Nonequilibrium stationary state for a damped rotator

G.Gallavotti, A.Iacobucci, S.Olla
INFN-Roma1 and Rutgers University
CEREMADE, Université Dauphine, Paris

Abstract: *Perturbative construction of the nonequilibrium steady state of a rotator under a stochastic forcing while subject to torque and friction*

20 Oct 2013 - arXiv: 1310.5379

1 Introduction and models

Nonequilibrium stationary states can be constructed in numerical simulations and, even for simple systems, show interesting nontrivial properties (see for instance [1]). There are very few examples, [2],[3], of systems that can be completely studied theoretically. Even apparently very simple systems can be quite difficult to analyze, if the aim is to describe in detail their stationary states properties.

Here we study the stationary state of a particle, "*rotator*", bound on a circle, in contact with a Langevin stochastic thermostat at temperature β^{-1} while subject to a constant torque of strenght τ.

The equation of motion is the stochastic equation on $T^1 \times R$

$$\dot q = \frac{p}{J}, \qquad \dot p = -\partial U - \tau - \frac{\xi}{J} p + \sqrt{\frac{2\xi}{\beta}}\,\dot w\,, \qquad U(q) \stackrel{def}{=} 2\,g\,V\cos q\,, \tag{1.1}$$

where J is the inertia moment of the rotator, ξ is the friction $\dot w$ is a standard white noise with increments $dw = w(t+dt) - w(t)$ of variance dt so that $\sqrt{\frac{2\xi}{\beta}}\dot w$ is a Langevin random force at inverse temperature β.

The potential U, Eq.(1.1), is a smooth function on the circle T^1, with $V > 0$ an energy parameter and g a dimensionless parameter measuring the strength of the conservative force. We chose the simplest possible function because the problem seems difficult even in such a case, The parameters β, J, V will be kept constant, hence the model is simply a pendulum subject to constant torque τ, friction ξ and white noise $\sqrt{\frac{2\xi}{\beta}}\dot w$.

When the torque $\tau = 0$, the stationary probability is simply given by the equilibrium Gibbs state proportional to $e^{-\beta H(p,q)} dp dq$, where $H(p,q) =$

$\frac{1}{2J}p^2 + U(q)$ is the Hamiltonian of the system. The torque τ is a non-conservative (or non-gradient) force and drives the system out of *equilibrium*. The thermostatting action of the noise acting on the rotator is essential, as it may take energy out, allowing reaching a steady state.

The *overdamped case* corresponds to the limit equation obtained rescaling time $t' = \lambda t$ and $\xi' = \lambda\xi$ and taking the limit $\lambda \to +\infty$: $q'_\xi(t')$ converges in law to the solution $\bar q(t)$ of the stochastic differential equation on T^1

$$\dot{\bar q} = -\frac{1}{\xi}(\partial U + \tau) + \sqrt{\frac{2}{\beta\xi}}\,\dot{\bar w}\,. \tag{1.2}$$

The generator for a distribution $F(q)\frac{dq}{2\pi}$ of such evolution is $\mathcal{L}^*_{od}F$ defined by $\mathcal{L}^*_{od}F = \xi^{-1}(\partial_q\Big((\tau + \partial_q U)F\Big) + \partial_q^2 F)$. The process therefore has an explicit stationary state given by

$$F_{od}(q) = e^{-\beta U(q)}\int_0^{2\pi} e^{\beta(\tau y + U(q+y))}dy/Z\,, \tag{1.3}$$

where Z is the normalization (to 1), [4]. In fact defining $B(y) = \tau y + U(y)$, it is $F_{od}(q) = Z^{-1}\int_q^{q+2\pi} e^{\beta(B(y)-B(q))}\,dy$ and $\partial F_{od}(q) = -\beta(\tau + \partial U(q))F_{od}(q)$, so that $\mathcal{L}^*_{od}F_{od} = 0$.

The study of the overdamped Langevin equation on the circle T^1 is surprisingly involved, [4]. There is indeed a remarkable lack of smoothness of some properties (large deviation functions) of the above stationary distribution in some region of the model parameters.

