MASTER EQUATION AND SECOND QUANTIZATION

Glauber Model in a Quantum Representation

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Master equation and Two Heat Reservoirs

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PROGRAM

- PROBABILITY DISTRIBUTION
- MASTER EQUATION
- QUANTUM APPROACH

- SIMPLE EXAMPLE
- COUPLING TO A SINGLE HEAT BATH
- INTERACTION
- TWO RESERVOIRS

1. **Equilibrium Statistical Mechanics**
   based on a secure foundation

- probability distribution
- interaction
- environment

2. **Nonequilbrium:**
   different approaches

- Markovian models
- Master equation

Input:
- set of states
- set of rates
- detailed balance coupling to a single heat bath

MASTER-EQUATION

- TYPICAL NON-EQUILIBRIUM SITUATION
- NO HAMILTONIAN-NO BOLTZMANN WEIGHT
- COARSE GRAINING OF SPATIAL SCALE
- REDUCTION OF DEGREES OF FREEDOM
- COARSE GRAINING OF TIME SCALE
- MESOSCOPIC APPROACH
- PROBABILITIC APPROACH

MASTER-EQUATION

- PROCESS
- CERTAIN CONFIGURATION
- MARKOV PROCESS
- UNIFORM IN TIME
- CONTINUOUS IN TIME

$$\partial_t P(S_1,\ldots,S_N,t) = \sum_i w(-S_i \rightarrow S_i) P(\ldots -S_i \ldots) - w(S_i \rightarrow -S_i) P(\ldots S_i \ldots)$$

GAIN LOST

$$\partial_t P(\vec{S}) = L P(\vec{S})$$

SIMPLE EXAMPLE: SPIN-FLIP

$$RATE \quad : \quad \lambda(T,\ldots) \qquad \uparrow \to \downarrow$$

$$RATE \quad : \quad \gamma(T,\ldots) \qquad \downarrow \to \uparrow$$

DESCRIPTION

$p_{\uparrow}(t), \quad p_{\downarrow}(t) \quad probab \quad .$

Markov process

$$p_{\uparrow}(t+\Delta t) = p_{\downarrow}(t)\gamma\Delta t + p_{\uparrow}(t)(1-\lambda\Delta t)$$

$$\frac{dp_{\uparrow}}{dt} = \gamma p_{\downarrow} - \lambda p_{\uparrow} \qquad \frac{dp_{\downarrow}}{dt} = -\gamma p_{\downarrow} + \lambda p_{\uparrow}$$

general .

$$\frac{d}{dt} p_a = L_{ab} p_b$$

$$L_{ab} = \begin{pmatrix} -\lambda & \gamma \\ \lambda & -\gamma \end{pmatrix}$$

QUANTUM DESCRIPTION

OTHER LANGUAGE:
CREATION AND ANNIHILATION OPERATORS

$$|0> = |\uparrow> \qquad |1> = |\downarrow>$$

$$d^{+}|0> = |1>$$

$$d\,|1> = |0>$$

$$d\,d^{+} + d^{+}d = 1$$

$$MAPPING \quad TO \quad SPINS \quad :$$

$$S = 1 - 2d^{+}d = 1 - 2n$$

$$S\,|1> = -1\,|1> \qquad S\,|0> = +1\,|0>$$

MAPPING TO A QUANTUM SYSTEM

$$|F(t)>=\sum_{n} p(\vec{n},t)\,|\vec{n}> \;\Rightarrow\; \frac{\partial}{\partial t}|F(t)>=\hat{L}\,|F(t)>$$

