Some exact results in systems of immobile interacting particles

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1. Motivation

Question : how to understand behaviour of interacting many-body systems ?

exactly solvable models $\Longrightarrow$ insight beyond mean-field concepts

much work done on $1D$ reaction-**diffusion** models $\Rightarrow$ Bethe ansatz/free fermions

process	rates: Glauber	rates: KDH	**dual** process
$\uparrow\downarrow\uparrow\longrightarrow\uparrow\uparrow\uparrow$	$\frac{1}{2}(1+\gamma)$	$\frac{1}{2}(1+3\delta)$	$AA \longrightarrow \emptyset\emptyset$
$\uparrow\uparrow\uparrow\longrightarrow\uparrow\downarrow\uparrow$	$\frac{1}{2}(1-\gamma)$	$\frac{1}{2}(1-\delta)$	$\emptyset\emptyset \longrightarrow AA$
$\uparrow\uparrow\downarrow\longrightarrow\uparrow\downarrow\downarrow$	$\frac{1}{2}$	$\frac{1}{2}(1-\delta)$	$\emptyset A \longrightarrow A\emptyset$
$\uparrow\downarrow\downarrow\longrightarrow\uparrow\uparrow\downarrow$	$\frac{1}{2}$	$\frac{1}{2}(1-\delta)$	$A\emptyset \longrightarrow \emptyset A$

KDH : Kimball '79 ; Deker & Haake '79 (exact magnetisation)

exact correlators/responses : Dutta, MH, Park 09

dynamical exponent $\tau \sim \xi^z$

$$z = \begin{cases} 2 & ; \text{ Glauber} \\ 4 & ; \text{ KDH} \end{cases}$$

 # stationary states (L sites, $T=0$)

$$\mathbf{N}_{\rm st} \simeq \begin{cases} 2 & ; \text{ Glauber} \\ g^L & ; \text{ KDH} \end{cases}$$

$g = (1+\sqrt{5}\,)/2 \simeq 1.618\ldots$ is the golden number

Here : consider opposite extreme, **without** diffusion (dual to KDH with $\delta = 1$)

applications to catalysis (e.g. ethanol oxydation) Dias, Araújo, Cadilhe 12

1. $A + A \to \emptyset + \emptyset$, with rate 2, **diffusionless particles**

descent dynamics : rapid local relaxation to stationary state
each single particle reacts **at most once** during its entire life
macroscopic averages depend sensitively on initial conditions

Kenkre & van Horn 81, Frederikson & Andersen 84, Prados & Brey 01-07,...

Analogies :

a) random sequential adsorption (RSA) $A \leftrightarrow \circ,\ \emptyset \leftrightarrow \bullet$

Evans 84, 93, Oliveira, Tomé, Dickman 92-94,...

b) metastable states in granular matter, tests of the Edwards' hypothesis

Edwards *et al.* 94, de Smedt, Godrèche, Luck 02, 05,...

2. $A + B \to \emptyset + \emptyset$, with rate 1, **diffusionless particles**

Majumdar & Privman 93

Duality with Ising model interfaces : if $\uparrow\downarrow \doteq A$ and $\downarrow\uparrow \doteq B$, then

$$(\uparrow\downarrow\uparrow \longrightarrow \uparrow\uparrow\uparrow) \doteq (AB \longrightarrow \emptyset\emptyset)\ ,\ (\downarrow\uparrow\downarrow \longrightarrow \downarrow\downarrow\downarrow) \doteq (BA \longrightarrow \emptyset\emptyset)$$

Aim : explicit exact calculation of particle-densities and correlators, for **arbitrary** initial conditions

2. Single-species model : the infinite lattice

Define ***n*-strings** of n **consecutive** particles $\underbrace{\bullet\bullet\ldots\bullet}_{n\ \text{particles}}$ $\qquad A+A\to\emptyset+\emptyset$

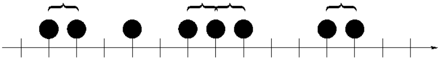
$$C_n(t) := \langle \eta_1(t)\eta_2(t)\ldots\eta_n(t)\rangle = \mathbf{P}\left(\underbrace{\bullet\bullet\ldots\bullet}_{n\ \text{particles}}\right)$$

Derive **closed** system of eqs. of motion, for all $n \geq 1$

$$\frac{\mathrm{d}}{\mathrm{d}t}C_n(t) = -2(n-1)C_n(t) - 4C_{n+1}(t)$$

simplify : change of variables

$$C_n(t) = u_n(s)e^{-2(n-1)t} \quad , \quad s = \frac{e^{-2t}-1}{2} \Longrightarrow \frac{\mathrm{d}}{\mathrm{d}s}u_n(s) = 4u_{n+1}(s)$$