Going beyond the overdamped motion assumption is the aim of the present work: hence the particle state will be described by a pair of coordinates $(q,p) \in T^1 \times R$.

The physical dimensions are $[J] = [time \times action]$, $[p] = [action]$, $q = [angle]$, $[V] = [U] = [\tau] = [energy] = [action/time]$, $[\xi] = [action]$, $[\beta] = [energy^{-1}]$ and $\dot w$ has dimension $[\dot w] = [action/\sqrt{time}]$: the "unusual" dimensions arise because q is dimensionless (an angle) rather than with dimension of a length.

The generator for the evolution of a distribution $F(q,p)\frac{dq\,dp}{2\pi}$ is

$$\begin{aligned}\mathcal{L}^*F = &-\Big\{\Big(\frac{p}{J}\partial_q F(q,p) - (\partial_q U(q) + \tau)\partial_p F(q,p)\Big)\\ &- \xi\,\Big(\beta^{-1}\partial_p^2 F(q,p) + \frac{1}{J}\partial_p(p\,F(q,p))\Big)\Big\}\,.\end{aligned} \tag{1.4}$$

The solution of $\mathcal{L}^*F = 0$ will be searched within the class of probability distributions satisfying the following hypotheses:

(H1) The function $F(p,q)$ is smooth and admits an expansion in Hermite polynomials (or "Wick monomials") H_n of the form

$$\begin{aligned} F(q,p) =&G_\beta(p)\sum_a \rho_a(q)\ :p^a:, \qquad G_\beta(p)=\frac{e^{-\frac{\beta}{2}p^2}}{\sqrt{2\pi\beta^{-1}}}\,,\\ :p^n:&\stackrel{def}{=}\Big(\frac{J\beta^{-1}}{2}\Big)^{\frac{n}{2}}H_n(\frac{p}{\sqrt{2J\beta^{-1}}}) \end{aligned}\,, \tag{1.5}$$

where $a\ge 0$ are integers; so that $\int :p^n::p^m:\,G_\beta(p)\,dp=\delta_{nm}n!\,(J\beta^{-1})^n$.
(H2) The coefficients $\rho_n(q)$ are C^∞-differentiable in q,g and the p,q,g-derivatives of F can be computed by term by term differentiation, obtaining convergent series.

It is known, [5], that the equation $\mathcal{L}^*F(p,q)=0$ admits a unique smooth and positive solution in $L_2(G_\beta(dp)dq)$, hence in $L_1(dpdp)\cap L_2(dpdq)$, with $\int F dpdq=1$.

In this paper we show that

Theorem: *There is a formal power series expansion in g for a solution of the equation $\mathcal{L}^*F=0$ with coefficients $\rho^{[r]}_n(q)$; their Fourier's transforms $\rho^{[r]}_{n,k}$ can be determined by a constructive algorithm, vanish for $|k|>r$ and satisfy the bounds*

$$\xi^n|\rho^{[r]}_{n,k}|\le A_r\frac{(B_r)^n}{n!}\delta_{|k|\le r},\qquad \forall r,k\,, \tag{1.6}$$

for A_r,B_r suitably chosen, depending also on the dimensionless parameters of the problem $\beta V,\beta\tau,\eta=\frac{\beta\xi^2}{2J}>0$.

The properties (H1),(H2) allow us to perform the algebra needed to turn the stationarity condition $\mathcal{L}^*F=0$ into a hierarchy of equations for the coefficients $\rho_n(q)$, $\forall n\ge 0$

$$\begin{aligned} n\beta^{-1}\partial\rho_n(q)+\Big[\frac{1}{J}\partial\rho_{n-2}(q)+\frac{\beta}{J}(\partial U(q)+\tau)\rho_{n-2}(q)\\ +(n-1)\frac{\xi}{J}\rho_{n-1}(q)\Big]=0\,, \end{aligned} \tag{1.7}$$

where ρ_{-1},ρ_{-2} are to be set equal to zero.