$$<\vec{n}'|\hat{L}\,|\vec{n}> \;=\; L_{n'n}$$

Example

$$d^{+}\,|0>=|1> \;\; \lambda-process$$

$$d\,|0> \;=|1> \;\; \gamma-process$$

$$\hat{L}_{f} \;=\sum_{i}[\gamma(1-d_{i}^{+})d_{i}+\lambda(1-d_{i})d_{i}^{+}]$$

RESULT

$$<A> = <s|A|F>$$

AVERAGE

$$\partial_t <A> = <[A,\hat{L}]>$$

EQUATION OF MOTION

$$\partial_t <n> = \lambda <1-n> - \gamma <n>$$

$$n = d^+ d$$

$$<n>_s = \frac{\lambda}{\lambda+\gamma} = \frac{1}{e^{\varepsilon/T}+1}$$

$$\lambda = \mu \exp(-\varepsilon/2T) \quad \gamma = \mu \exp(\varepsilon/2T)$$

COUPLING TO A HEAT BATH

$$\hat{L}_f = \mu \sum_i [\ (1-d_i^+)\exp(-\frac{H}{2kT})d_i \exp(\frac{H}{2kT}) +$$

$$+\ (1-d_i)\exp(-\frac{H}{2kT})\ d_i^+ \exp(\frac{H}{2kT})\ ]$$

$$\lambda \equiv \mu \exp(-\frac{\varepsilon}{kT}); \quad \gamma \equiv \mu \exp(\frac{\varepsilon}{kT})$$

$$H = \sum \varepsilon n_i$$

$$\lambda < \gamma \quad T \to 0 : \gamma >> \lambda$$

GLAUBER MODEL

- TYPICAL NON-EQUILIBRIUM SYSTEM
- ISING MODEL WITHOUT INTRINSIC DYNAMIC
- COARSE GRAINING OF TIME SCALE
- SINGLE FLIP

$$\partial_t P(\sigma_1,..,\sigma_N,t) = \sum_i w(-\sigma_i \to \sigma_i) P(...-\sigma_i...) - w(\sigma_i \to -\sigma_i) P(..\sigma_i..)$$

$$\partial_t P(\vec{\sigma}) = L(\sigma) P(\vec{\sigma})$$

ISING MODEL and A SINGLE BATH

$$H = -h\sum_i \sigma_i - \frac{1}{2}\sum_{<i,j>} J_{ij}\sigma_i\sigma_j$$

$$H = (2h + 2Jz)\sum_i n_i - 2\sum_{<i,j>} J_{ij} n_i n_j$$

$$\sigma_i = 1 - 2n_i$$

Glauber Model

$$\hat{L} = \kappa \sum_i [\,(1-d_i^+)\,d_i \exp(E_i\,/\,T) + (1-d_i\,)\exp(-E_i\,/\,T)\,]$$

$$E_i = h_i + J(0) - 2\sum_{j(i)} J_{ij}\, d_j^+\, d_j\ ; \quad J(0) = \sum_j J_{ij}$$

$$\frac{\partial}{\partial t}\langle\sigma_i\rangle = -2\langle\, \sigma_i\, w_i(\sigma_i)\,\rangle\,,$$

PHENOMENOLIGICAL ANSATZ
GLAUBER/SUZUKI

$$w_i^G(\sigma_i) = \frac{1}{2\alpha}\left[1 - \sigma_i \tanh\left(\frac{E_i}{T}\right)\right]\,.$$

OUR EXACT RESULT

$$\frac{1}{2\kappa}\frac{\partial}{\partial t}\langle\sigma_i\rangle = \left\langle \sinh\left(\frac{E_i}{T}\right)\right\rangle - \left\langle \sigma_i \cosh\left(\frac{E_i}{T}\right)\right\rangle\,.$$

$$w_i(\sigma_i) = \kappa \exp(-\frac{E_i\sigma_i}{T}) \equiv \kappa \cosh\left(\frac{E_i}{T}\right)\left[1 - \sigma_i \tanh\left(\frac{E_i}{T}\right)\right]\,.$$

