Formal perturbation analysis of a non equilibrium stationary state

by A.Iacobucci, S.Olla, G.G.

Non-equilibrium: statistics is often shown to exist.

(By) “compactness methods”: very unsatisfactory.

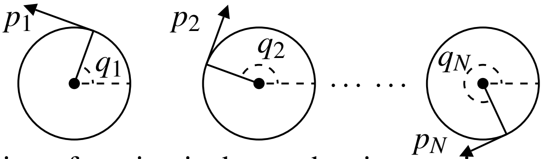
Dissatisfaction: when physical quantities are needed “no answers”.

E.g. for hard spheres systems continuity of correlation of a stationary nonequilibrium distibution is not known $\Rightarrow$ no answer to simple questions like $\langle \partial_q \rho(q-q') \rangle$.

Particularly valuable are therefore exactly soluble models.

Unfortunately they are very few , most involve stochastic forces.

Even so the study is very difficult. Here the question of "computing" correlations for a "trivial" system. The $N=1$ **case**



The equation of motion is the stochastic equation

$$\dot{q} = \frac{p}{J} \qquad \dot{p} = -\partial U - \tau - \frac{\xi}{J} p + \sqrt{\frac{2\xi}{J}}\,\dot{\mathbf{w}}$$

$\dot{\mathbf{w}}$ w.n. of width $(\frac{J}{\beta_0\, dt})^{\frac{1}{2}}$,
$U = -gV\cos(q)$ conservative force, τ torque, ξ friction, J inertia

β_0 inverse temperature

Problem: find the stationary state distribution

It is hard to believe that this in not known **???**.

The limit case with $\xi \to \lambda\xi$, $t \to \lambda t$, $\lambda \to \infty$ overdamped is exactly soluble: generator is

$$\mathscr{L}^*_{od} F = \xi^{-1}\big(\partial_q \Big((\tau + \partial_q U)F\Big) + \partial_q^2 F\big)$$

and the stationary state is

$$F_{od}(q) = e^{-\beta U(q)} \int_0^{2\pi} e^{\beta(\tau y + U(q+y))} dy/Z$$

In the non overdamped case the generator for the evolution of density $F(p,q)dpdq$ yields the PDE $\mathscr{L}^* F = 0$

$$\mathscr{L}^* F = -\Big\{\Big(\frac{p}{J}\partial_q F(q,p) - (\partial_q U(q) + \tau)\partial_p F(q,p)\Big) - \xi\,\Big(\beta_0^{-1}\partial_p^2 F(q,p) + \frac{1}{J}\partial_p(p\,F(q,p))\Big)\Big\}$$

It is hard to believe that this in not known **???**.

General results: **most interesting: simulations, ILOS1: [1]**

(1) There exists a smooth solution (Hormander)

(2) is exponentially approached by initial δ (Mattingly-Stuart)

(3) it is positive $F(q,p) = \frac{e^{-\frac{\beta}{2J}p^2}\rho(p,q)}{\sqrt{2J\beta^{-1}}} = G(p)\rho(p,q)$ (MS)

(4) $\int G(p)\rho(p,q)^2 < \infty$, (Olla)

(5) $\int G(p)\partial\rho(p,q)^2 < \infty$, (Olla)

(6) $\Rightarrow$ if $:p^n: := \left(\frac{J\beta^{-1}}{2}\right)^{\frac{n}{2}} H_n(\frac{p}{\sqrt{2J\beta^{-1}}})$ (Wick,Hermite poly.)

$\rho(p,q) = G(p)(\rho_0(q) + \rho_1(q)p + \rho_2(q) :p^2: + \rho_3(q) :p^3: + \dots)$

Problem: Find the expansion in g of $\rho_n(q)$ (why care?)

By algebra $\mathscr{L}^* F = 0$ becomes: $n \geq 0$ ($\rho_{<0} \equiv 0$)

$$n\beta^{-1}\partial\rho_n(q) + \Big[\frac{1}{J}\partial\rho_{n-2}(q) + \frac{\beta}{J}(\partial U(q) + \tau)\rho_{n-2}(q)$$
$$+ (n-1)\frac{\xi}{J}\rho_{n-1}(q)\Big] = 0$$

Messy! compute the $\rho_n^{[r]}(q)$ and go dimensionless with

$$\sigma_n(q) \stackrel{def}{=} \rho_n(q)\xi^n n!, \quad \eta \stackrel{def}{=} \beta\xi^2/J, \beta\tau, \quad \beta V$$

(1) Recursion is linear: take the F.T. $\sigma_{n,k}$

(2) Recursion is second degree: hence take $\mathbf{S}_{n,k} \stackrel{def}{=} \binom{\sigma_{n,k}}{\sigma_{n-1,k}}$
for $k \neq 0$: *i.e.* Fourier modes of the $\sigma' s$

