LECTURE NOTES
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J. Gemmer
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Quantum Thermodynamics

Emergence of Thermodynamic Behavior Within Composite Quantum Systems

Springer

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Authors

J. Gemmer
Universität Osnabrück
FB Physik
Barbarastr. 7
49069 Osnabrück, Germany

M. Michel
G. Mahler
Universität Stuttgart
Pfaffenwaldring 57
70550 Stuttgart, Germany

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Preface

This monograph views thermodynamics as an *incomplete description* of many freedom quantum systems. Left unaccounted for may be an environment with which the system of interest interacts; closed systems can be described incompletely by focussing on any subsystem with fewer particles and declaring the remainder as the environment. Any interaction with the environment brings the open system to a mixed quantum state, even if the closed compound state is pure. Moreover, observables (and sometimes even the density operator) of an open system may relax to equilibrium values, while the closed compound state keeps evolving unitarily à la Schrödinger forever.

The view thus taken can hardly be controversial for our generation of physicists. And yet, the authors offer surprises. Approach to equilibrium, with equilibrium characterized by maximum ignorance about the open system of interest, does not require excessively many particles: some dozens suffice! Moreover, the precise way of partitioning which might reflect subjective choices is immaterial for the salient features of equilibrium and equilibration. And what is nicest, quantum effects are at work in bringing about universal thermodynamic behavior of modest size open systems. Von Neumann's concept of entropy thus appears as being much more widely useful than sometimes feared, way beyond truely macroscopic systems in equilibrium.

The authors have written numerous papers on their quantum view of thermodynamics, and the present monograph is a most welcome coherent review.

Essen,
June 2004

Fritz Haake

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List of Symbols

$\hat{1}$	Unit operator
$\hat{1}^{(\mu)}$	Unit operator in Hilbert space of subsystem μ
∇	Nabla operator
δ_{ij}	Kronecker delta
$\delta(\dots)$	Dirac δ-function
$\otimes$	Dyadic product
$\mathrm{d}A$	Infinitesimal change of an integrable quantity, complete differential
ΔA	Finite change of A
δA	Infinitesimal change of a non-integrable quantity
$\mathcal{C}_N\{f\}$	Convolution of N identical functions f
$[\![f]\!]$	Hilbert space average of a quantity f
$\mathcal{O}(R,n)$	Surface of an n-dimensional hypersphere with radius R
$\left[\hat{A},\hat{B}\right]$	Commutator of $\hat{A}$ with $\hat{B}$
$\mathcal{F}\{f\}$	Fourier transformation of f
$\overline{f}$	Mean value of f
$\langle i\|j\rangle$	Scalar product in Hilbert space
$\{\eta_i,\xi_i\}$	Set of all coordinates $i=1,\dots n$
$\{\eta_{ab}^{AB},\xi_{ab}^{AB}\}$	Set of coordinates in subspace AB
$\{\eta_i^J,\xi_i^J\}$	Subset of coordinates in subspace J
$\{r,\phi_i\}$	Generalized spherical coordinates
$\{r^J,\phi_i^J\}$	Spherical coordinates of subspace J
$\{r^{AB},\phi_i^{AB}\}$	Spherical coordinates of subspace AB
$\langle\hat{A}\rangle$	Expectation value of operator $\hat{A}$
$\hat{A}$	Operator
$\hat{A}^{(\mu)}$	Operator in subspace μ
$\hat{A}^\dagger$	Adjoint operator
$\hat{A}_{\mathrm{H}}(t)$	Time-dependent operator in Heisenberg picture
$\hat{A}_{\mathrm{I}}$	Operator in the interaction picture
$\|A,a\rangle$	Basis state of the gas system g
A	Index of the energy subspace of the gas system with energy E_A^{g}
a	Index of the degenerate eigenstates belonging to one energy subspace A of the gas system