Define auxiliary quantity $u_0(s)$ such that eq. of motion also valid for $n \geq 0$

Define generating function $F(x,s) := \sum_{n=0}^{\infty} \frac{u_n(s)}{n!} x^n$

from the recursion of the $u_n(s)$ obtain the equation

$$\frac{\partial}{\partial s} F(x,s) = \sum_{n=0}^{\infty} \frac{4u_{n+1}(s)}{n!} x^n = 4 \sum_{n=1}^{\infty} \frac{u_n(s)}{(n-1)!} x^{n-1} = 4 \frac{\partial}{\partial x} F(x,s)$$

with the general solution $F(x,s) = f(x+4s) = F(x+4s,0)$. Re-expand :

$$C_n(t) = \sum_{m=0}^{\infty} \frac{2^m}{m!} C_{m+n}(0) \left(e^{-2t} - 1\right)^m \; e^{-2(n-1)t}$$

for **arbitrary** initial values $C_n(0) = u_n(0)$

N.B. no dependence of physical quantities on the auxiliary initial value $C_0(0)$
if initially uncorrelated $C_n(0) = \rho^n$: reproduces known classical result

Kenkre & van Horn 81, Evans 84, Oliveira & Tomé 92, Prados & Brey 01, de Smedt *et al.* 02, ...

Calculation of **correlators** of n-strings : observables with **hole** of r sites

$$C^{r}_{n,m}(t) := \langle \eta_1(t)\ldots\eta_n(t)\eta_{n+r+1}(t)\ldots\eta_{n+m+r}(t)\rangle = \mathbf{P}\left(\underbrace{\bullet\bullet\ldots\bullet}_{n}\boxed{r}\underbrace{\bullet\bullet\ldots\bullet}_{m}\right)$$

Spatially translation-invariant initial conditions, equation of motion $r \geq 2$, $n, m \geq 1$

$$\partial_t C^{r}_{n,m}(t) = -2\big[C^{r}_{n+1,m}(t) + C^{r}_{n,m+1}(t) + (n+m-2)C^{r}_{n,m}(t) + C^{r-1}_{n+1,m}(t) + C^{r-1}_{n,m+1}(t)$$

$$\partial_t C^{1}_{n,m}(t) = -2\big[C^{1}_{n+1,m}(t) + C^{1}_{n,m+1}(t) + (n+m-2)C^{1}_{n,m}(t) + 2C_{n+m+1}(t)\big]$$

Change of variables : $C_n(t) = u_n(s)e^{-2(n-1)t}$, $C^{r}_{n,m}(t) = u^{r}_{n,m}(s)e^{-2(n+m-2)t}$

Extend to $n, m \geq 0$. Solve recursion for generating function, for $r \geq 1$

$$\begin{aligned} C^{r}_{n,m}(t) \;=\; & e^{-2(n+m-2)t}\sum_{k,l=0}^{\infty}\sum_{q=0}^{r-1}\sum_{q'=0}^{q}\binom{q}{q'} \\ & \times C^{r-q}_{n+k+q-q',m+l+q'}(0)\,\frac{(e^{-2t}-1)^{k+l+q}}{k!\;l!\;q!} \\ & + 2^{r}\left(\frac{(e^{-2t}-1)^{r}}{r!} + \frac{(e^{-2t}-1)^{r+1}}{(r+1)!}\right)e^{2(r+1)t}C_{n+m+r}(t) \end{aligned}$$

; for **arbitrary** initial conditions

Illustration 1 :

$A + A \to \emptyset + \emptyset$

initially uncorrelated particles, mean density ρ : $C_{n,m}(0) = \rho^{n+m}$

$$C^r_{n,m}(t) - C_n(t)C_m(t) = \frac{\rho^{n+m}}{r!} e^{-2(n+m-2)t} \left(2\rho\left(e^{-2t}-1\right)\right)^r$$
$$\times \left[\frac{r+e^{-2t}}{r+1} \exp\left(2\rho\left(e^{-2t}-1\right)\right) - {}_1F_1\left(r, r+1; 2\rho\left(1-e^{-2t}\right)\right)\right]$$

