Kinetics in a non-glauberian Ising model: some exact results

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Contents :

I. Kinetic Ising models

study relaxation of $1D$ Ising spin systems coupled to a heat bath
classical equilibrium Hamiltonian : $\mathcal{H} = -J \sum_n \sigma_n \sigma_{n+1}$, $\sigma_n = \pm 1$
consider probability $P(\{\sigma\}; t)$ of configuration $\{\sigma\} = (\sigma_1, \ldots, \sigma_{\mathcal{N}})$
Markovian dynamics, described by a master equation

$$\partial_t P(\{\sigma\}; t) = -\sum_n \left[W(F_n\sigma|\sigma) P(\{\sigma\}; t) - W(\sigma|F_n\sigma) P(\{F_n\sigma\}; t) \right]$$

with single-spin flips $\{F_n\sigma\} = (\sigma_1, \ldots, \sigma_{n-1}, -\sigma_n, \sigma_{n+1}, \ldots, \sigma_{\mathcal{N}})$
and transition rates $W(\sigma \to \tau) = W(\tau|\sigma)$.

experimentally observed, e.g. in single-chain magnets :
$[Mn_2(saltmen)_2Ni(pao)_2(py)_2](ClO_4)_2$ Coulon et al. '04

Local transition rates, with
(i) parity and (ii) spin-reversal symmetries (for $h_n = 0$) :

$$W(F_n\sigma|\sigma) = \alpha\,(1 - (\gamma/2)\sigma_n\,(\sigma_{n-1} + \sigma_{n+1}) + \delta\sigma_{n-1}\sigma_{n+1})$$
$$-\quad \alpha\tanh(\beta h_n)\,(\sigma_n - (\gamma/2)\,(\sigma_{n-1} + \sigma_{n+1}) + \delta\sigma_{n-1}\sigma_n\sigma_{n+1})$$

Detailed balance guarantees relaxation towards equilibrium state at temperature β^{-1} :

$$\gamma = (1+\delta)\tanh(2\beta J).$$

Almost universally chosen :
Glauber dynamics : $\delta = 0$ **integrable** in one dimension

GLAUBER '63

here : **KDH dynamics** : $\boxed{\gamma = 2\delta}$

KIMBALL '79, DEKER & HAAKE '79

physical interest : consider transition rates

process	rates: Glauber	rates: KDH	dual process
$\uparrow\downarrow\uparrow \longrightarrow \uparrow\uparrow\uparrow$	$\alpha(1+\gamma)$	$\alpha(1+3\delta)$	$AA \longrightarrow \emptyset\emptyset$
$\uparrow\uparrow\uparrow \longrightarrow \uparrow\downarrow\uparrow$	$\alpha(1-\gamma)$	$\alpha(1-\delta)$	$\emptyset\emptyset \longrightarrow AA$
$\uparrow\uparrow\downarrow \longrightarrow \uparrow\downarrow\downarrow$	α	$\alpha(1-\delta)$	$\emptyset A \longrightarrow A\emptyset$
$\uparrow\downarrow\downarrow \longrightarrow \uparrow\uparrow\downarrow$	α	$\alpha(1-\delta)$	$A\emptyset \longrightarrow \emptyset A$

here : $\gamma = \tanh(2\beta J)$, $\delta = \tanh(2\beta J)/(2-\tanh(2\beta J))$.

for $J > 0$ always **two** stationary states : $\cdots\uparrow\uparrow\uparrow\uparrow\cdots, \cdots\downarrow\downarrow\downarrow\downarrow\cdots$
unique stationary states for $\beta^{-1} > 0 \Longleftrightarrow \gamma < 1, \delta < 1$

additional absorbing states for KDH dynamics if $\delta = 1$
periodic chain with $\mathcal{N}$ sites : $\approx 2 \cdot 1.618^{\mathcal{N}}$ absorbing states

Carlon, MH, Schollwöck '01

Questions :

- effect of additional absorbing states on dynamics ?
- value of dynamical exponent z ? DEKER & HAAKE '79, HAAKE & THOL '80
- consequences for ageing behaviour ? (two-time quantities)
- relationships with kinetically constained models ?

