统计物理基础的近期进展、以及小量子系统的统计性质

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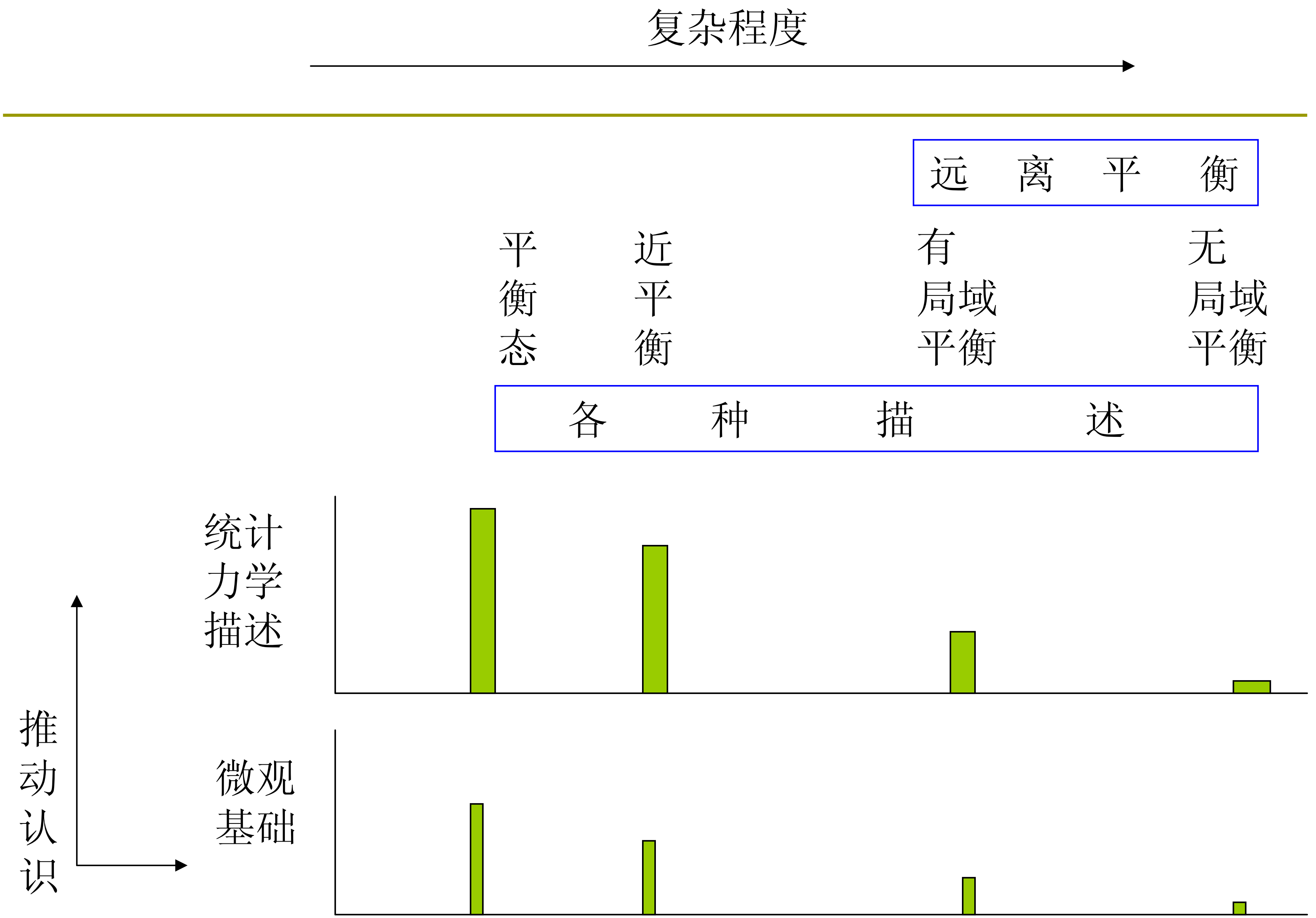
概述

- (1) 经典统计力学基础与混沌现象
- (2) 量子统计基础研究中遇到的问题
- (3) 对微正则系综适用性的一个新理解
- (4) 从微正则系综到正则系综
- (5) 热化——系统的趋平衡过程与ETH
- (6) 非极弱耦合下小量子系统的统计描述


复杂程度
远离平衡
平衡态
近平衡
有局域平衡
无局域平衡
各种描述
统计力学描述
微观基础
推动认识

经典统计力学基础与混沌现象

经典统计物理的等几率原理：

具有一定能量的孤立系统，其统计性质由微正则系综描述。

微正则系综：系统以同样的几率处于其能量面上的每个态。

实验根据：该原理的预言与热力学一致，且其对涨落的预言也与实验结果一致。

理论论证与依据：—— 动力学系统的混沌性质（波尔兹曼—分子混沌）。

平衡态——遍历性（ergodic）

扩散过程——混合性（mixing）

热传导——混沌性（chaotic）

Ergodicity: A system is said to be **ergodic**, if the time average of an arbitrary function f(q,p) with almost every possible initial states is equal to the average over (energy surface in) phase space.

$$\langle f \rangle_t = \langle f \rangle_{ps}$$

$$\langle f \rangle_t = \lim_{T\to\infty} \frac{1}{T} \int_0^T f(q,p)dt$$

$$\langle f \rangle_{ps} = \int_{\mathcal{M}} f(q,p)d\mu$$

Where dμ is the invariant measure in the phase space.

The meaning of ergodicity is that almost every trajectory explores all the possible regions (on the energy surface) in phase space, with a weight proportional to dμ.

对平衡态的描述（长时间一致的行为）

—— 对应动力学系统的遍历性（ergodicity）

Mixing: One may use the following picture to illustrate the concept of mixing

Imagine the dispersion of a drop of ink in a glass of water，

or the following procedure.

(a) Take a shaker that consists of 20% rum and 80% cola, with the part of rum representing the initial distribution of the considered initial states as “incompressible fluid” in phase space.

(b) Shaking the shaker for a time long enough, then, every part of the shaker (of macroscopic scale), however small, will contain “approximately” 20% rum, representing that every part of the phase space contains 20% of the trajectories at time t.