(3) u_n = average of σ_n; then $(r = 1)$

$$\mathbf{S}^{[r]}_{n,k} = M_{n,k}\mathbf{S}^{[r]}_{n-1,k} + \mathbf{X}^{[r]}_{n,k}, \qquad \mathbf{S}^{[r]}_{2,k} = \mathbf{Y}^{[r]}_k$$
$$u^{[r]}_n = -\beta\tau u^{[r]}_{n-1} + v^{[r]}_n, \qquad u^{[r]}_2 = u^{[r]}$$

Explicitly $r = 1$ (to start) for $n > 2$ with data at $n = 2$

$$v_n^{[1]} = 0 \;\Rightarrow\; u_n^{[1]} = (-\beta\tau)^n$$

Let $m \equiv n - 1$:

$$a_k \stackrel{def}{=} (1 - i\frac{\beta\tau}{k})i, \quad |1\rangle \stackrel{def}{=} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle \stackrel{def}{=} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$M_{n,k} \stackrel{def}{=} \begin{pmatrix} \frac{m}{k} i\eta & ima_k\eta \\ 1 & 0 \end{pmatrix}, \; M_{n,k}^{-1} \stackrel{def}{=} \begin{pmatrix} 0 & 1 \\ \frac{1}{ima_k\eta} & -\frac{1}{k\,a_k} \end{pmatrix},$$

$$\mathbf{Y}_1 \stackrel{def}{=} \Big(-\eta a_k \sigma_{0,1}^{[1]} - \eta\beta V\Big)|1\rangle$$

$$\mathbf{X}_{n,k} \stackrel{def}{=} -\frac{\beta V}{ia_k} + (-\beta\tau)^n$$

Conclusion: $\sigma_{0,1}^{[1]}$ determines everything at order 1

at order r it must be $|k| \le r$ and again $\sigma_{0,k}^{[r]}$.

So infinitely many solutions! however $\rho(q,p)$ must be L_2:

Required: $|\sigma_n(q)| \le \frac{\varepsilon^n}{\sqrt{n!}}$. **Formally**

$$\mathbf{S}_n = \lambda M_{n+1}^{-1} \ldots M_N^{-1} \ldots . + \sum_{h=n+1}^{\infty} M_{n+1}^{-1} \ldots M_h^{-1} \mathbf{X}_h$$

A cut-off version is

$$\mathbf{S}_n(N) = \lambda_N M_{n+1}^{-1} \ldots M_N^{-1} |2\rangle + \sum_{h=n+1}^{N-n} M_{n+1}^{-1} \ldots M_h^{-1} \mathbf{X}_h$$

Need a theorem: for $|\beta\tau|, \eta^{-1}$ small enough

Theorem 1: *Given k, if η is large enough there is a sequence $\Lambda_k(n_1,N)$ such that for all $n_1 \ge 2$ and all $k \ne 0$ the*

$$\zeta_k(n_1,N) \stackrel{def}{=} \begin{pmatrix} \zeta_k(n_1,N)_1 \\ 1 \end{pmatrix} = \Lambda_k(n_1,N) M_{n_1+1}^{-1} \ldots M_N^{-1} |2\rangle$$

is s.t. $|\zeta_k(n_1,N)_1| \le 1$ and $\zeta_k(n_1) \stackrel{def}{=} \lim_{N\to\infty} \zeta_k(n_1,N)$ exists.

Corollary: *A solution, unique exponentially, is*

$$\mathbf{S}^{[1]}_{n,k} = \lambda\,\zeta_{n,k} + \xi_{n,k}, \qquad n \ge 2, \qquad \text{where}$$

$$\zeta_{n,k} = M_n \cdots M_3\,\zeta_k(2), \qquad \xi_{n,k} = \sum_{h=n+1}^{\infty} -\beta V \eta M^{-1}_{n+1} \dots M^{-1}_h \mathbf{X}^{[1]}_h$$

$$|\zeta_{n,k}| \le B\,|1 - \frac{i\beta\tau}{k}|^n, \qquad |\mathbf{S}_n| \le B\beta V|1 - i\beta\tau|^n$$

Once $\zeta(2) = \lim_{N\to\infty} \Lambda_k(2,N)^{-1} M_3^{-1} \cdots M_N^{-1} |2\rangle$ get initial data

$$\mathbf{S}^{[1]}_{2,1} \equiv (\sigma^{[1]}_{0,1}\overline{y}^{[1]}_1 - \eta\beta V)\,|1\rangle = \lambda\,\zeta_{2,1} + \xi_{2,1}$$