$A, B/E$	Index operation under the constraint $E_A^{\mathrm{g}} + E_B^{\mathrm{c}} = E$
A_{ij}	Matrix elements of an operator $\hat{A}$
A_{ij}^*	Complex conjugate matrix elements of an operator $\hat{A}$
AR	Accessible region
$\lvert B, b\rangle$	Basis state of the container system c
B	Index of the energy subspace of the container system with energy E_B^{c}
b	Index of the degenerate eigenstates belonging to one energy subspace B of the container system
c	Label for container
$D^2_{\hat{\rho}\hat{\rho}'}$	Distance measure (Bures metric)
D	Diagonal deviation matrix
d	Dimension of the Liouville space
d_A	Dimension of special subspace A
E_i	Energy of the state $\lvert i\rangle$
E	Energy
E_0	Zero-point energy
E^{c}	Total energy of container system
E_B^{c}	Energy eigenvalues of the container system
E^{g}	Total Energy of gas system g
E_A^{g}	Energy eigenvalues of the gas system g
E	Off-diagonal part of a matrix, deviation matrix
$F_{\hat{\rho}\hat{\rho}'}$	Fidelity between $\hat{\rho}$ and $\hat{\rho}'$
$F(T, V)$	Free energy
F	Jacobian matrix (functional matrix)
F^J	Jacobian matrix in subspace J
F^{AB}	See F^J
F	Force
$G(T, p)$	Gibbs free energy
$g(E)$	State density of subsystems
$g(\boldsymbol{\gamma}, E)$	Energy spectrum of wave package $\lvert\gamma\rangle$
$G^{\mathrm{c}}(E_B^{\mathrm{c}})$	State density of the container system
$G^{\mathrm{g}}(E_A^{\mathrm{g}})$	State density of the gas system
$G(E)$	State density at energy E
g	Label for gas subsystem
$H(S, p)$	Enthalpy
$H(\boldsymbol{q}, \boldsymbol{p})$	Hamilton function
$\hat{H}$	Hamiltonian
$\hat{H}_{\mathrm{loc}}^{(\mu)}$	Local Hamiltonian of subsystem μ
$\hat{H}_{\mathrm{F}}^{(\mu,\mu+1)}$	Next neighbor Förster coupling
$\hat{H}_{\mathrm{R}}^{(\mu,\mu+1)}$	Next neighbor random coupling
$\hat{H}_{\mathrm{NR}}^{(\mu,\mu+1)}$	Next neighbor non-resonant coupling
$\hat{H}_0$	Unperturbed Hamiltonian
$\hbar = h/2\pi$	Planck's constant

$\hat{H}^{\mathrm{c}}$	Hamiltonian of the container system c
$\hat{H}^{\mathrm{g}}$	Hamiltonian of the gas system g
$\mathscr{H}$	Hilbert space
$\mathscr{H}^{(\mu)}$	Hilbert space of subsystem μ
i	Imaginary unit
$\hat{I}$	Interaction operator
$\hat{I}^{\mathrm{gc}}$	Interaction between gas system and container system
$\|i\rangle$	Basis state
$\langle i\|$	Adjoint basis state
$\|i,j,\ldots\rangle$	Product state of several subsystems
$\|i,t\rangle$	Time-dependent state
$\|i\rangle \otimes \|j\rangle = \|ij\rangle$	Product state of two subsystems
J	Label for a side condition
$\boldsymbol{j}$	Current
$\boldsymbol{j}_u$	Energy current
$\boldsymbol{j}_s$	Entropy current
$\hat{J}$	Current operator
$\hat{J}^{(\mu,\mu+1)}$	Local current operator between subsystem μ and $\mu+1$
k_{B}	Boltzmann constant
$\hat{\mathcal{L}}$	Super-operator acting on operators of the Liouville space (Lindblad operator)
$\hat{\mathcal{L}}_{\mathrm{coh}}$	Coherent part of Lindblad super-operator
$\hat{\mathcal{L}}^{1,2}_{\mathrm{inc}}$	Incoherent part of Lindblad super-operator
L	Transport coefficient (in general a matrix)
m	Number of micro states accessible for a system; mass
N_0^{c}	Number of levels in lower band
N_1^{c}	Number of levels in upper band
$N^{\mathrm{c}}(E_B^{\mathrm{c}})$	Total number of states in a subspace B, degeneracy
$N(E)$	Number of levels under the constraint $A, B/E$
$N^{\mathrm{g}}(E_A^{\mathrm{g}})$	Total number of states in a subspace A, degeneracy
n_{var}	Number of macro variables
$n^{(\mu)}$	Number of levels of subsystem μ
n_{tot}	Dimension of the total Hilbert space
N	Number of subsystems, particle number
n	Number of levels of a subsystem
$N_{AB} = N_A N_B$	Number of states in subspace AB
N_A	See $N^{\mathrm{g}}(E_A^{\mathrm{g}})$
N_B	See $N^{\mathrm{c}}(E_B^{\mathrm{c}})$
X_i	Extensive macro variable
$\boldsymbol{p}$	Vector of all momentum coordinates
$\boldsymbol{p}_\mu$	Momentum of the μ^{th} particle
$\hat{\boldsymbol{p}}_\mu$	Momentum operator of the μ^{th} particle
$\hat{P}^{\mathrm{ex}}$	Projector projecting out some part ex of the total state space

