi_{\boldsymbol{\sigma}} \rangle = \frac{1}{4N} \ll 1$$
FOR ANY $\boldsymbol{\sigma}$

$\hat{A}$ IS THERMODYNAMICALLY NORMAL FOR ANY E, ΔE

ONE CAN EVEN START FROM THE STATE WITH ALL SPINS POINTING THE x-DIRECTION, WHERE $\langle \varphi(0) | \hat{A} | \varphi(0) \rangle = 1/2$

BUT STILL HAVE $\hat{A} \ll 1$ AFTER A LONG TIME

EXAMPLE 1
INDEPENDENT SPINS

THE OPERATOR $\hat{A} = \frac{1}{N}\sum_{j=1}^{N}\hat{S}_j^{(x)}$ EXHIBITS THE "APPROACH TO EQUILIBRIUM"

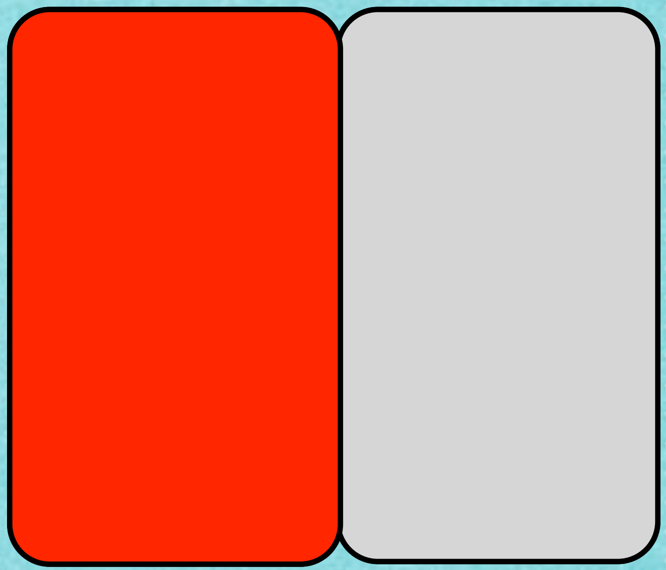
BUT THIS IS A TRIVIAL CONSEQUENCE OF THE INDEPENDENT SPIN PRECESSION AROUND THE z-AXIS

THE STORY IS TOTALLY DIFFERENT IF WE CHOSSE

$$\hat{A} = \frac{1}{N}\sum_{j=1}^{N}\hat{S}_j^{(z)}$$

EXAMPLE 2
THERMAL CONTACT

A TOY MODEL FOR TWO MACROSCOPIC BODIES IN THERMAL CONTACT



$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\rm int}$$

$$\hat{H}_1 \, \xi_j = E_j^{(1)} \, \xi_j \quad \hat{H}_2 \, \chi_k = E_k^{(2)} \, \chi_k$$

DENSITY OF STATES $\rho_1(E), \rho_2(E)$

AS ALWAYS, WE ASSUME $\rho_\nu(E) \simeq \exp[V \, \sigma_\nu(E/V)]$

WITH INCREASING ENTROPY DENSITIES $\sigma_\nu(\epsilon)$

AND LARGE VOLUME V

$$\nu = 1, 2$$

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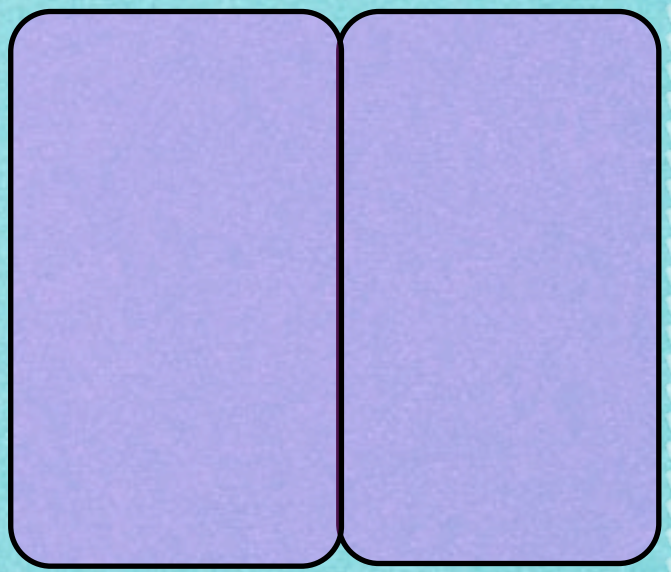