Mathematical expression

An area preserving map $\mathbf{M}$ of a compact region S is mixing on S, if given any two subsets σ and σ' of S, where σ and σ' have positive Lebesgue measure ($\mu_L(\sigma) > 0, \mu_L(\sigma') > 0$), then,

$$\frac{\mu_L(\sigma)}{\mu_L(S)} = \lim_{m\to\infty} \frac{\mu_L[\sigma' \cap \mathbf{M}^m(\sigma)]}{\mu_L(\sigma')}$$

Mixing implies ergodicity, but, the converse is not true.

对扩散过程的描述——需要混合性（mixing）性质（Krylov）

K-systems have invariant sets with positive KS (Krylov, Kolmogorov, Sinai) entropy.

It has been proved that KS entropy is the summation of positive Lyapunov exponents.

$$h_k = \sum_{\sigma_i > 0} \sigma_i$$

Therefore, a K-system has positive Lyapunov exponent.

When we speak of a chaotic system, we usually mean a K-system.

We mention that σ_1 is not usually the same constant for all stochastic regions; distinct, isolated regions of stochasticity generally have different values of σ_1.

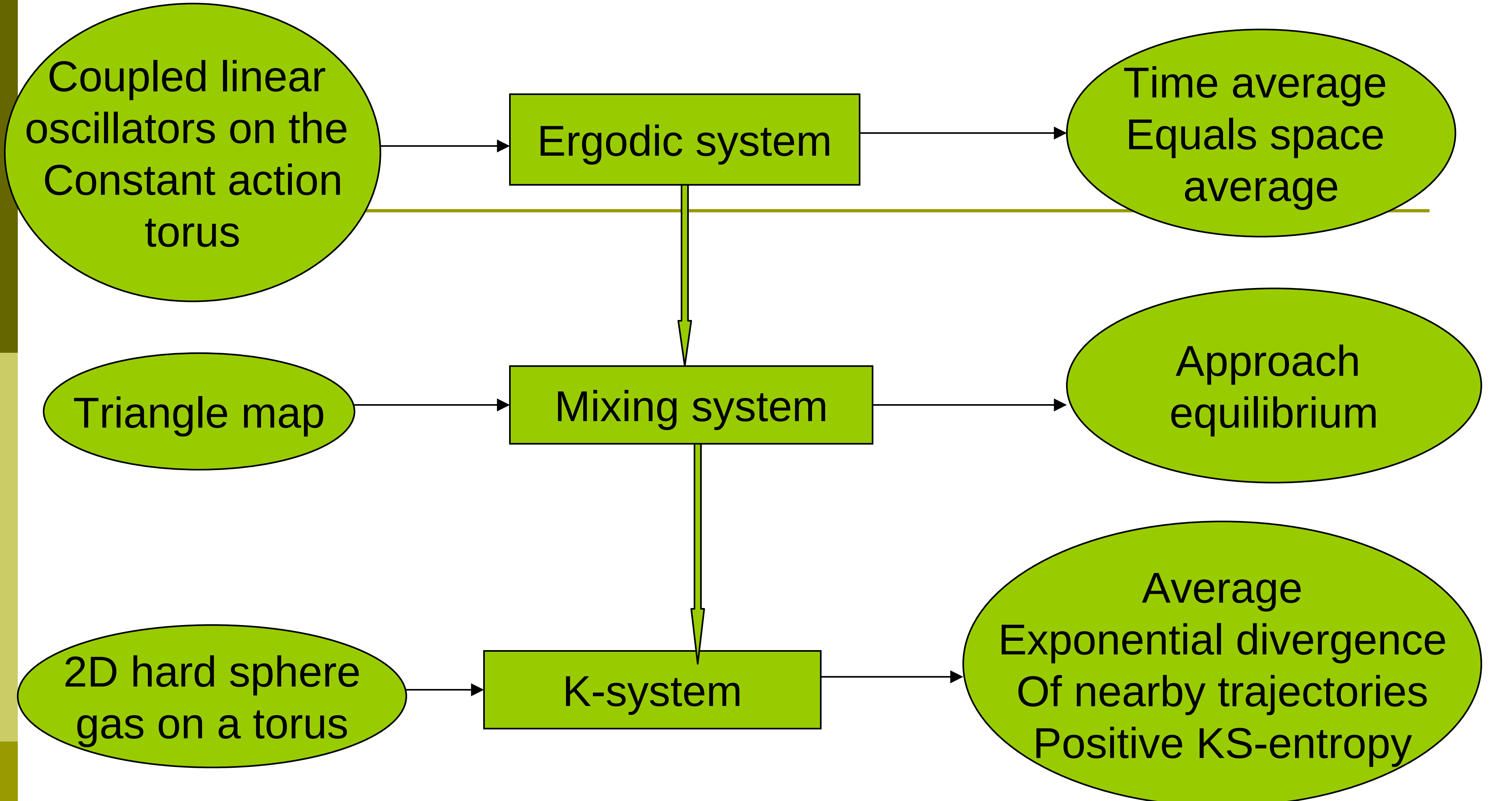
正常热传导，满足傅里叶定律。

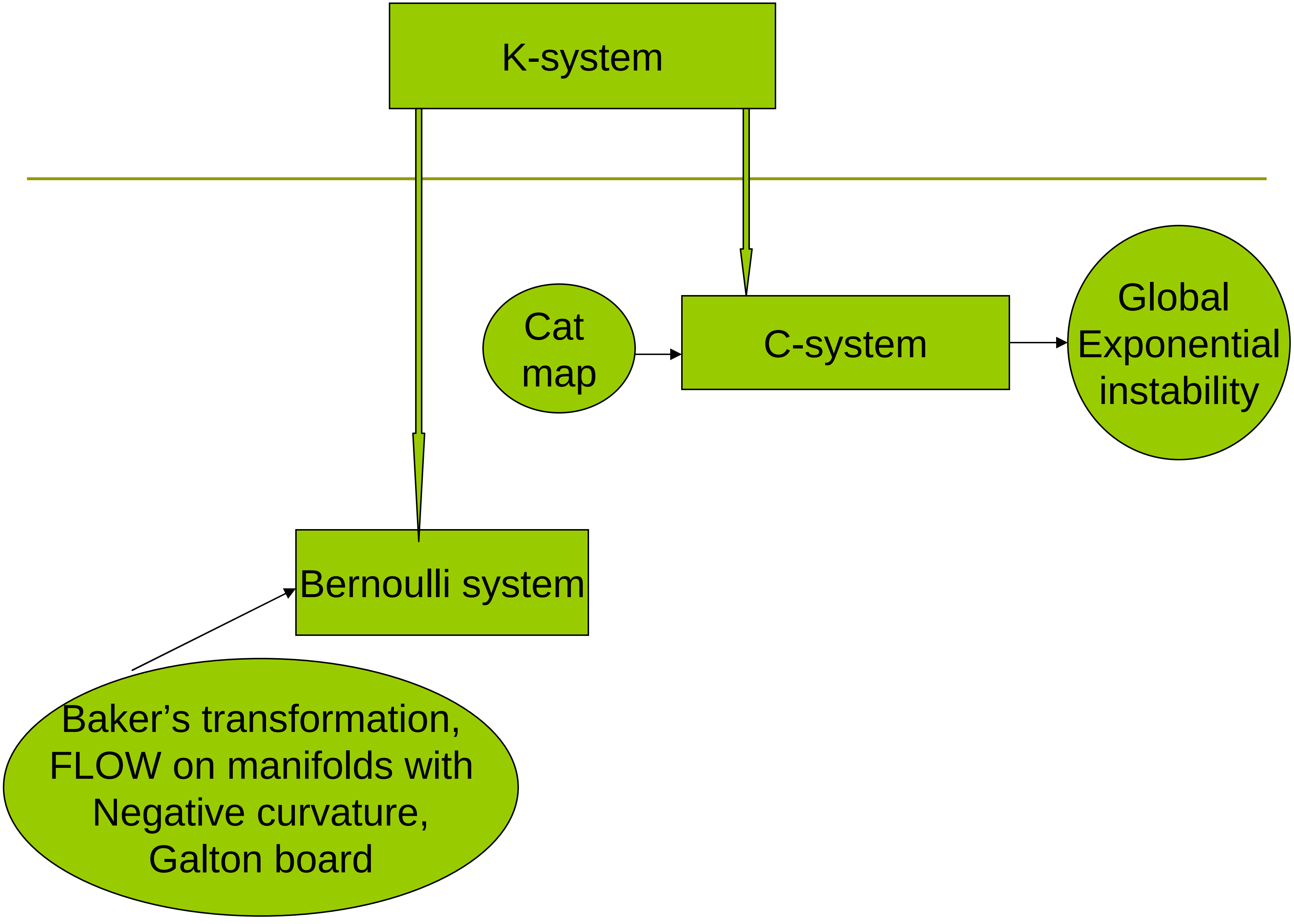
其机制——通常与系统动力学运动的混沌性（chaotic）有关。

（注：言“通常”，是因为存在反例。）

A C-system, also called Anosov-system, is one which is chaotic and is hyperbolic at every point in the phase space (not just on the invariant set).

A Bernoulli system is a system which can be represented as a symbolic dynamics consisting of a full shift on a finite number of symbols.


Coupled linear oscillators on the Constant action torus
Ergodic system
Time average Equals space average
Triangle map