p	Pressure
$\hat{P}_{ii}^{(\mu)}$	Projector within subspace μ
$\hat{P}_{ij}$	Transition operator, projector for $i = j$
P	Purity
Q	Heat
$\hat{\boldsymbol{q}}_\mu$	Position operator of the μ^{th} particle
q	Position
$\boldsymbol{q}$	Vector of position coordinates of N particles
$\boldsymbol{q}_\mu$	Position of the μ^{th} particle
$\{\boldsymbol{q}_\nu^{\text{c}}\}$	Set of position coordinates of all container particles
$\{\boldsymbol{q}_\mu^{\text{g}}\}$	Set of position coordinates of all gas particles
r	Radial coordinate of a hypersphere
R^J	Radius of hypersphere in subspace J
R^{AB}	See R^J
S	Entropy
S^{tot}	Entropy of system and environment
S_{lin}	Linearized von Neumann entropy
$s(\boldsymbol{q}, t)$	Entropy density
$s(U, V)$	Specific entropy
$\text{sph}(n)$	n-dimensional hypersphere
$T(\boldsymbol{q}, t)$	Temperature field
T	Temperature
$T^{(\mu)}$	Local temperature of subsystem μ
t	Time
$\text{Tr}\{\dots\}$	Trace operation
$\text{Tr}_\mu\{\dots\}$	Partial trace over subsystem μ
$u(\boldsymbol{q}, t)$	Energy density
U	Internal energy
$\hat{U}$	Unitary transformation
$\hat{U}_0(t, t_0)$	Unitary transformation into the interaction picture
U_{ij}	Unitary matrix
$\hat{U}(t)$	Time evolution operator
$\hat{U}^{(\mu)}(t)$	Time evolution operator of subsystem μ
$\boldsymbol{v}$	Velocity vector
$\hat{V}$	Potential
$\hat{V}_{\text{I}}(t)$	Potential in the interaction picture
V	Volume
v	Hilbert space velocity
$W(E_A^{\text{g}}, E_B^{\text{c}})$	See W_{AB}
$W(E_B^{\text{c}})$	See W_B
$W^{\text{d}}(E_B^{\text{c}})$	Dominant probability of finding the container in E_B^{c}
$W^{\text{d}}(E_A^{\text{g}})$	Dominant probability of finding the gas in E_A^{g}
$W(E)$	Probability of finding the complete system at energy E
$W(E_A^{\text{g}})$	See W_A