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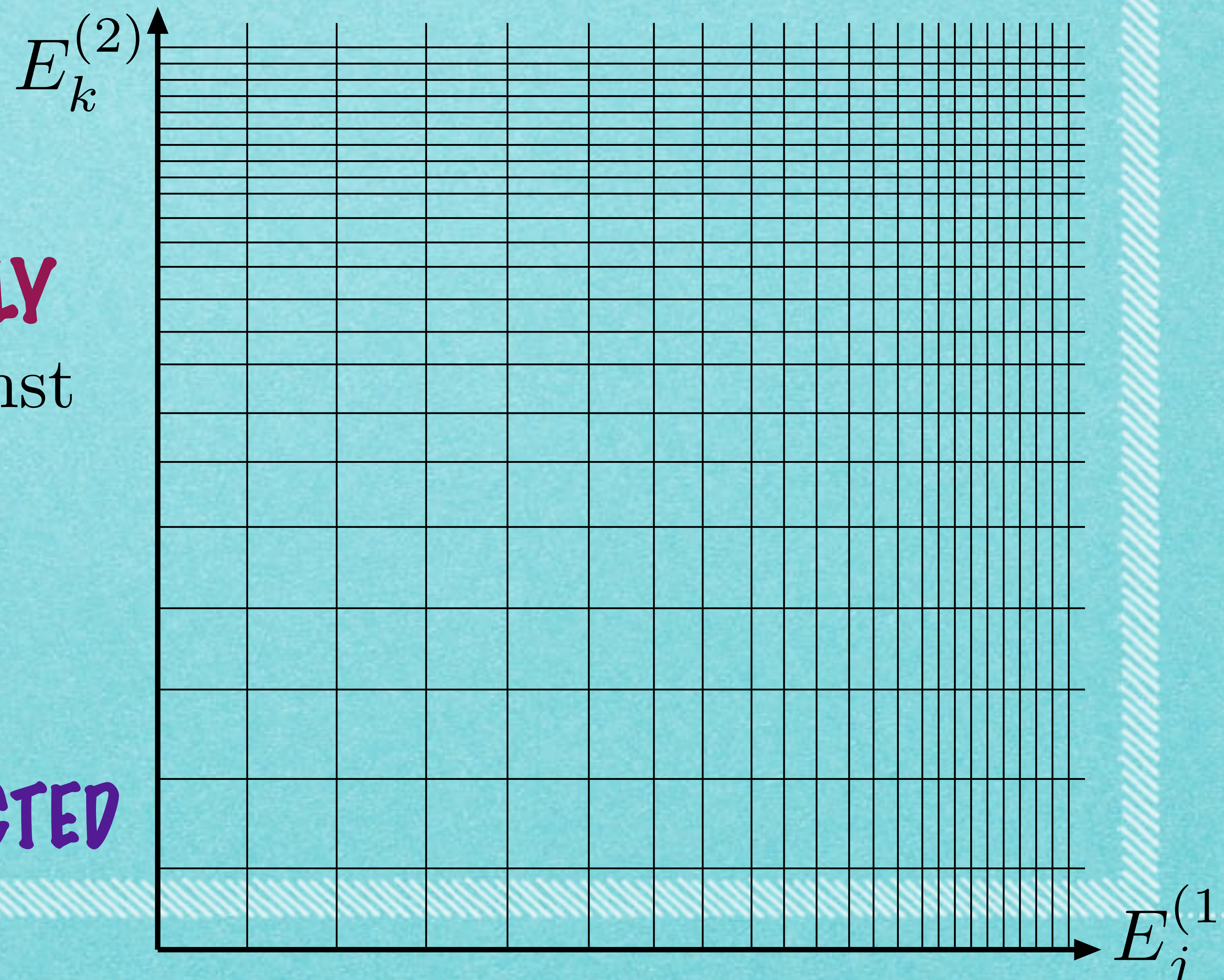
INTERACTION HAMILTONIAN (WHICH IS ARTIFICIAL)