Remarks: (1) Adapting [5], it can be seen that $\mathcal{L}^*F(p,q)=0$ admits a unique solution smooth in p,q. However its analyticity in g and the properties of its representation in the form in Eq.(1.5), are not proven by the above Theorem,

as it only deals with the Taylor coefficients of a formal expansion in powers of g.
(2) Identities follow immediately by normalization or by integration. Let $\overline{\rho}_n \stackrel{def}{=} \int \rho_n(q)\frac{dq}{2\pi}$ and $\widetilde{\rho}_n(q) \stackrel{def}{=} \rho_n(q) - \overline{\rho}_n$; then for $n = 1$

$$\int \rho_0(q)\frac{dq}{2\pi} = 1, \quad \widetilde{\rho}_1 = 0\,. \tag{1.8}$$

(3) The bound in Eq.(1.6) yields a convergent expression for the $\rho_n^{[r]}(q)$ or for $F^{[r]}(q,p)$ or, for bounded f, of $\int F^{[r]}(q,p)\cdot f(p)dp$. Such expressions can possibly be compared with results of numerical simulations.

The above Theorem is the main result.

2 Dimensionless equations

It is convenient to introduce the dimensionless quantities

$$\sigma_n(q) \stackrel{def}{=} \rho_n(q)\xi^n n!, \qquad \eta \stackrel{def}{=} \beta\xi^2/J, \qquad \beta\tau, \qquad \beta V, \tag{2.1}$$

which will be relevant in the following.

Let a tilde over a function $f(q)$ mean $f - \overline{f}$, with $\overline{f} \stackrel{def}{=} \int_0^{2\pi} f(q)\frac{dq}{2\pi} \stackrel{def}{=} \langle\, f \,\rangle$. If $\sigma_n(q) \stackrel{def}{=} \widetilde{\sigma}_n(q) + \overline{\sigma}_n$ with $\langle\, \widetilde{\sigma}_n \,\rangle = 0$, consider the sequence of functions $\sigma(q) = (\widetilde{\sigma}_n(q), \overline{\sigma}_n)_{n\ge 1}$. The stationarity Eq.(1.7), for $n \ge 1$ and using the Hermite polynomials properties $p : p^n := p^{n+1} : +\frac{J}{\beta} : p^{n-1} :$, $\partial_p : p^n := n : p^{n-1}:$ and $\partial_p G(p) = -\frac{\beta}{J}\, p\, G(p)$, becomes, after dividing both sides by n

$$\begin{aligned} \partial\widetilde{\sigma}_n =& -\eta\Big((n-1)\Big(\partial\widetilde{\sigma}_{n-2} + \beta\widetilde{\partial U\widetilde{\sigma}_{n-2}} + \beta\partial U\overline{\sigma}_{n-2} \\ &+ \beta\tau\widetilde{\sigma}_{n-2} + \widetilde{\sigma}_{n-1}\Big)\Big)\,, \\ \overline{\sigma}_n =& -\Big(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau\,\overline{\sigma}_{n-1}\Big)\,, \end{aligned} \tag{2.2}$$

where $\sigma_j = 0$ for $j < 0$. For $n = 0$, Eq.(1.7) is an identity, thus Eq.(2.2) holds only for $n \ge 1$. By normalization $\overline{\sigma}_0 \equiv 1$, as also implied by the second of Eqs.(2.2).

The Fourier transform of Eqs.(2.2) for $n \ge 1$ is

$$\begin{aligned}
\widetilde{\sigma}_{n,k} =& -\frac{\eta(n-1)}{ik}\widetilde{\sigma}_{n-1,k} - \eta(n-1)(1+\frac{\beta\tau}{ik})\widetilde{\sigma}_{n-2,k}\\
&- \eta(n-1)\Big(\frac{\beta g V}{ik}\sum_{k'=\pm1} ik'\widetilde{\sigma}_{n-2,k-k'} + \beta g V\overline{\sigma}_{n-2}\delta_{k,\pm1}\Big)\,,\\
\overline{\sigma}_n =& -\Big(\overline{\beta\partial U\widetilde{\sigma}_{n-1}} + \beta\tau\overline{\sigma}_{n-1}\Big)\\
\equiv& (-\beta\tau)^n + \sum_{j=0}^{n-1}(-\beta\tau)^j\overline{(-\beta\partial U)\widetilde{\sigma}_{n-1-j}}\,.
\end{aligned} \tag{2.3}$$