$W(\boldsymbol{q},\boldsymbol{p},t)$	Probability of finding a point in phase space at position $(\boldsymbol{q},\boldsymbol{p})$ at time t
$W_{ij}^{(12)}$	Probability of finding subsystem 1 in state i and subsystem 2 in state j
$W_{1\to 0}$	Rate for a decay from $\|1\rangle$ to $\|0\rangle$
$W_{ij}(t)$	Transition probability from state j into state i
$W_i = \rho_{ii}$	Statistical weight of, or probability of finding the system in the pure state $\hat{P}_{ii}$
W_{AB}	Joint probability of finding the gas system at energy E_A^{g} and the container system at energy E_B^{c}
W_B	Probability of finding the container system at energy E_B^{c}
W_{AB}^{d}	Dominant probability distribution for the whole system
W_A	Probability of finding the gas system at energy E_A^{g}
$\{W_{AB}\}$	Set of all probabilities W_{AB}, probability distribution
$\{W_{AB}^{\mathrm{d}}\}$	Set of dominant probabilities
W_A^{d}	Dominant probability distribution for the gas system, equivalent to $W^{\mathrm{d}}(E_A^{\mathrm{g}})$
W_B^{d}	Dominant probability distribution for the container system, equivalent to $W^{\mathrm{d}}(E_B^{\mathrm{c}})$
$\|x\rangle$	State vector indexed by position x
Z_i	Macro variables
Z	Canonical partition function
α	Lagrange parameter or exponent for spectra
β	Lagrange parameter; inverse temperature
$\gamma_i = (p_i, q_i)$	Wavepackage coordinates
$\|\boldsymbol{\gamma}\rangle$	Complete but not necessarily orthogonal basis
$\delta\epsilon$	Band width
ΔE_0^{c}	Energy level spacing in lower band
ΔE_1^{c}	Energy level spacing in upper band
$\Delta_{\mathrm{H}}^2(f)$	Hilbert space variance of a quantity f
ΔW_A	Variance of W_A
ε_i	Deviation, small quantity
ε_{AB}	Deviation from W_{AB}^{d}
η	Carnot efficiency
η_i	Real part of ψ_i
κ	Heat conductivity
λ	Coupling constant
λ_0	Mean absolute value of interaction matrix element
μ	Subsystem index; chemical potential
ξ_i	Imaginary part of ψ_i; intensive macro variable
$\hat{\rho}_{\mathrm{eq}}^{\mathrm{g}}$	Equilibrium state of subsystem g
$\hat{\rho}$	Density operator
$\hat{\rho}^{(\mu)}$	Reduced density operator subsystem μ
$\hat{\rho}_{\mathrm{irrel}}$	Irrelevant part of density operator

$\hat{\rho}_{\mathrm{rel}}$	Relevant part of density operator
$\rho_{\mathrm{irrel}}(\boldsymbol{q},\boldsymbol{p})$	Irrelevant part of the prob. dist. func. $\rho(\boldsymbol{q},\boldsymbol{p})$
$\rho_{\mathrm{rel}}(\boldsymbol{q},\boldsymbol{p})$	Relevant part of the prob. dist. func. $\rho(\boldsymbol{q},\boldsymbol{p})$
$\rho(\boldsymbol{q},\boldsymbol{p})$	Probability distribution function
ρ_{ij}	Density matrix
$\hat{\rho}$	Density operator
$\hat{\rho}^{\mathrm{g}}_{\mathrm{min}}$	Minimum purity state of the gas g
$\hat{\sigma}_{\pm}$	Raising/lowering operator
$\hat{\sigma}_i$	Pauli operator
σ	Standard deviation
$\|\psi\rangle$	Wave function, arbitrary pure state
$\|\psi_{\mathrm{I}}(t)\rangle$	Arbitrary wave function in the interaction picture
$\|\psi^{(\mu)}\rangle$	Pure state of subsystem μ
ψ^{AB}_{ab}	Amplitute of a product state $\|Aa\rangle \otimes \|Bb\rangle$
ψ^{A}_{a}	Product state amplitude of gas system
ψ^{B}_{b}	Product state amplitude of container system
ψ_{ij}	Amplitude of a basis product state $\|ij\rangle$
ψ_i	Amplitude of basis state $\|i\rangle$
ω_{ji}	Transition frequency from state j into state i
$\Omega(E)$	Total volume of phase space below the energy surface $H(\boldsymbol{q},\boldsymbol{p}) = E$
$\mathcal{V}\ (\{W_{AB}\})$	Size of region in Hilbert space with probability distribution $\{W_{AB}\}$
$\mathcal{V}^{\,d}$	Size of dominant region in Hilbert space

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