Mixing system
Approach equilibrium
2D hard sphere gas on a torus
K-system
Average Exponential divergence Of nearby trajectories Positive KS-entropy


K-system
Cat map
C-system
Global Exponential instability
Bernoulli system
Baker’s transformation, FLOW on manifolds with Negative curvature, Galton board

(2) 量子统计力学基础研究中

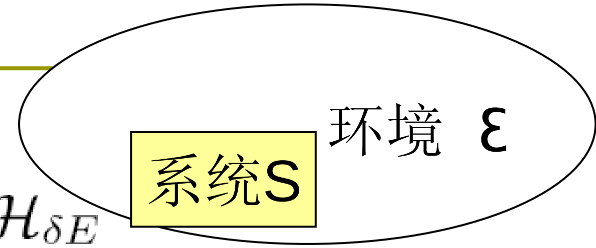
——希尔伯特空间的性质所带来新问题

（1） 非简并情况下，一个能级仅对应一个状态，因此，无法谈论能量面上的各态遍历。

（2） 系综的数学描述为密度矩阵，为算子，在任何基矢上有对角与非对角元。

能量本征态

量子系统的描述：　大系统 = 子系统+环境



微正则描述：$\rho_{mic}=\Sigma_{\eta}|E^T_{\eta}\rangle\langle E^T_{\eta}|$,　　$|E^T_{\eta}\rangle\in \mathcal{H}_{\delta E}$

$\mathcal{H}_{\delta E}$：能量在 $[E, E+\delta E]$ 内的大系统能量本征态所张子空间.

对于子系统的正则描述：　$\rho_{\rm can}=Z^{-1}e^{-\beta H^S}$

An approach proposed by Schrodinger:

Relating ρ_{can} to the reduced density matrix ρ^s of the system S, which is weakly coupled to a huge environment.

$\rho^S=\mathrm{Tr}_{\mathcal{E}}\rho_{mic}$

（3）对微正则系综适用性的一个新理解：

就描述子系统的性质而言，大系统微正则系综的预言，与其（希尔伯特空间的）能量壳子空间 $\mathcal{H}_{\delta E}$ 中大多数矢量的预言基本一样。

S.Popescu, A.J.Short, and A.Winter, Nature Physics ***2****, 754 (2006).*

具体内容

三 $\mathcal{H}_{\delta E}$

ARTICLES

Entanglement and the foundations of statistical mechanics

SANDU POPESCU[1,2], ANTHONY J. SHORT[1]* AND ANDREAS WINTER[3]

$\rho^{S} = \mathrm{Tr}_{\mathcal{E}} \rho_{mic}$

主要结果: $\rho^S \simeq \rho^S_{\delta E}$ $\rho^S_{\delta E} = \mathrm{Tr}_{\mathcal{E}} |\Psi^{\delta E}_{\mathrm{ty}}\rangle\langle\Psi^{\delta E}_{\mathrm{ty}}|$