(recall $\overline{y}^{[1]} = -\eta(1 + \frac{\beta\tau}{i})$) determines the only unknown $\sigma^{[1]}_{0,1}$ by

$$\sigma^{[1]}_{0,1}\overline{y}^{[1]}_1 - \lambda\,\zeta(2)_1 = (\xi(2)_1 + \eta\beta V) - \lambda = \xi(2)_2$$

Hence the key is the theorem

Once more this is a problem on a Ising system controlled by γ

$$\gamma = -\frac{4ia_k k^2}{m\eta}, \qquad \lambda_{n,k,\pm} \stackrel{def}{=} -\frac{1 \pm \sqrt{1+\gamma}}{2\,k\,a_k}, \qquad m = n-1$$

and spectral decomposition of M_n^{-1}:

$$M_{n,k}^{-1} = \sum_{\sigma=\pm 1} \lambda_{n,k,\sigma} \frac{|v_{n,\sigma}\rangle\langle w_{n,\sigma}|}{\langle w_{n,\sigma}|v_{n,\sigma}\rangle},$$

$$|v_{n,\sigma}\rangle = \lambda_{n,\sigma}^{-1} \begin{pmatrix} 1 \\ \lambda_{n,\sigma} \end{pmatrix},$$

$$\langle w_{n,\sigma}| = \Big(\varepsilon_n, \lambda_{n,\sigma}\Big), \qquad \varepsilon_n = \frac{\gamma}{4k^2 a_k^2}$$

The Ising model arises because $M_n^{-1} \cdots M_N^{-1} |2\rangle$ is writing explicitly the matrix product $M_n^{-1}\cdots M_N^{-1}|2\rangle$ as

$$\sum_{\sigma_3,\ldots,\sigma_N} |v_{3,\sigma_3}\rangle \cdot \Big(\prod_{j=3}^{N} \lambda_{j,\sigma_j}\Big) \prod_{j=3}^{N} \frac{\langle w_{j,\sigma_j}|v_{j+1,\sigma_{j+1}}\rangle}{\langle w_{j,\sigma_j}|v_{j,\sigma_j}\rangle}$$

"expectation" of $|v_{3,\sigma_3}\rangle$ in a Gibbs state. Gibbs factor?

Spin configuration = intervals of $-$ separated $+$, then

$$\overline{\Lambda}_N \prod_{i=1}^{p} I_J \qquad \text{is the Gibbs weight}$$

$$\rho(J) \stackrel{def}{=} \frac{\sum_{p\ge1} \sum^{*}_{J_1<\ldots<J_p} \Big(\prod_{s=1}^{p} I_{J_s}\Big)}{\Omega_2(N)}$$

$$P_- \stackrel{def}{=} \sum_{\{3\}\in J} \rho(J),\ \zeta(2) = |v_{3,-}\rangle P_- + |v_{3,+}\rangle P_+$$

$$\overline{\Lambda}_N^{[2]} \stackrel{def}{=} \Big(\prod_{j=3}^{N} \lambda_{j,+}\Big)\Big(\prod_{j=3}^{N} \frac{\langle w_{j,+}|v_{j+1,+}\rangle}{\langle w_{j,+}|v_{j,+}\rangle}\Big)$$

$$I_J \stackrel{def}{=} \Big(\prod_{j=k}^{k'} \frac{\lambda_{j,-}}{\lambda_{j,+}}\Big)\Big(\prod_{j=k}^{k'} \frac{\langle w_{j,-}|v_{j+1,-}\rangle}{\langle w_{j,-}|v_{j,-}\rangle}\,\frac{\langle w_{j,+}|v_{j,+}\rangle}{\langle w_{j,+}|v_{j+1,+}\rangle}\Big)$$
$$\cdot\,\frac{\langle w_{k-1,+}|v_{k,-}\rangle}{\langle w_{k-1,+}|v_{k,+}\rangle}\,\frac{\langle w_{k',-}|v_{k'+1,+}\rangle}{\langle w_{k',+}|v_{k'+1,+}\rangle}\,\frac{\langle w_{k',+}|v_{k',+}\rangle}{\langle w_{k',-}|v_{k',-}\rangle}$$

$$|I_J| \le W_J \stackrel{def}{=} \Big(\frac{\sqrt{2}k^2}{\eta}\Big)^{|J|}\Big(\prod_{j\in J}\frac{1}{j-1}\Big)\frac{2k^4}{\eta^2(k'-1)^3}$$

Non transl. inv. but very small already for J close to the origin.

Hence the $P_\pm$ can be computed as convergent series in I_J's as well as the partition function $exp(\Omega_N)$ which amits a limit as $N \to \infty$ (no logarithm necessary).