DISCUSSION: TRANSITION RATE

$$w_i(\sigma_i) = \kappa \cosh\left(\frac{E_i}{T}\right)\left[\ 1 - \sigma_i \tanh\left(\frac{E_i}{T}\right)\ \right]$$

$$E_i = \sum J_{ij}\,\sigma_j$$

High temperature: same behavior-microscopic time scale
Low temperature E>>T: different behavior

$$\sigma_i = 1$$

$$(i)\ E_i < 0\ \ not\ \ adapted$$

$$w(1)_{T\to 0} = \kappa \exp(|\ E_i\ |/T) \Leftrightarrow \qquad w^G = 1/\alpha$$

$$short\ \ time\ \ flips$$

$$(ii)\ E_i > 0\ \ w(1) = \kappa \exp(-E_i/T)$$

DISCUSSION: TRANSITION RATE

$$w_i(\sigma_i) = \kappa \cosh\left(\frac{E_i}{T}\right) [\, 1 - \tanh\left(\frac{E_i}{T}\right) \,]$$

Low temperature E>>T: different behavior

$$\sigma_i = -1$$

$$(i)\, E_i < 0 \;\; not \;\; adapted$$

$$w(-1)_{T \to 0} = \kappa \exp(-|E_i|/T) \Rightarrow 0 \;\; flips \;\; \mathrm{sup}\, .$$

$$(ii)\;\; E_i > 0 \;\;\; w(-1) = \kappa \exp(E_i/T) \;\; high \;\; rate$$

Coupling to two reservoirs

$$L = \nu \sum_i \left[(1 - d_i^\dagger) e^{-H_i/2T'} d_i e^{H_i/2T} + (1 - d_i) e^{-H_i/2T'} d_i^\dagger e^{H_i/2T} \right].$$

Two different reservoirs: T and T'

Local energy:

$$H_i = (\varepsilon_i - \mu) n_i$$

Coupling to two reservoirs

$$L = \nu \sum_i [(1 - d_i^\dagger) d_i \exp((\varepsilon_i - \mu)/2T)$$

$$+ (1 - d_i) d_i^\dagger \exp(-(\varepsilon - \mu)/T')].$$

$$\exp(-H_i/2T') d_i \exp(H_i/2T) |1\rangle = \exp(\varepsilon_i - \mu)/2T |0\rangle,$$

$$\exp(-H_i/2T') d_i^\dagger \exp(H_i/2T) |0\rangle = \exp(-(\varepsilon_i - \mu)/2T') |1\rangle.$$

$\uparrow \rightarrow \downarrow \quad \lambda - process\ activated\ by\ T'$

Result

$$\nu^{-1}\partial < n_i > = \exp[-(\varepsilon_i - \mu)/2T'] < 1 - n_i > - \exp(\varepsilon_i - \mu)/2T < n_i >$$

$$\langle n_i \rangle_s = \frac{1}{\exp((\varepsilon_i - \mu)/T_e) + 1} \quad \text{with} \quad \frac{1}{T_e} = \frac{1}{2}\left[\frac{1}{T} + \frac{1}{T'}\right].$$

Induced phase transition

$$\varepsilon_i = 2\left[h_i + \sum_j J_{ij}\langle\sigma_j\rangle \right],$$

$$\nu^{-1}\partial_t\langle\sigma\rangle = -r\langle\sigma\rangle + b\langle\sigma\rangle^2 - u\langle\sigma\rangle^3,$$

with $r = 2T_0\left[\frac{1}{T_e} - \frac{1}{T_0}\right]$, $\quad b = T_0^2\left[\frac{1}{T} - \frac{1}{T'}\right]\left[\frac{1}{T_e} - \frac{1}{T_0}\right]$,

$$u = \frac{T_0^2}{2}\left[\frac{1}{T^2} + \frac{1}{T'^2}\right] - \frac{T_0^3}{6}\left[\frac{1}{T^3} - \frac{1}{T'^3}\right]. \qquad (23)$$