$|\Psi^{\delta E}_{\mathrm{ty}}\rangle$ 是 $\mathcal{H}_{\delta E}$ 中的一个典型态矢量。

$$|\Psi^{\delta E}_{\mathrm{ty}}\rangle = \mathcal{N}^{-1}_{\delta E} \sum_{\eta \in \Gamma_{\delta E}} C_\eta |E^{\mathcal{T}}_\eta\rangle$$

$|E^{\mathcal{T}}_\eta\rangle$ 为大系统能量本征态。

C_η 为高斯无规数。

所用数学性质：Levy引理

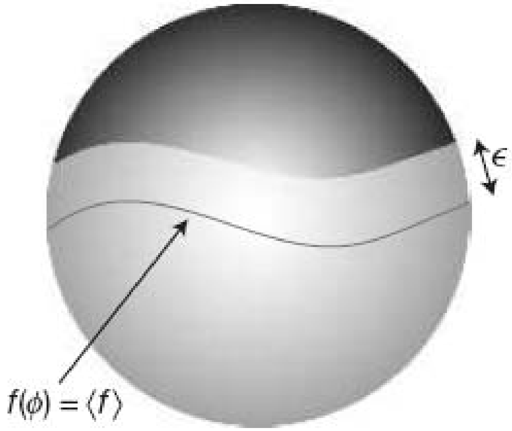


Figure 2 Bounding deviations from the average using Levy's lemma. Levy's lemma[14] is a result in high-dimensional geometry, which states that for almost all points ϕ on a hypersphere of dimension d (where $d \gg 1$) and area $V[\{\phi\}]$, and all functions f that do not vary too rapidly ($|\nabla f| \leq 1$), $f(\phi)$ is approximately equal to its mean value $\langle f \rangle$. The diagram shows the case $d = 2$, in which the hypersphere corresponds to the surface of a normal sphere. The shaded region corresponds to the maximum area $V[\{\phi | f(\phi) - \langle f \rangle \geq \epsilon\}]$ in which f is ϵ greater than average. Although this area is relatively large for $d = 2$, when d becomes large, the relative size of this region compared with the entire hypersphere becomes exponentially small. Specifically, Levy's lemma states that $V[\{\phi | f(\phi) - \langle f \rangle \geq \epsilon\}] / V[\{\phi\}] \leq 4 \exp(-(1/9\pi^3)(d+1)\epsilon^2)$.

Levy's lemma: Let $f : \mathbb{S} \to \mathbb{R}$ be a real-valued function on a $(D-1)$-dimensional Euclidean sphere $\mathbb{S}$ (embedded in a D-dimensional Euclidean space), with $\lambda = \sup_{x_1,x_2} |f(x_1) - f(x_2)|/|x_1 - x_2|$, then, for a uniformly random point $x \in \mathbb{S}$,

$$\mathrm{Pr}_x\{f(x) > \langle f \rangle + \epsilon\} \leq 2\exp[-D\epsilon^2/(9\pi^3\lambda^2)], \qquad (16)$$

where Pr means probability and $\langle f \rangle$ is the average of f over the sphere. Thus, $|f(x) - \langle f \rangle| \lesssim a\lambda D^{-1/2}$ for a typical point x, where a is a number determined by the accuracy required.

(4) 从量子微正则系综到正则系综 （极弱耦合情况）

从量子微正则描述到正则描述推导中所遇到的困难。

经典情况（见诸教科书）：

对子系统的描述 —— 系统处于各可能状态的几率。

从微正则描述到正则描述的推导 ——用到近似 $e^{S(E-E_i^{(S)})} \approx e^{S(E)-\beta E_i^{(S)}} \sim e^{-\beta E_i^{(S)}}$

相当于假设环境的态密度局部地随能量按指数增长。

量子情况中出现的问题：

对子系统的描述——系统的约化密度矩阵。 $\rho^S = \mathrm{Tr}_{\mathcal{E}} \rho_{micro}$

推导中所遇到的问题——证明子系统的约化密度矩阵在系统能量本征基矢上为对角的。

S.Goldstein, et al, Phys.Rev.Lett. ***96****, 050403 (2006).*

PRL **96,** 050403 (2006) PHYSICAL REVIEW LETTERS

Canonical Typicality

Sheldon Goldstein,[1,*] Joel L. Lebowitz,[1,†] Roderich Tumulka,[2,‡] and Nino Zanghì[3,§]

Consider a system S and a huge environment $\mathcal{E}$

$$H = H^S + H^I + H^{\mathcal{E}}.$$

The interaction, described by H^I, is assumed to be weak. Normalized eigenstates of the self-Hamiltonian H^S with eigenenergies E^S_α are denoted by $|E^S_\alpha\rangle$, and normalized eigenstates of the environment Hamiltonian $H^{\mathcal{E}}$ with eigenenergies $E^{\mathcal{E}}_i$ are denoted by $|E^{\mathcal{E}}_i\rangle$.

To use typicality to derive useful results, δE should not be too small.

极弱互作用情况。

考虑子空间 $$\mathcal{H}_d = \bigoplus_{\alpha} |E_\alpha^S\rangle \otimes \mathcal{H}_\alpha^{(\mathcal{E})}$$

$\mathcal{H}_\alpha^{(\mathcal{E})}$ ← a subspace in the Hilbert space of the environment $\mathcal{E}$, which is spanned by $|E_i^{\mathcal{E}}\rangle$ with energies lying in the region $[E-E^S_\alpha, E-E^S_\alpha+\delta E]$.