$$\langle \xi_j \otimes \chi_k | \hat{H}_{\text{int}} | \xi_{j'} \otimes \chi_{k'} \rangle = \begin{cases} \delta & \text{if } (j,k) \leftrightarrow (j',k') \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta E \gg \delta \gg (\text{level spacing})$$

DRAW A SINGLY-CONNECTED LINE ROUGHLY ALONG $E_j^{(1)} + E_k^{(2)} = \text{const}$



$(j,k) \leftrightarrow (j',k')$ MEANS THAT THEY ARE CONNECTED

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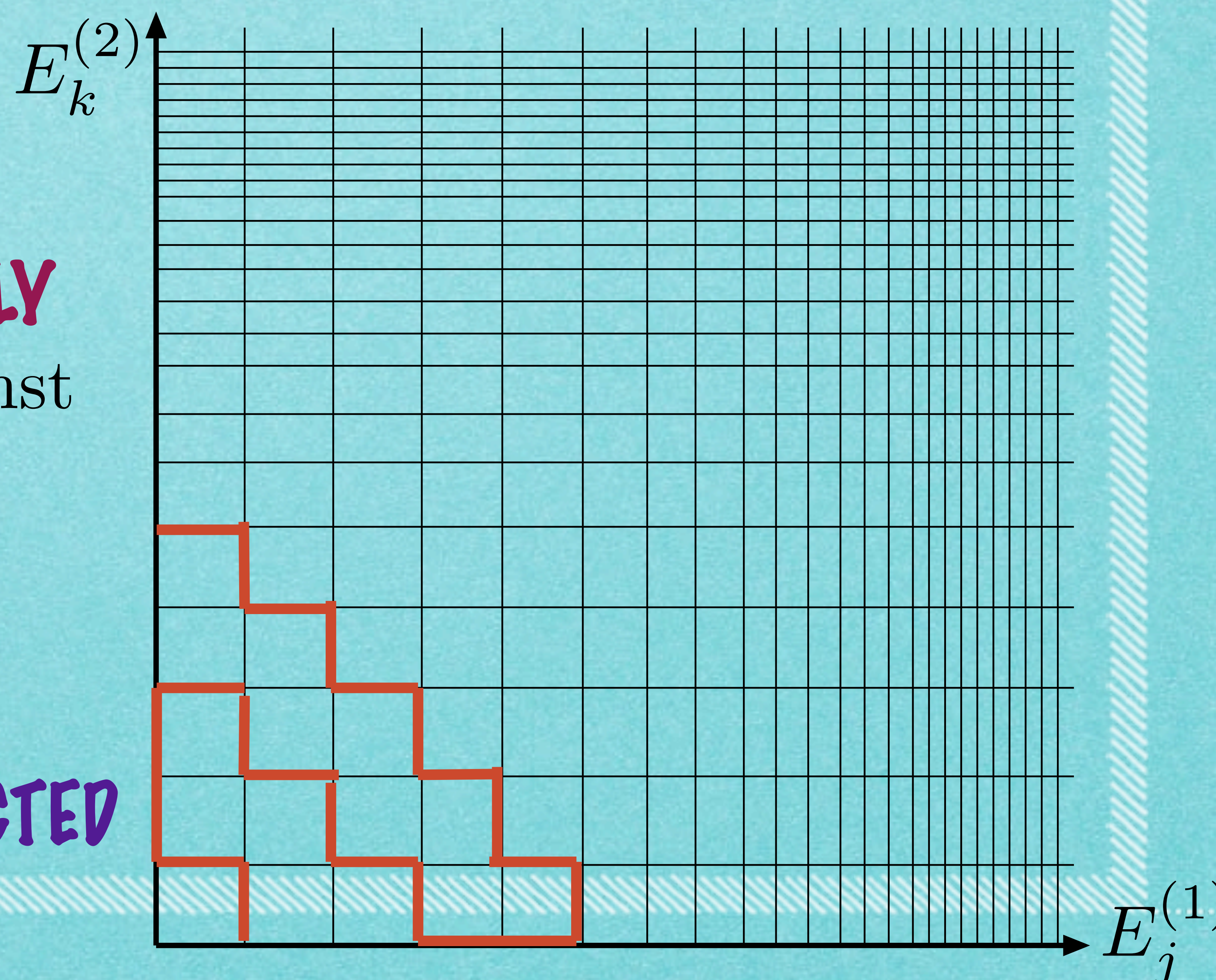