Symmetry:

$$\sigma \leftrightarrow -\sigma \qquad T \leftrightarrow T'$$

OUTLOOK

Diffusion and two different reservoirs

$$L = \mu \sum_{ij} (1 - d_i \; d_j^+) \; d_i^+ d_j \; \exp[\varepsilon / 2(1/T_j \; - 1/T_i \;)]$$

Continuous model for n(x,t)

$$\partial_t n = -\nabla \bullet \vec{j} \qquad \vec{j} = -D \nabla n + \lambda n \nabla T$$

Stationary solution

$$n(\vec{x}) = c \; \exp(\lambda / D \;\; T(\vec{x}))$$

Summary

- ❖Master equation in a quantum representation
- ❖Transition probability distribution
- ❖Extension to two reservoirs
- ❖Induced phase transition

oDiffusion and heat transport
oCoupled equations

INTRODUCTION

Different levels

•Microscopic	quantum approach
•Macroscopic	thermodynamics
•Mesoscopic	hydrodynamic, phase transitions probabilistic approach
Aim:	characterization of states evolution process, equations

Stochastic models on a mesoscopic level

Joint probability density distribution

$P_n(1,2,...n)$ $\quad 1 = (x_1, t_1);$ $\quad t_1 > ...> t_n$

Conditional probability

$P_n(1,2..,n) = P(1|2,...,n)$

Reduced distribution $P_{n-1}=\sum\int P_n$

1. Simplification: Markov Process

$P_n(1,2..,n) = P(1|2)$

Consequence

$P_n(1,2,...n) = P(1|2)\, P(2|3)..\, P(n-1|n)\, P_1(n)$

Chapman-Kolmogorov Equation

$P(1|3) = \int\sum P(1|2)P(2|3)$

2. **Simplification:** Uniform in time

$$P_2(x_1,t_1;x_2,t_2) = P(x_1,t_1\text{-}t_2\,|x_2)\;P_1(x_2)$$

Consequence: **Master equation**

3.Simplification: Contin. Time

$P(1|1`) = T_\tau(x|x`) \qquad \tau\ = t - t`$

$T_\tau(x|x`) = T_0(x|x`) + \hat{w}(x|x`)\,\tau + 0(\tau^2)$

$$\frac{\partial T_\tau(x\,|\,x`)}{\partial \tau} = \sum \int d\bar{x}\, \hat{w}(x\,|\,\bar{x}) T_\tau(\bar{x}\,|\,x`)$$

Constraint $\sum \int dx\, \hat{w}(x\,|\,x`) = 0$

Define new function to resolve the constraint

$$\hat{w}(x\,|\,x`) = w(x\,|\,x`) - \delta(x - x`) \sum \int d\bar{x} w(\bar{x}\,|\,x`)$$

Master Equation **gain** **lost**

$$\frac{\partial T_\tau(x\,|\,x`)}{\partial \tau} = \sum \int d\bar{x} \left[ w(x\,|\,\bar{x}) T_\tau(\bar{x}\,|\,x`) - w(\bar{x}\,|\,x) T_\tau(x\,|\,x`) \right]$$

$$\partial_t p(n,t) = \sum_{n'} \left[\, w(n \mid n')\, p(n',t) - w(n' \mid n)\, p(n,t) \,\right] \equiv \sum_{n'} L(n,n')\, p(n',t)\,.$$

$$w(n' \mid n) = \exp[-\beta H(n')/2]\, V(n' \mid n)\ \exp[\beta H(n)/2]\,.$$

$$\frac{p_s(n')}{p_s(n)} = \frac{V(n' \mid n)}{V(n \mid n')} \exp(\beta[H(n) - H(n')])\,.$$

$$\begin{aligned} \partial_t p(n,t) \ &= \ \sum_{n'} [\exp(-\beta H(n)/2)\, V(n \mid n')\ \exp(\beta H(n')/2)\, p(n',t) \\ &- \ \exp(-\beta H(n')/2) V(n' \mid n) \exp(\beta H(n)/2)\, p(n,t)\,]\,. \end{aligned}$$