其维数远大于S的Hilbert空间维数。

$$|E^T_\eta\rangle \approx |E_\alpha^S E_i^{\mathcal{E}}\rangle$$

极弱耦合

因此， $$\mathcal{H}_{\delta E} \simeq \mathcal{H}_d$$

$\mathcal{H}_d$ 中的典型态矢量

$$|\Psi\rangle = \mathcal{N} \sum_{\alpha} |E_{\alpha}^{S}\rangle |\Phi_{\alpha}^{\mathcal{E}}\rangle,$$

where $\mathcal{N}$ is the normalization coefficient and

$$|\Phi_{\alpha}^{\mathcal{E}}\rangle = \sum_{j_\alpha} C_{j_\alpha} |E_{j_\alpha}^{\mathcal{E}}\rangle \quad \text{with } |E_{j_\alpha}^{\mathcal{E}}\rangle \in \mathcal{H}_{\alpha}^{(\mathcal{E})}.$$

Real and imaginary parts of $C_{j\alpha}$ are Gaussian random numbers with mean zero and variance 1/2

给出相应的约化密度矩阵 ρ_d^S。

Goldstein 等人工作的主要结果：

$\mathcal{H}_d$ 中的典型态矢量所给出的约化密度矩阵 ρ_d^S,

（1）在系统S的能量本征态基矢上为对角的，

（2）其对角元正比于 $\mathcal{H}_\alpha^{(\mathcal{E})}$ 子空间的维数。

假设环境的态密度局部地随能量按指数增长

ρ_d^S 为正则分布

$\rho^S \simeq \rho_{\delta E}^S$ $\mathcal{H}_{\delta E} \simeq \mathcal{H}_d$

$$\rho_{\rm can} = Z^{-1} e^{-\beta H^S}$$

大系统微正则分布所给的 ρ S 有正则分布形式。

更实际的弱互作用强度情况

大系统的Hilbert空间的维数，随系统大小按指数增加。

因此，未扰动（大）系统的近邻能级间距，随系统大小按指数减小。

（大系统的能量随系统大小最多按幂次增长）

固定强度的弱互作用下，当环境足够大， $|E^T{}_\eta> \neq |E_\alpha^S E_i^{\mathcal{E}}\rangle$

$\mathcal{H}_{\delta E} \simeq \mathcal{H}_d$ 不再成立，Goldstein等人的推导不适用。

Riera, Gogolin, and Eisert (PRL,108,080402 (2012))证明，互作用足够弱时，约化密度矩阵仍然为正则分布。

（5）热化（thermalization）机制、系统的趋平衡过程与ETH

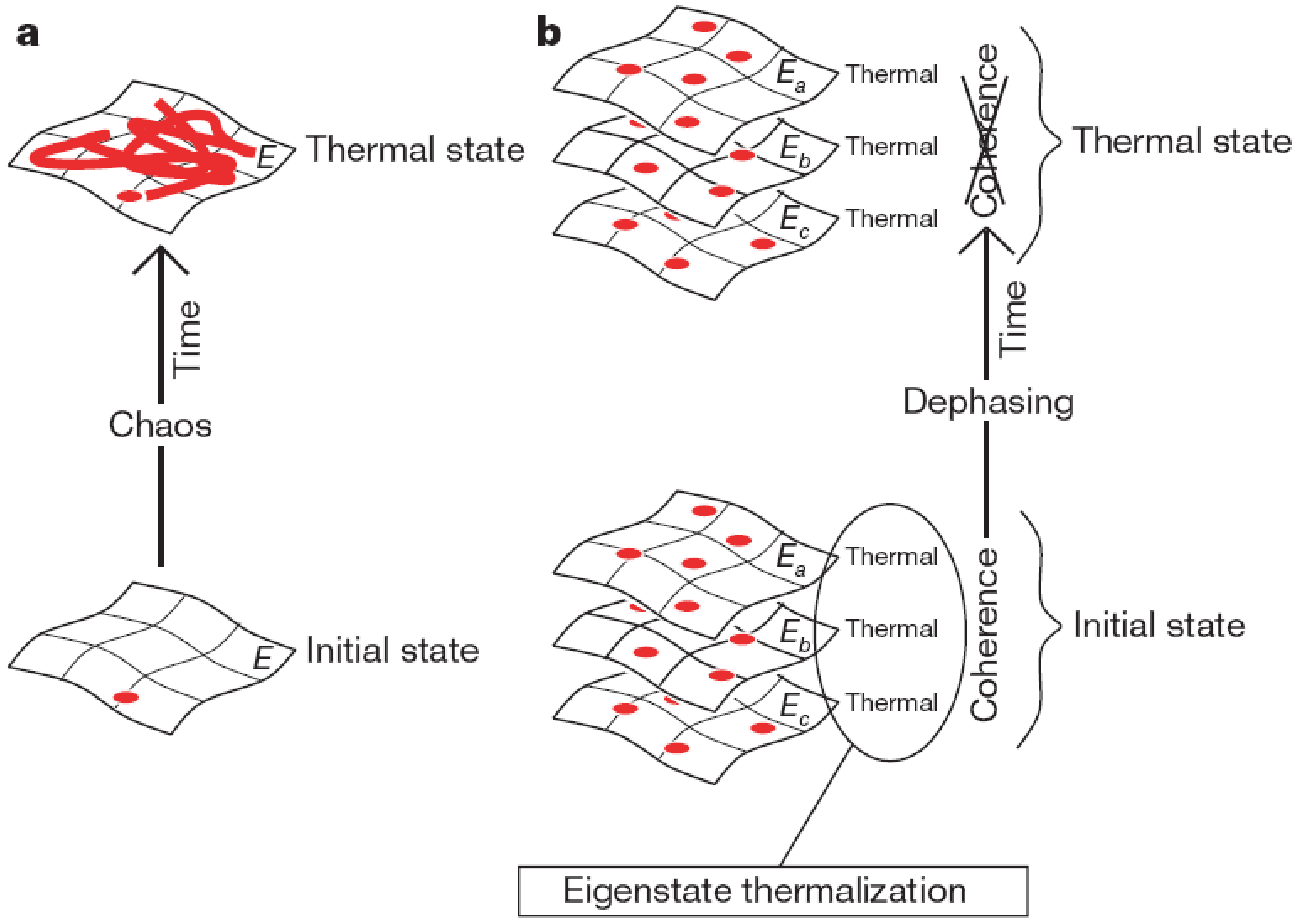
Deutsch and Srednicki independently proposed the third scenario, which, following Srednicki, we call the 'eigenstate thermalization hypothesis (ETH)'[12,13]: the expectation value $\langle \Psi_\alpha | \hat{A} | \Psi_\alpha \rangle$ of a few-body observable $\hat{A}$ in an energy-E_α eigenstate $|\Psi_\alpha\rangle$ of the hamiltonian of a large, interacting many-body system equals the thermal (microcanonical in our case) average $\langle A \rangle_{\text{microcan}}(E_\alpha)$ of $\hat{A}$ at the mean energy E_α

$$\langle \Psi_\alpha | \hat{A} | \Psi_\alpha \rangle = \langle A \rangle_{\text{microcan}}(E_\alpha)$$

12. Deutsch, J. M. Quantum statistical mechanics in a closed system. *Phys. Rev. A* **43**, 2046–2049 (1991).
13. Srednicki, M. Chaos and quantum thermalization. *Phys. Rev. E* **50**, 888–901 (1994).