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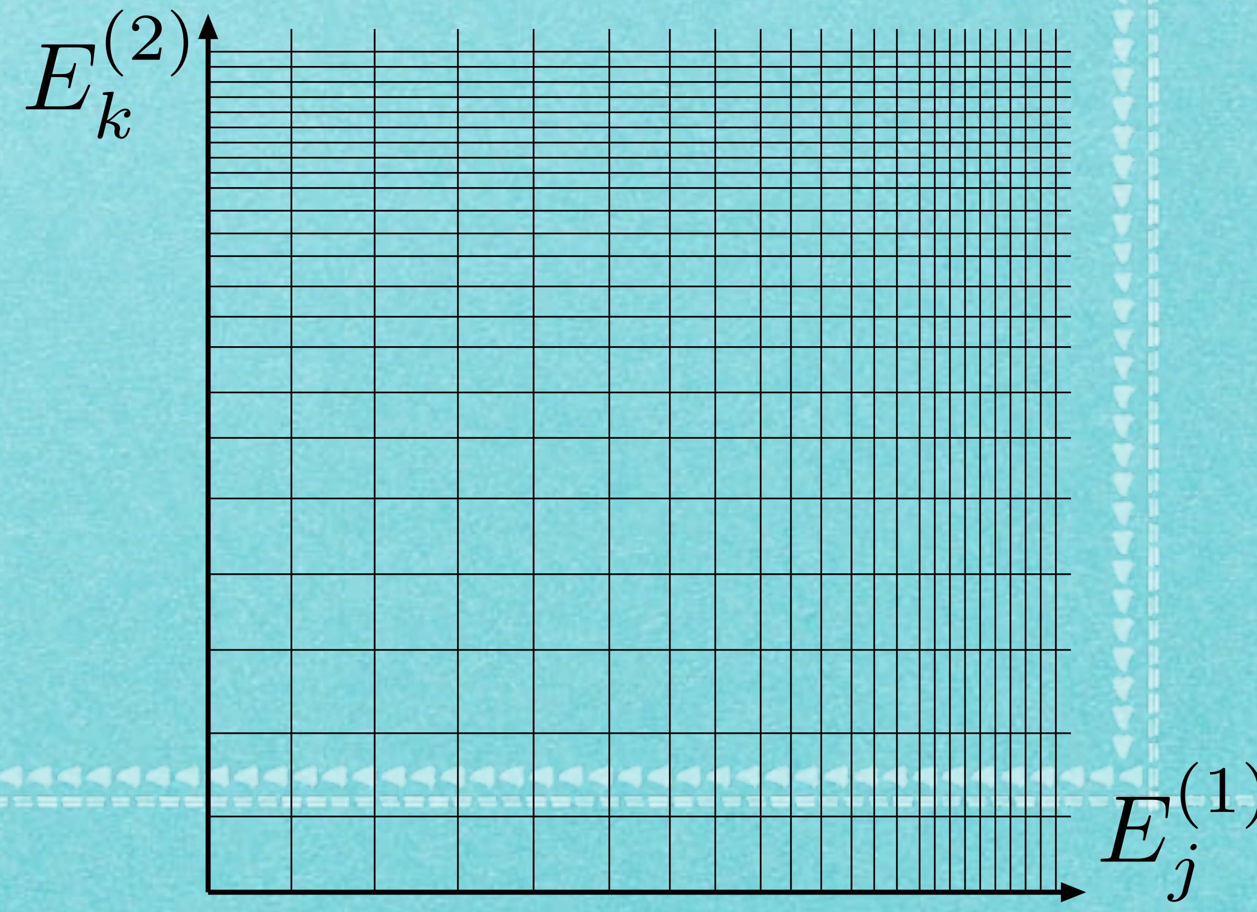
EXAMPLE 2
THERMAL CONTACT