* double exponential relaxation, typical for $1D$ systems — DE SMEDT *et al.* 02

* factorial spatial decay, inconsistent with Edwards' *a priori* ensemble

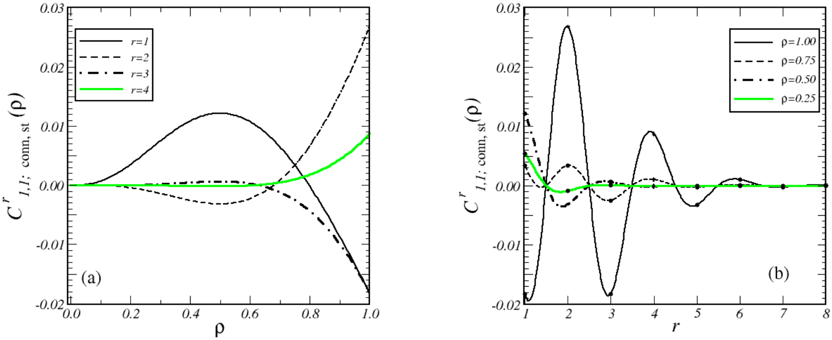


Illustration 2 : Numerical test

$A + A \rightarrow \emptyset + \emptyset$

three initial conditions : (b and c correlated)

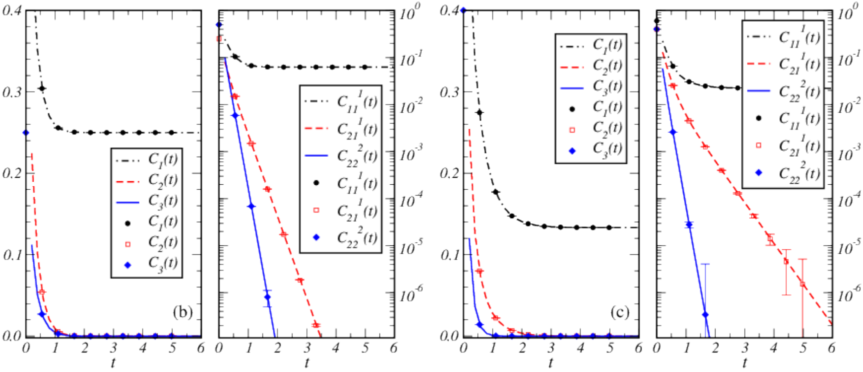
a) $\ldots AAAAAAAAAAA \ldots$

b) $\ldots AAA\emptyset AAA\emptyset AAA\emptyset AAA\emptyset \ldots$

c) $\ldots AAAA\emptyset AAAA\emptyset AAAA\emptyset AAAA\emptyset \ldots$

find : (i) n-string density $C_n(t)$, (ii) (n, m)-correlator $C^r_{n,m}(t)$

compare with Monte Carlo simulations $L = 65536$ sites, $2 \cdot 10^5$ histories



3. Single-species model : the semi-infinite lattice

Define ***n*-strings** of n **consecutive** particles $\underbrace{\bullet\bullet\ldots\bullet}_{n \text{ particles}}$ $\quad A + A \to \emptyset + \emptyset$

do **not** assume spatial translation-invariance

$$C_{a;n}(t) := \langle \eta_a(t)\eta_{a+1}(t)\ldots\eta_{a+n-1}(t)\rangle$$

From the master equation, derive eqs. of motion,
for all $n \geq 1$ and all **hole positions** $a \in \mathbb{Z}$

$$\frac{\mathrm{d}}{\mathrm{d}t} C_{a;n}(t) = -2(n-1)C_{a;n}(t) - 2C_{a-1;n+1}(t) - 2C_{a;n+1}(t)$$

later : restrict to halfspace $a \geq 0$

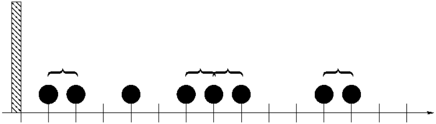


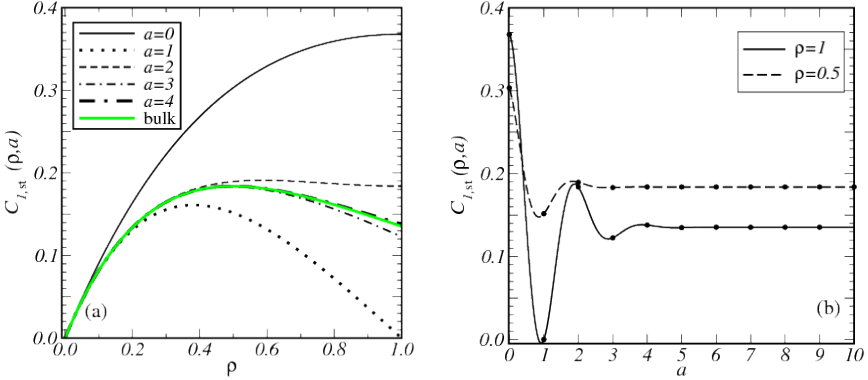
Illustration :