Theorem: **Fixed $r > 0$ the equation $\mathscr{L}^* F(p,q) = 0$, for τ, g, ξ^{-1} small,**

(1) admits a formal C^r (in g,p,q) solution in $L_1(dpdq)$

(2) The coefficients $F^{[r]}(p,q)$ of its Taylor expansion at $g = 0$ can be determined, analytic in q,p, requiring decay as $n!^{-\frac{1}{2}}$ of the Hermite expansion of F

(3) are explicitly computable.

Question: $r = \infty$ and F analytic in g.

Non believers in CE: the CE can be avoided by making use of the theory of continued fractions because

$$\zeta_k(h,s) \stackrel{def}{=} \langle 1|M_{h+1}^{-1}\ldots M_s^{-1}|2\rangle$$

Theorem:

If $\quad \gamma \stackrel{def}{=} -\frac{ia_k k^2}{\eta}, \quad \zeta_k(h,s) = \binom{(-ka_k)\varphi_k(h,s)_1}{1}$: then

$$\varphi_k(h,s)_1 = \cfrac{1}{1+\frac{\gamma}{h}\cfrac{1}{1+\frac{\gamma}{h+1}\cfrac{1}{1+\frac{\gamma}{h+2}\cdots\cfrac{1}{1+\frac{\gamma}{s-1}}}}}$$

$$
\begin{aligned}
(\widetilde{\sigma}^{[r]}_{n,k})_1 = & \sum_{h=2}^{n} x^{[r]}_{h+1,k} \Big(\prod_{j=3}^{h-1} \zeta(j,h)_1^{-1}\Big)\Big(\prod_{j=2}^{n}\zeta(j,\infty)_1\Big) \\
& - \sum_{h=n+1}^{\infty} x^{[r]}_{h+1,k}\Big(\prod_{j=n+2}^{h-1}\frac{1}{\zeta(j,h)_1}\Big)\Big(1-\prod_{j=2}^{n}\frac{\zeta(j,\infty)_1}{\zeta(j,h)_1}\Big)
\end{aligned}
$$

and component 2 is with n replaced by $n-1$. The initial data

$$
\begin{aligned}
\widetilde{\sigma}^{[r]}_{2,k} = & -\sum_{h=3}^{\infty} x^{[r]}_{h+1}\Lambda(3,h)\Big(1-\frac{\Lambda(2,h)\Lambda(3,\infty)}{\Lambda(2,\infty)\Lambda(3,h)}\Big) \\
\widetilde{\sigma}^{[r]}_{0,k} = & \frac{1}{i\eta a_k}\Big(\widetilde{\sigma}^{[r]}_{2,k} + \eta\beta V\Big(\delta_{|k|=1}\delta_{r=1} + \sum_{|k-k'|=1}\frac{k'}{k}\widetilde{\sigma}^{[r-1]}_{0,k-k'}\Big)\Big)
\end{aligned}
$$

At order $r=0$: $\widetilde{\sigma}^{[0]}_{n,k}=0, u^{[0]}_n=(-\beta\tau)^n$ hence $x^{[0]}_{n,k}\equiv 0$.

Assuming that $x^{[r']}_{n,k}, u^{[r']}_n$ *are known for* $r'<r$ it is:

Assuming that $x_{n,k}^{[r']}, u_n^{[r']}$ are known for $r' < r$

$$u_0^{[r]} = 0, \quad u_1^{[r]} = -\beta V \sum_{k'} ik' \widetilde{\sigma}_{0,-k'}^{r-1}, \quad u_2^{[r]} = -\beta\tau u_1^{[r]},$$

$$u_n^{[r]} = -\beta V \sum_{k'=\pm 1} ik' \Big(\sum_{h=0}^{n-3} (-\beta\tau)^h \widetilde{\sigma}_{n-1-h,-k'}^{[r-1]} + (-\beta\tau)^{n-1} \widetilde{\sigma}_{0,-k'}^{[r-1]} \Big)$$

$$x_{n,k}^{[r]} = -\frac{\beta V}{ia_k} \Big(u_{n-2}^{[r-1]} \delta_{|k|=1} + \sum_{|k-k'|=1} \frac{k'}{k} \widetilde{\sigma}_{n-2,k-k'}^{[r-1]} \Big)$$

Need convergence: mainly need exponential bounds on the coefficients of $\widetilde{\sigma}_{n,k}^{[r]}$: *i.e.* on:

$$\Big| \Big(1 - \frac{\Lambda(2,h)\Lambda(3,\infty)}{\Lambda(2,\infty)\Lambda(3,h)} \Big) \Big| < \varepsilon^{h-n}, \qquad h \geq n$$

which are an easy consequence of the CE or of the continued fractions if $\gamma \stackrel{def}{=} -\frac{ia_k k^2}{\eta} << 1$ however at order r it is $|k| \leq r$ hence doubts on analyticity

A. Iacobucci, F. Legoll, S. Olla, and G. Stoltz.
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