对ETH的理解：

若能量本征态可视为典型态，则ETH是Levy lemma的特例。


a
Thermal state
E
Time
Chaos
Initial state
E
b
E_a
Thermal
E_b
Thermal
E_c
Thermal
Coherence
Thermal state
Time
Dephasing
E_a
Thermal
E_b
Thermal
E_c
Thermal
Coherence
Initial state
Eigenstate thermalization

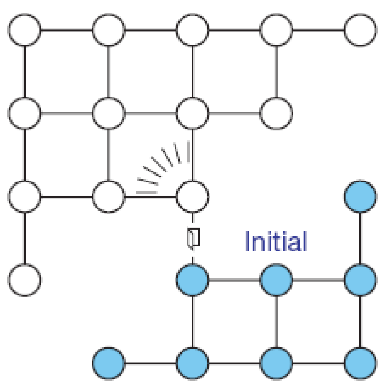
?

nature Vol 452|17 April 2008|doi:10.1038/nature06838

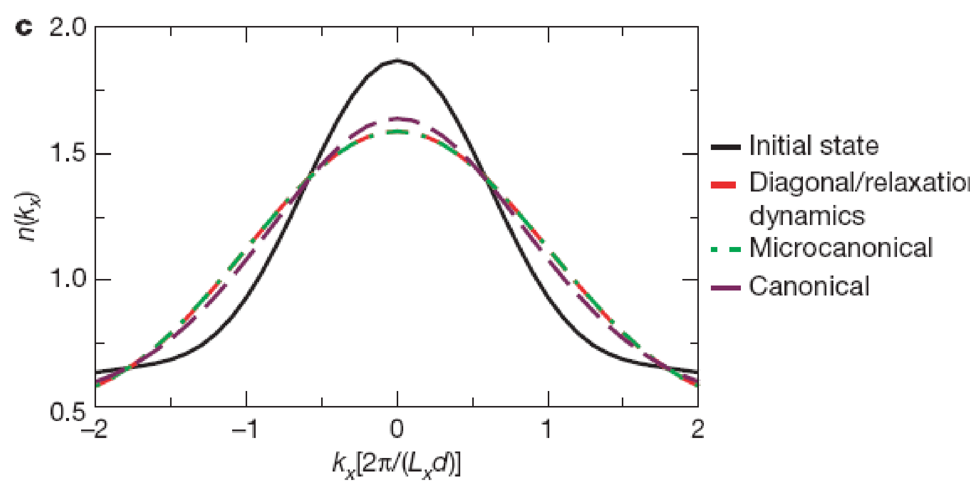
LETTERS

Thermalization and its mechanism for generic isolated quantum systems

Marcos Rigol[1,2], Vanja Dunjko[1,2] & Maxim Olshanii[2]



To study relaxation of an isolated quantum system, we considered the time evolution of five hard-core bosons with additional weak nearest-neighbour repulsions, on a 21-site, two-dimensional lattice,



nature Vol 440|13 April 2006|doi:10.1038/nature04693

LETTERS

A quantum Newton's cradle

Toshiya Kinoshita[1], Trevor Wenger[1] & David S. Weiss[1]