initially uncorrelated particles, in **right half-space** : $C_{a;n}(0) = \rho^n \Theta(a)$

$$C_{1,\mathrm{st}}(\rho; a) \;:=\; \lim_{t\to\infty} C_{a;1}(t) = \rho e^{-\rho} \sum_{k=0}^{a} \frac{(-\rho)^k}{k!}$$

$$= \rho e^{-2\rho} \left[1 + (-1)^a \rho^{1+a} \,{}_1F_1\left(a+1, a+2; \rho\right) / \Gamma(a+2)\right]$$

* double exponential relaxation, typical for $1D$ systems
* surface $C_{0;1\mathrm{st}} = \rho e^{-\rho}$ different from bulk $C_{\infty;1,\mathrm{st}} = C_1(\infty) = \rho e^{-2\rho}$



Calculation of **correlators** of n-strings :

observables $\underbrace{\bullet\bullet\ldots\bullet}_{n}\boxed{\text{r}}\underbrace{\bullet\bullet\ldots\bullet}_{m}$ with a **hole** of r sites

$$C^{r}_{a;n,m}(t) := \langle \eta_a(t)\ldots\eta_{a+n}(t)\eta_{a+n+r+1}(t)\ldots\eta_{a+n+m+r+1}(t)\rangle$$

and do **not** assume spatial translation-invariance

Needed : reductions to n-string for $r=1$ and to smaller holes for $r \geq 2$

An analogous computation finally gives

$$C^{r}_{a;n,m}(t) = 2^r \left(\frac{\left(e^{-2t}-1\right)^r}{r!} + \frac{\left(e^{-2t}-1\right)^{r+1}}{(r+1)!} \right) e^{2(r+1)t} C_{a;n+m+r}(t)$$
$$+e^{-2(n+m-2)t} \sum_{\ell,k=0}^{\infty} \sum_{q=0}^{r-1} \sum_{q'=0}^{q} C^{r-q}_{a-\ell;n+\ell+q-q',m+k+q'}(0) \begin{pmatrix} q \\ q' \end{pmatrix} \frac{\left(e^{-2t}-1\right)^{k+\ell+q}}{k!\ \ell!\ q!}$$

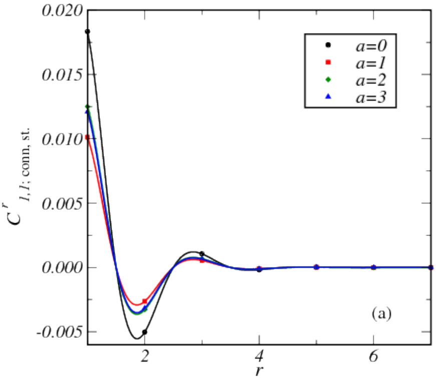
Illustration :

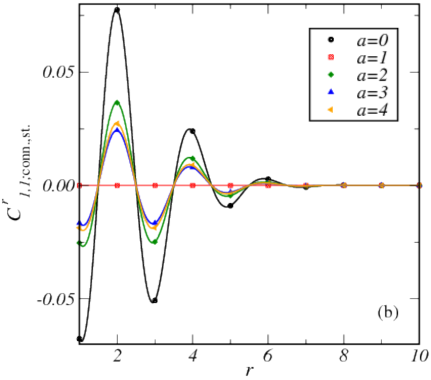
$|A + A \to \emptyset + \emptyset$

initially uncorrelated particles, in **right half-space** : $C_{a;n,m}(0) = \rho^{n+m}\Theta(a)$

$$C^r_{a;1,1} - C_{a;1}(\infty)C_{a+r+1;1}(\infty) = \rho^2 e^{-2\rho}\frac{\Gamma(1+a,-\rho)}{\Gamma(1+a)}\left[\frac{e^{-\rho}\Gamma(1+r,-2\rho)}{\Gamma(1+r)} - \frac{e^{-2\rho}\Gamma(1+r+a,-\rho)}{\Gamma(1+r+a)} - \frac{2^r(-\rho)^r}{\Gamma(r+2)}\right]$$

$\rho = 0.5$ $\rho = 1$





4. Two-species model

there are $\mathbf{N}_{\mathrm{st}} \sim (\sqrt{2}+1)^L$ stationary states on a chain with L sites