ENERGY EIGENSTATE $\hat{H}\,\psi_\alpha = E_\alpha\,\psi_\alpha \qquad \psi_\alpha = \sum_{j,k} c_{j,k}\,\xi_j \otimes \chi_k$

ONE CAN PROVE THAT $c_{j,k}$ ARE NEARLY EQUAL WHEN $|E_j^{(1)} + E_k^{(2)} - E_\alpha| \lesssim \delta$, AND SMALL OTHERWISE

"DEMOCRACY" IN ENERGY EIGENSTATES



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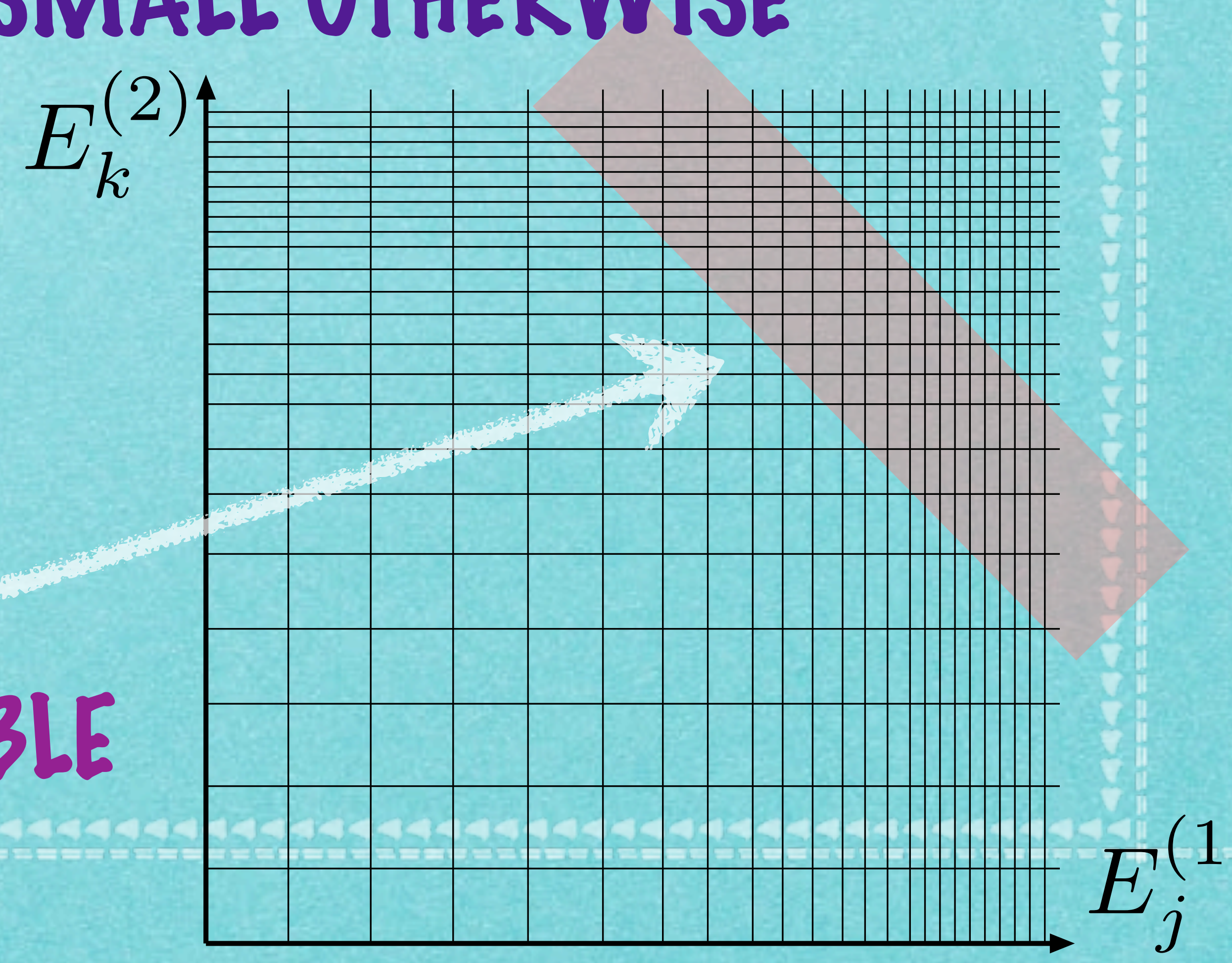
"DEMOCRACY" IN ENERGY EIGENSTATES