FREDERIKSON & ANDERSEN '84

II. Calculation of global averages

Find single-time and two-time observables

$$\langle X\rangle_t := \sum_{\sigma} X(\{\sigma\})P(\{\sigma\};t)$$

$$\langle X(t)Y(s)\rangle := \sum_{\sigma,\widetilde{\sigma}} X(\{\sigma\})Y(\{\widetilde{\sigma}\})P(\{\sigma\},t|\{\widetilde{\sigma}\},s)$$

Consider single-spin and three-spin quantities

$$\sigma_n \quad , \quad q_n := \sigma_{n-1}\sigma_n\sigma_{n+1}$$

Single-time averages can be found from ($n_i \neq n_j$ if $i \neq j$) : GLAUBER '63

$$\frac{\partial}{\partial t}\langle \sigma_{n_1}\cdots\sigma_{n_N}\rangle_t = -2\left\langle \sigma_{n_1}\cdots\sigma_{n_N}\sum_{i=1}^{N} W(F_{n_i}\sigma|\sigma)\right\rangle_t ,$$

find explicit equations of motion (for external field $h_n = 0$) :

$$\begin{aligned} \frac{\partial}{\partial t}\langle \sigma_n \rangle &= -\langle \sigma_n \rangle + \frac{\gamma}{2}\langle \sigma_{n-1} + \sigma_{n+1} \rangle - \delta \langle q_n \rangle \\ \frac{\partial}{\partial t}\langle q_n \rangle &= -3\langle q_n \rangle + \gamma \langle \sigma_{n-1} + \sigma_{n+1} \rangle - \delta \langle \sigma_n \rangle + \delta \, \langle A_n \rangle \end{aligned}$$

$$\text{where} \quad A_n := \left[\frac{\gamma}{2\delta} \sigma_{n-2}\sigma_n\sigma_{n+1} - \sigma_{n-1}\sigma_{n+1}\sigma_{n+2} \right] + \left[\frac{\gamma}{2\delta} \sigma_{n-1}\sigma_n\sigma_{n+2} - \sigma_{n-2}\sigma_{n-1}\sigma_{n+1} \right]$$

Define **global observables** : Kimball '79, Deker & Haake '79

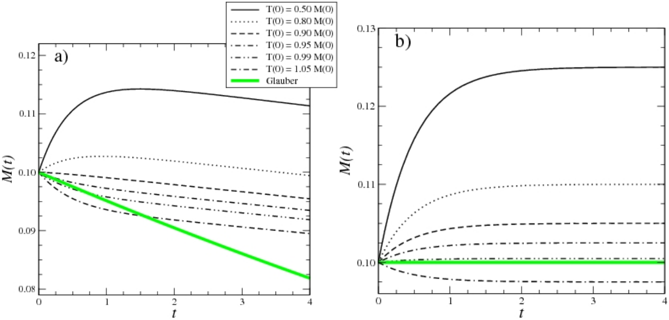
$$M(t) := \frac{1}{\mathcal{N}} \sum_n \langle \sigma_n \rangle_t \ , \quad T(t) := \frac{1}{\mathcal{N}} \sum_n \langle q_n \rangle_t$$

find for $\boxed{\gamma = 2\delta}$ (KDH) a **closed system** of equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} M(t) \\ T(t) \end{pmatrix} = \begin{pmatrix} 2\delta - 1 & -\delta \\ 3\delta & -3 \end{pmatrix} \begin{pmatrix} M(t) \\ T(t) \end{pmatrix} \ , \quad \mathcal{N} \to \infty$$

Solution : $M(t) = M_- e^{-t/\tau_-} + M_+ e^{-t/\tau_+}$
with $\tau_\pm^{-1} = 2 - \delta \pm \sqrt{1 + 2\delta - 2\delta^2}$.
1. **Dynamical exponent** : equilibrium correlation length
$\xi^{-1} = -\ln\tanh(\beta J) \approx 2e^{-2\beta J}$, hence $\delta \simeq 1 - \xi^{-2}$ DEKER & HAAKE '79