热化：几十年前即有人研究，近来受到很多关注。

—— 实验、数值计算方面有许多进展。

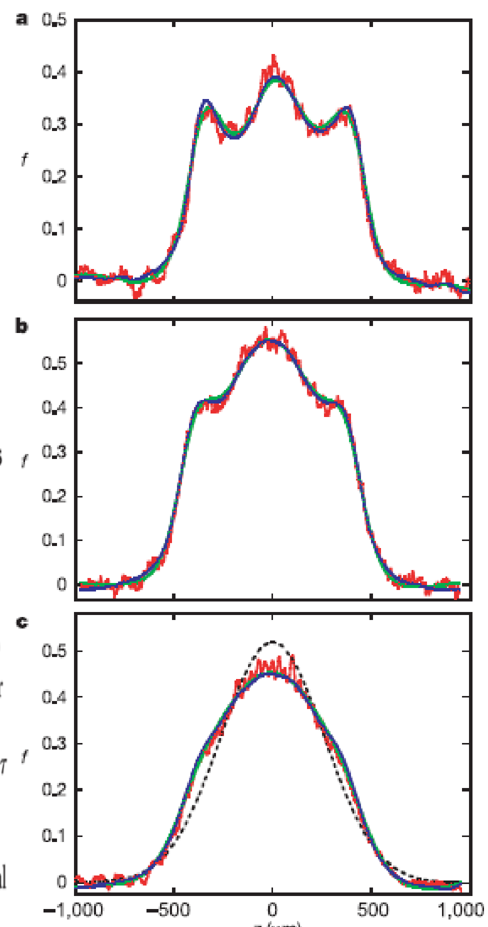
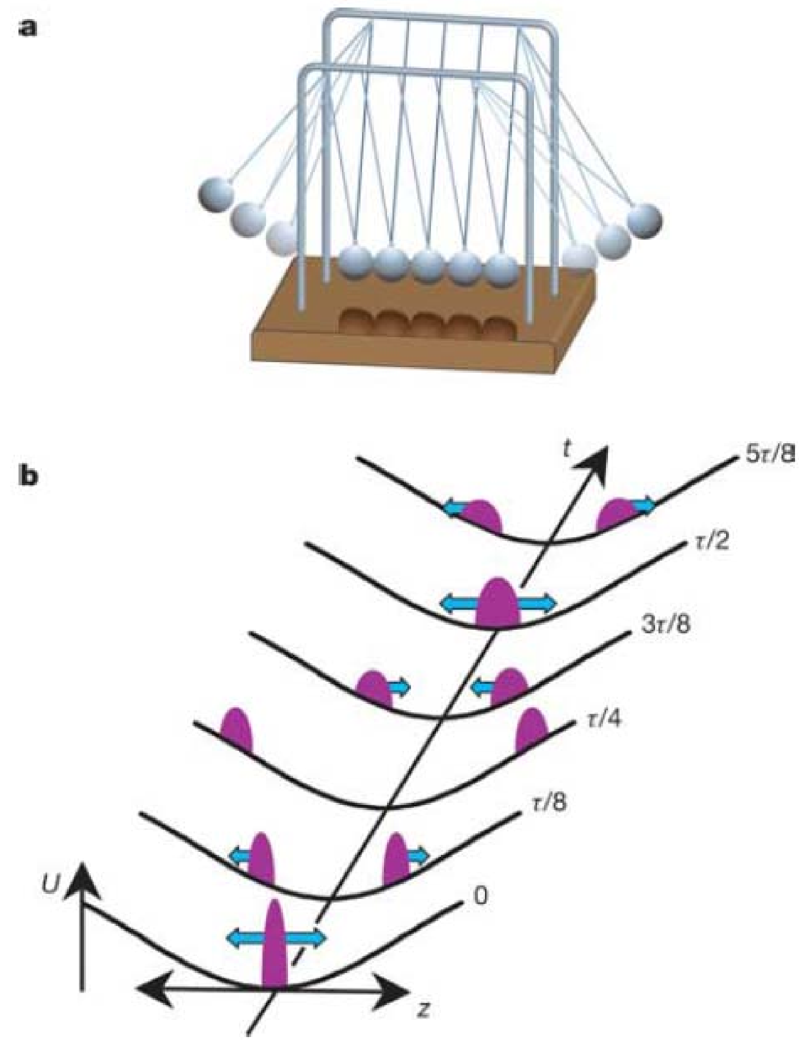
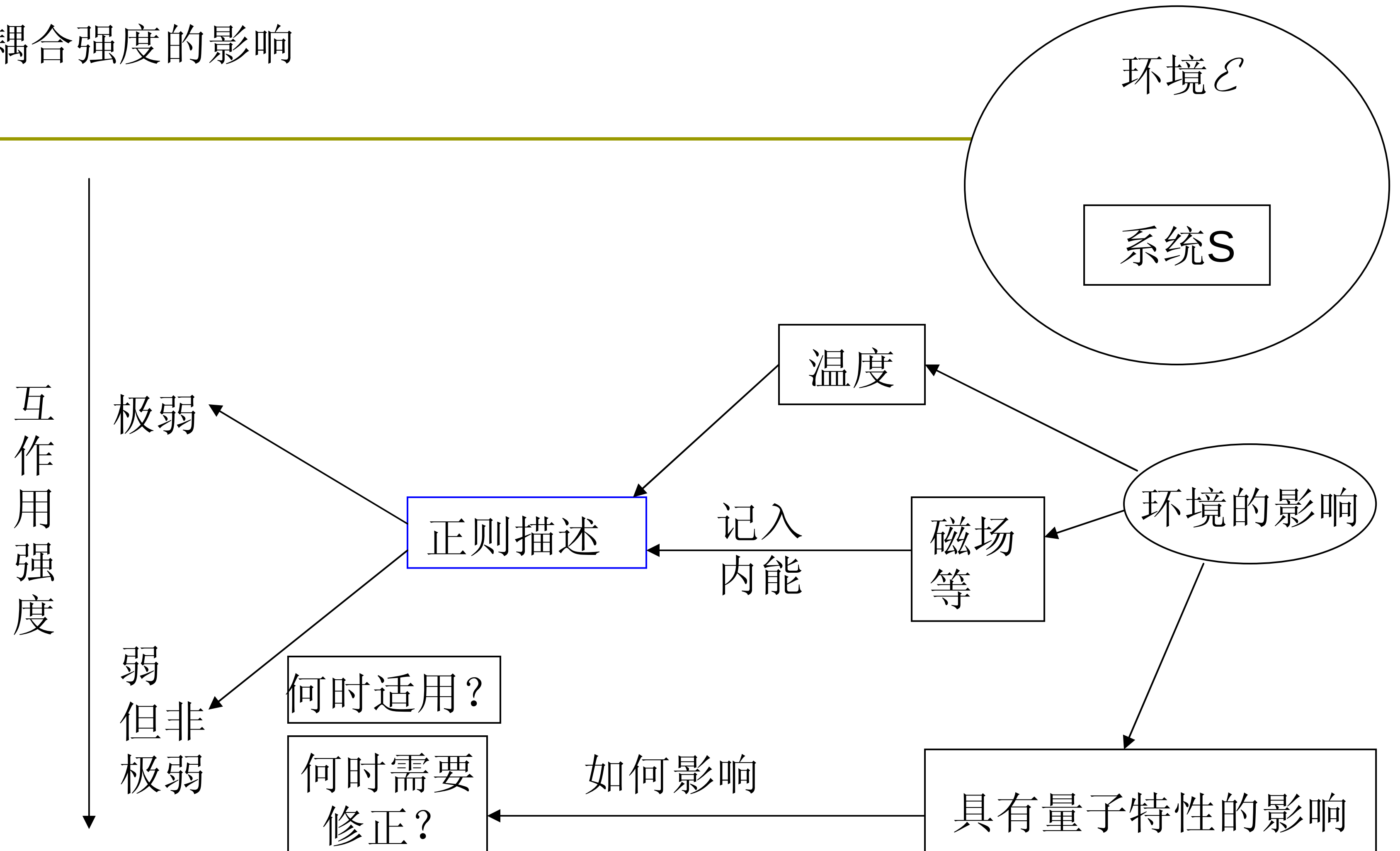


Figure 3 | The expanded momentum distribution, $f(p_{ex})$, for three values of γ_0. The curves are obtained by transversely integrating absorption images like those in Fig. 2. The spatial position, z, is approximately proportional to the expanded momentum, p_{ex}. The vertical scale is arbitrary, but consistent among the curves. **a**, $\gamma_0 = 4$; **b**, $\gamma_0 = 1$; and **c**, $\gamma_0 = 0.62$. The highest (green) curve in each set is the average of $f(p_{ex})$ from the first cycle, that is, from the images like those in Fig. 2. The lower curves in each set are $f(p_{ex})$ taken at single times, t, after the atoms have dephased: **a**, $\tau = 34$ ms, $t = 15\tau$ (blue) and 30τ (red); **b**, $\tau = 13$ ms, $t = 15\tau$ (blue) and 40τ (red); and **c**, $\tau = 13$ ms, $t = 15\tau$ (blue) and 40τ (red). The changes in the distribution with time are attributable to known loss and heating. (See Supplementary Information for a discussion of the fine spatial structure in these curves.)