ALMOST LIKE MICROCANONICAL ENSEMBLE



EXAMPLE 2
THERMAL CONTACT

THIS IMPLIES THAT $\hat{A} = \hat{H}_1$ IS THERMODYNAMICALLY NORMAL IN THE SENSE THAT

$$\langle\psi_\alpha|\,\hat{H}_1\,|\psi_\alpha\rangle \simeq E_1^{\mathrm{eq}} \quad \langle\psi_\alpha|\,(\hat{H}_1 - E_1^{\mathrm{eq}})^2\,|\psi_\alpha\rangle = \mathrm{small}$$

FOR ANY α SUCH THAT $E \leq E_\alpha \leq E + \Delta E$

E_1^{eq} **IS THE SOLUTION OF**

$$\frac{d}{dE_1}\log\rho_1(E_1) = -\frac{d}{dE_1}\log\rho_2(E - E_1)$$

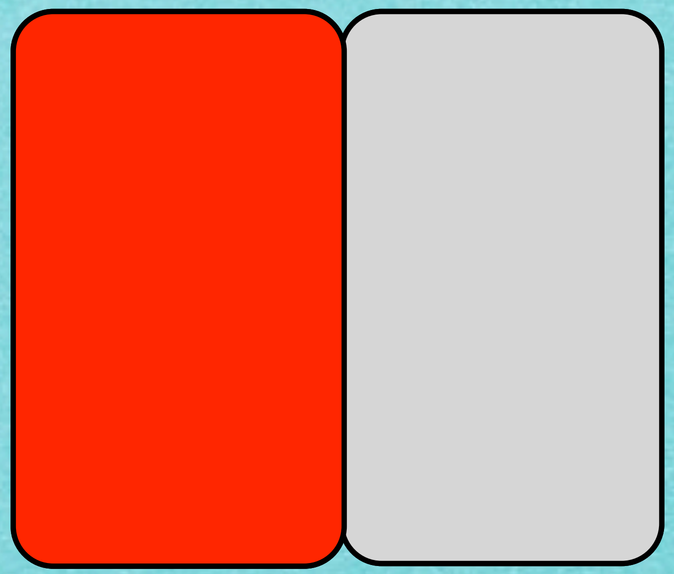
TEMPERATURE BALANCE

EXAMPLE 2
THERMAL CONTACT

ONE CAN EVEN START FROM THE STATE WHERE THE TWO SYSTEMS HAVE DRASTICALLY DIFFERENT TEMPERATURES

BUT ONE HAS $\hat{H}_1 \simeq E_1^{\mathrm{eq}}$ AFTER A LONG TIME

WE HAVE THUS RIGOROUSLY DERIVED THE EQUILIBRATION OF TWO MACROSCOPIC QUANTUM BODIES IN THERMAL CONTACT



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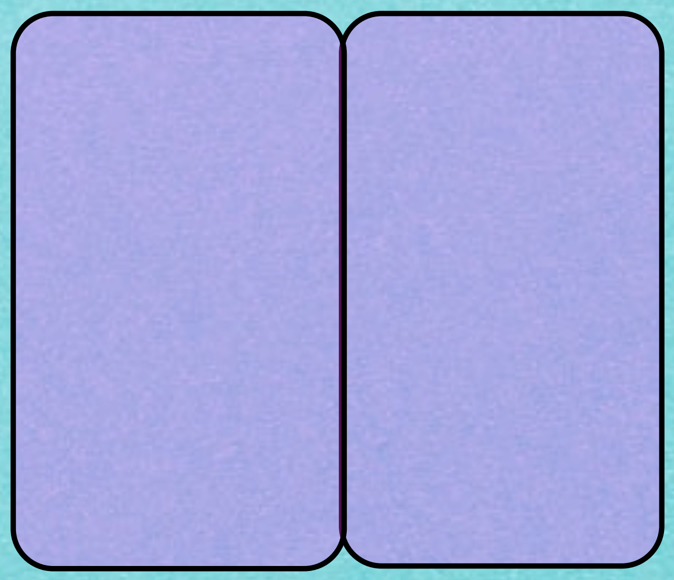

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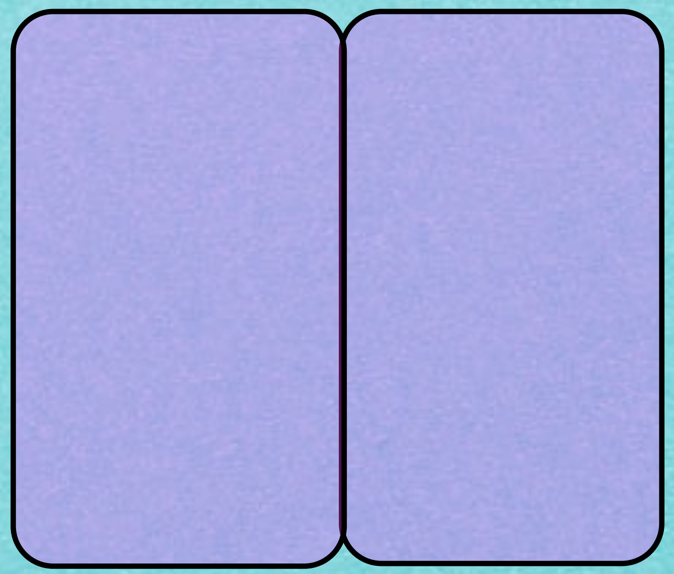

SO FAR FOR A TOY MODEL....

SUMMARY AND FUTURE ISSUES