For large times & $\beta \to \infty$, relaxation time $\tau_- \simeq \frac{2}{3}\xi^4 \Longrightarrow \boxed{z = 4}$
distinct from result $z = 2$ of Glauber dynamics as $\beta^{-1} \to 0$
2. **non-monotonous behaviour** of global magnetisation, in contrast to Glauber dynamics



magnetisation $M(t)$ in KDH model (a) $\delta = 0.90476$ (b) $\delta = 1$

Global single-time correlators :

$$C^{\sigma\sigma}_{m,n}(t) := \langle \sigma_m \sigma_n \rangle_t \quad , \quad C^{q\sigma}_{m,n}(t) := \langle q_m \sigma_n \rangle_t \quad , \quad C^{qq}_{m,n}(t) := \langle q_m q_n \rangle_t$$

and $C^{ab}(t) := \mathcal{N}^{-2} \sum_{m,n} C^{ab}_{m,n}(t)$. We find, for $\mathcal{N} \to \infty$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} C^{\sigma\sigma}(t) \\ C^{q\sigma}(t) \\ C^{qq}(t) \end{pmatrix} = \begin{pmatrix} 4\delta - 2 & -2\delta & 0 \\ 3\delta & 2\delta - 4 & -\delta \\ 0 & 6\delta & -6 \end{pmatrix} \begin{pmatrix} C^{\sigma\sigma}(t) \\ C^{q\sigma}(t) \\ C^{qq}(t) \end{pmatrix}$$

with the explicit solutions ($\alpha_\pm := 1 + \delta \pm \sqrt{1 + 2\delta - 2\delta^2}$) :

$$\begin{aligned} C^{\sigma\sigma}(t) &= B_- e^{-2t/\tau_-} + B_0 e^{-t(\tau_-^{-1} + \tau_+^{-1})} + B_+ e^{-2t/\tau_+} \\ C^{q\sigma}(t) &= \frac{\alpha_- B_-}{\delta} e^{-2t/\tau_-} + \frac{(1+\delta) B_0}{\delta} e^{-t(\tau_-^{-1} + \tau_+^{-1})} + \frac{\alpha_+ B_+}{\delta} e^{-2t/\tau_+} \\ C^{qq}(t) &= \frac{3\alpha_-}{\alpha_+} B_- e^{-2t/\tau_-} + 3 B_0 e^{-t(\tau_-^{-1} + \tau_+^{-1})} + \frac{3\alpha_+}{\alpha_-} B_+ e^{-2t/\tau_+} \end{aligned}$$

NB : the $B_{\pm,0}$ depend on the initial conditions

III. Ageing behaviour

a) Define **two-time** (linear) **response functions** to an external magnetic field $h(s)$:

$$\widehat{R}(t,s) := \frac{1}{\beta\mathcal{N}} \sum_n \left. \frac{\delta\langle\sigma_n\rangle_t}{\delta h(s)} \right|_{h=0} \;,\quad \widehat{Q}(t,s) := \frac{1}{\beta\mathcal{N}} \sum_n \left. \frac{\delta\langle q_n\rangle_t}{\delta h(s)} \right|_{h=0}$$

such that for $t > s$, we have

$$\frac{\partial}{\partial t} \begin{pmatrix} \widehat{R}(t,s) \\ \widehat{Q}(t,s) \end{pmatrix} = \begin{pmatrix} 2\delta - 1 & -\delta \\ 3\delta & -3 \end{pmatrix} \begin{pmatrix} \widehat{R}(t,s) \\ \widehat{Q}(t,s) \end{pmatrix} \;,\quad \mathcal{N} \to \infty$$

with the boundary conditions for $t = s$:

$$\begin{aligned} \widehat{R}(s,s) &= 1 + \delta C_0^{q\sigma}(s) - 2\delta C_1^{\sigma\sigma}(s) \\ \widehat{Q}(s,s) &= \delta + (1-2\delta) C_0^{q\sigma}(s) + 2(1-\delta) C_1^{q\sigma}(s) \\ &\quad -2\delta C_2^{q\sigma}(s) + 2\delta C_1^{qq}(s) \end{aligned}$$

NB : the non-global correlators $C_n^{ab}(t) = \mathcal{N}^{-1} \sum_m C_{n+m,m}^{ab}(t)$ are not yet known in general

Solution : $\widehat{R}(t,s) = A_-(s)e^{-(t-s)/\tau_-} + A_+(s)e^{-(t-s)/\tau_+}$.