耦合强度的影响



环境$\mathcal{E}$
系统S
互作用强度
极弱
温度
环境的影响
正则描述
记入内能
磁场等
弱但非极弱
何时适用？
何时需要修正？
如何影响
具有量子特性的影响

$$\mathcal{H}_d = \bigoplus_\alpha |E_\alpha^S\rangle \otimes \mathcal{H}_\alpha^{(\mathcal{E})}$$

(6) 非极弱耦合下小量子系统的统计描述

回顾前述思路

$\rho^S \equiv \mathrm{Tr}_{\mathcal{E}} \rho_{mic} \approx \mathcal{H}_{\delta E}$ 中典型矢量所给约化密度矩阵

$\mathcal{H}_{\delta E} \simeq \mathcal{H}_d$

$\mathcal{H}_d$ 中典型矢量所给约化密度矩阵≈ $\rho_{\mathrm{can}} = Z^{-1} e^{-\beta H^S}$

非极弱互作用下， $|E^T{}_\eta\rangle \neq |E_\alpha^S E_i^{\mathcal{E}}\rangle$

$\mathcal{H}_{\delta E} \simeq \mathcal{H}_d$ 不再成立。

$$\mathcal{H}_d = \bigoplus_\alpha |E_\alpha^S\rangle \otimes \mathcal{H}_\alpha^{(\mathcal{E})}$$

我们的处理方法：

(i) 引入系统S的重整化的自哈密顿量，转动能量本征矢，使新的$\mathcal{H}_d$ 接近于$\mathcal{H}_{\delta E}$

$$H^{SR} = H^{S0} + H_S^I, \quad H^{IR} = H^{I0} - H_S^I,$$

(ii)假设系统S仅与环境的很小部分有直接的相互作用。

具体手段：

减小H在$|E_\alpha^S E_i^{\mathcal{E}}\rangle$ 基上的非对角元，使 $\mathcal{H}_d^R \doteq \mathcal{H}_{\delta E}$

基本结果：

系统S的统计描述为由重整化哈密顿量H^{SR}所给出的正则描述。

$$H_S^I = \sum_{\alpha\beta} (H_S^I)_{\alpha\beta} |E_\alpha^S\rangle\langle E_\beta^S|,$$

$$(H_S^I)_{\alpha\beta} \simeq \langle H_{\alpha\beta}^{I0}\rangle_{\gamma_{\alpha\beta}}$$

where $\gamma_{\alpha\beta} = \alpha$ if $E_\alpha^S < E_\beta^S$ and $\gamma_{\alpha\beta} = \beta$ if $E_\alpha^S > E_\beta^S$.

$\langle H_{\alpha\beta}^{I0}\rangle_\alpha$ 是 $H_{\alpha\beta}^I \equiv \langle E_\alpha^S|H^I|E_\beta^S\rangle$ 在子空间 $\mathcal{H}_\alpha^{(\mathcal{E})}$ 中的期待值的平均值。

特例：互作用哈密顿量为直积形式 $H^{I0} = \epsilon K^S K^A$ （比如自旋情况）

$$\langle H^{I0}_{\alpha\beta}\rangle_\gamma = \epsilon K^S_{\alpha\beta}\langle K^A\rangle_\gamma$$

$$H^{SR} \approx H^{S0} + \epsilon\overline{K^A}K^S + \epsilon\sum_{\alpha\beta}\Delta K^A_{\alpha\beta}K^S_{\alpha\beta}\,|E^S_\alpha\rangle\langle E^S_\beta|,$$

where $\overline{K^A}$ is the average of $\langle K^A\rangle_\gamma$ over γ and $\Delta K^A_{\alpha\beta} = \langle K^{\mathcal{E}}\rangle_{\gamma_{\alpha\beta}} - \overline{K^A}$.

（1） ε 足够小，得到通常的正则描述

（2）$\langle K^A\rangle_\gamma$ 为常数，则$\Delta K^A_{\alpha\beta} \simeq 0$

$$H^{SR} \approx H^{S0} + \epsilon\overline{K^A}K^S.$$

$\overline{K^A}$ 相当于环境所产生的经典场。

例如在外磁场中的单自旋， $-\mu\mathbf{s}\cdot\mathbf{B}$ 一般被视为自哈密顿量的一部分

统计力学基础中未解决问题：

（1）趋平衡过程，即约化密度矩阵趋向于正则分布的过程。（热化）

（2）与环境有非极弱耦合情况下，系统的统计描述。

（3）局域平衡系统的微观描述。

（4）远离平衡态的微观动力学描述。

（4）启示、以及对平衡态性质（本质？）的一种新理解

What is an equilibrium state of a system S?

The canonical typicality approach suggests:

An equilibrium state of a subsystem is described by the reduced density matrix given by a typical vector in an appropriate energy eigen-subspace of the Hilbert space of the total system.

——unnecessary to consider an ensemble.

暂时摆脱系综框架

How could we explain the fact that an equilibrium state behaves like an ``attractor''?

Because, typical vectors give almost identical reduced density matrices.

启示

建立远离平衡态的普遍理论所遇到的关键难题之一：

如何将统计描述与动力学描述更协调、自然地统一起来？

前述理解：平衡态统计理论的成功，可能部分根植于高维线性空间中典型态的某些数学性质。
这为描述子系统非平衡态的性质预留了空间。
（1）大系统若处于非典型态 —— 有非平凡的动力学演化。
（2）若在某子空间中的分量有典型态的特征
—— 可部分应用统计描述。

该新思路在未来几（十几）年会有效推动对非平衡态的理解吗？

Thank you!