Define 2 **alternating n-strings** of n **consecutive** particles $\qquad A + B \to \emptyset + \emptyset$

$$A_n := \mathbf{P}\big(\underbrace{ABABAB\ldots}_{n\ \text{sites}}\big) = \langle \delta_{\eta_1,A}\delta_{\eta_2,B}\delta_{\eta_3,A}\delta_{\eta_4,B}\ldots\rangle$$

$$B_n := \mathbf{P}\big(\underbrace{BABABA\ldots}_{n\ \text{sites}}\big) = \langle \delta_{\eta_1,B}\delta_{\eta_2,A}\delta_{\eta_3,B}\delta_{\eta_4,A}\ldots\rangle$$

$$\frac{\mathrm{d}}{\mathrm{d}t}A_n = -B_{n+1} - (n-1)A_n - A_{n+1}\ , \ \frac{\mathrm{d}}{\mathrm{d}t}B_n = -A_{n+1} - (n-1)B_n - B_{n+1}$$

new variables $A_n(t) = u_n(s)e^{-(n-1)t}$, $B_n(t) = v_n(s)e^{-(n-1)t}$, $s := e^{-t} - 1$

decouples : let $\boxed{X_n(s) := u_n(s) - v_n(s),\ Y_n(s) := u_n(s) + v_n(s)}$:

$\frac{\mathrm{d}}{\mathrm{d}s}X_n(s) = 0$, $\frac{\mathrm{d}}{\mathrm{d}s}Y_n(s) = 2Y_{n+1}(s)$ $\to$reduces to single-species model !

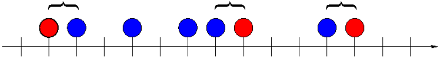


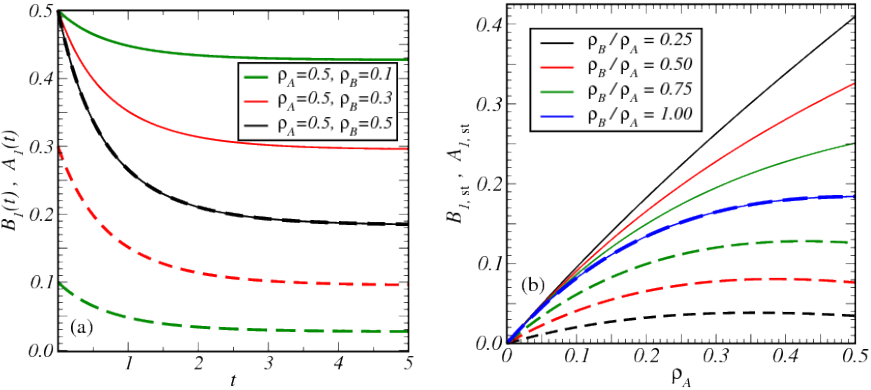
Illustration : initially uncorrelated particles, densites ρ_A, ρ_B

$A + B \to \emptyset + \emptyset$

MAJUMDAR & PRIVMAN 93

$$A_n(0) = \rho_A^{[(n+1)/2]}\rho_B^{[n/2]} = (\rho_A\rho_B)^{n/2}\left[\frac{1+(-1)^n}{2} + \frac{1-(-1)^n}{2}\sqrt{\frac{\rho_A}{\rho_B}}\right]$$

$$\begin{aligned} A_n(t) = &\frac{1}{2}(\rho_A\rho_B)^{n/2}e^{-(n-1)t}\left\{\left[\left(1+\frac{1}{2}\frac{\rho_A+\rho_B}{\sqrt{\rho_A\rho_B}}\right)e^{2\sqrt{\rho_A\rho_B}\,(e^{-t}-1)} + \frac{1}{2}\frac{\rho_A-\rho_B}{\sqrt{\rho_A\rho_B}}\right]\right. \\ &\left. +(-1)^n\left[\left(1-\frac{1}{2}\frac{\rho_A+\rho_B}{\sqrt{\rho_A\rho_B}}\right)e^{-2\sqrt{\rho_A\rho_B}\,(e^{-t}-1)} - \frac{1}{2}\frac{\rho_A-\rho_B}{\sqrt{\rho_A\rho_B}}\right]\right\} \end{aligned}$$



5. Conclusions

AB-**correlators :** consider two alternating strings at a distance r leads to closed pairs of closed systems $\Rightarrow$ explicit solution known

- simple models of descent dynamics (diffusionless particles)
- exact solution in $1D$ permits study of non-mean-field properties
- identify n-strings (alternating n-strings for two-species model) as main observable
- exact densities and correlators for arbitrary initial conditions via generating functions
- earlier results on initially uncorrelated particles included as special cases