Quench from **fully disordered state** ($\delta = 0$ or $\beta^{-1} = \infty$)
to some finite $\delta \in (0,1]$:
then $\widehat{R}(0,0) = 1$ and $\widehat{Q}(0,0) = \delta$.
In particular, at **zero** temperature $\delta = 1$, we find $\widehat{R}(t,0) \sim \mathrm{cste.}$.

Interpretation : space-time response with respect to a fluctuation in the initial state : $R(t,0;\mathbf{r}) = t^{-\lambda_R/z} f_R(|\mathbf{r}|^z/t)$
our results are in Fourier space at zero momentum $\mathbf{k} = \mathbf{0}$:

$$\begin{aligned}\widehat{R}(t,0) &= \widehat{R}_{\mathbf{0}}(t,0) = \int_{\mathbb{R}^d} \mathrm{d}\mathbf{r}\, e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} R(t,0;\mathbf{r}) \\ &= \int_{\mathbb{R}^d} \mathrm{d}\mathbf{r}\, t^{-\lambda_R/z} f_R(|\mathbf{r}|^z/t) \sim t^{(d-\lambda_R)/z}\end{aligned}$$

hence **autoresponse exponent** of $1D$ KDH model : $\boxed{\lambda_R = 1}$

b) **two-time correlation function** $\widehat{C}^{ab}(t,s) := \mathcal{N}^{-2}\sum_{m,n} C^{ab}_{m,n}(t,s)$
For $t > s$, we have the equations of motion

$$\frac{\partial}{\partial t}\left(\begin{array}{c}\widehat{C}^{\sigma f}(t,s)\\ \widehat{C}^{qf}(t,s)\end{array}\right) = \left(\begin{array}{cc}2\delta-1 & -\delta\\ 3\delta & -3\end{array}\right)\left(\begin{array}{c}\widehat{C}^{\sigma f}(t,s)\\ \widehat{C}^{qf}(t,s)\end{array}\right)$$

and boundary condition for $t = s$: $\widehat{C}^{ab}(s,s) = C^{ab}(s)$.
For example, the global spin-spin correlator is

$$C^{\sigma\sigma}(t,s) = B_- e^{-(t+s)/\tau_-} + \frac{B_0}{2}\left[e^{-t/\tau_- - s/\tau_+} + e^{-t/\tau_+ - s/\tau_-}\right] + B_+ e^{-(t+s)/\tau_+}$$

Quench from $\delta = 0$ to criticality $\delta = 1$: we find $\widehat{C}^{\sigma\sigma}(t,s) \sim \text{cste.}$.
Interpretation : result in Fourier space at zero momentum $\mathbf{k} = \mathbf{0}$:

$$\widehat{C}(t,0) = \widehat{C}_{\mathbf{0}}(t,0) = \int_{\mathbb{R}^d} \mathrm{d}\mathbf{r}\; e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} C(t,0;\mathbf{r}) \sim t^{(d-\lambda_C)/z}$$

hence **autocorrelation exponent** of $1D$ KDH model : $\boxed{\lambda_C = 1}$

IV. Conclusions

1. $1D$ KDH model $\gamma = 2\delta$ gives closed equations of motion for global magnetisation $\sum_n \langle \sigma_n \rangle$ and three-spin average $\sum_n \langle \sigma_{n-1}\sigma_n\sigma_{n+1} \rangle$ — KIMBALL '79, DEKER & HAAKE '79
2. at zero temperature **many** new absorbing states
   dual system : reaction(-diffusion) processes
3. find closed system of equations of motion for **global** single-time and two-time correlators and responses
4. exponents : $\boxed{z = 4,\ \lambda_C = \lambda_R = 1}$
   for comparison : Glauber dynamics : $z = 2$, $\lambda_C = \lambda_R = 1$.

Some open questions :

- extension to higher dimensions ?
- extension to different spin systems ?
- closed systems of equations for non-vanishing momenta ?