SMALLER ISSUES

CAN WE CONSTRUCT FURTHER EXAMPLES? ESPECIALLY LESS ARTIFICIAL MODELS OF THERMAL CONTACT

IS IT POSSIBLE TO SHOW THERMODYNAMIC NORMALITY IN AN EXACTLY SOLVABLE MODEL?
FREE FERMION IS DONE, BUT HOW ABOUT "DIFFICULT" ONES?

CAN WE FORMULATE USEFUL SUFFICIENT CONDITIONS FOR THERMODYNAMIC NORMALITY? (BASICALLY, DECAY OF CORRELATION WILL DO)

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Deguchi

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BIGGER ISSUES

CAN ONE ESTIMATE RELAXATION TIME??

IS THERMODYNAMIC NORMALITY VALID IN REALISTIC SYSTEMS???
IF NOT, WE HAVE TO LIVE WITH RESULTS WHICH HOLD FOR MOST (NOT ANY) INITIAL STATES

IS IT REASONABLE TO STUDY COMPLETELY ISOLATED SYSTEMS????
NOTHING (WE CAN OBSERVE) IS ISOLATED!!

BIGGER ISSUES

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IS THERMODYNAMIC NORMALITY VALID IN REALISTIC SYSTEMS???
IF NOT, WE HAVE TO LIVE WITH RESULTS WHICH HOLD FOR MOST (NOT ANY) INITIAL STATES Monnai, Ikeda

IS IT REASONABLE TO STUDY COMPLETELY ISOLATED SYSTEMS????
NOTHING (WE CAN OBSERVE) IS ISOLATED!!