After defining $\mathbf{S}_{n,k}\stackrel{def}{=}\begin{pmatrix}\widetilde{\sigma}_{n,k}\\ \widetilde{\sigma}_{n-1,k}\end{pmatrix}$, it is natural to introduce the g–independent 2×2 matrices $M_{n,k}$

$$M_{n+1,k}\stackrel{def}{=}\begin{pmatrix}-\frac{n}{ik}\eta & ina_k\eta\\ 1 & 0\end{pmatrix}, \qquad a_k\stackrel{def}{=}(i+\frac{\beta\tau}{k})\,, \tag{2.4}$$

so that Eqs.(2.3) can be written more concisely, for $n\ge 0$,

$$\begin{aligned}
\mathbf{S}_{n+1,k} =& M_{n+1,k}\Big(\mathbf{S}_{n,k}+\mathbf{X}_{n+1,k}\Big), \quad \mathbf{X}_{n+1,k}\stackrel{def}{=}\begin{pmatrix}0\\ x_{n+1,k}\end{pmatrix},\\
x_{n+1,k}\stackrel{def}{=}& -\frac{\beta g V}{ia_k}\Big(\delta_{|k|=1}\overline{\sigma}_{n-1} + \sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}_{n-1,k-k'}\Big)\,,\\
\overline{\sigma}_{n+1} =& -(\overline{\beta\partial U\widetilde{\sigma}_n} + \beta\tau\overline{\sigma}_n)\,.
\end{aligned} \tag{2.5}$$

Notice that $M_{n,k}$ is defined for $n\ge 1$, while $M^{-1}_{n,k}$ is defined for $n\ge 2$.

Remarks: (1) The case $g=0$ is an exercise: $\sigma_n(q)$ must be constant simply by symmetry, and $\sigma_0=1$. It follows, from Eqs.(2.2) and (1.4) $\sigma_n\equiv\overline{\sigma}_n = (-\beta\tau)^n$ and the series in Eq.(1.4) becomes

$$\begin{aligned}
\sigma_n \equiv& \overline{\sigma}_n = (-\beta\tau)^n\,,\\
F(p,q) =& G_\beta(p)\sum_{n=0}^\infty \frac{(-1)^n}{n!}\Big(\frac{\beta\tau}{\xi}\Big)^n\Big(\frac{J\beta^{-1}}{2}\Big)^{\frac{n}{2}} H_n(\frac{p}{\sqrt{(2\beta^{-1}J)}})\,,
\end{aligned} \tag{2.6}$$

which, by the definition of the Hermite polynomials via their generating function ([6, 8.957]), is

$$F(p,q) = G_\beta(p-v), \qquad v = -\frac{J\tau}{\xi}\,. \tag{2.7}$$

(2) Eqs.(2.5) implies for $n = 0, 1$ (*i.e.* for $n = 1, 2$ in Eq.(2.3)) that

$$\mathbf{S}_1 = \begin{pmatrix} 0 \\ \widetilde{\sigma}_0 \end{pmatrix}, \quad \mathbf{S}_2 = \begin{pmatrix} \widetilde{\sigma}_2 \\ 0 \end{pmatrix}. \tag{2.8}$$

It is important to notice that Eq.(1.8) (hence also (2.3)) implies $\widetilde{\sigma}_1 \equiv 0$*.*

If $\widetilde{\sigma}_2$ is known, $\widetilde{\sigma}_0$ can be derived by solving, if possible, the equation (see the first of Eqs.(2.3) or (2.5))

$$\widetilde{\sigma}_{2,k} = i\eta a_k \widetilde{\sigma}_{0,k} - \eta \frac{\beta g V}{ik} \sum_{k'=\pm 1} ik' \widetilde{\sigma}_{0,k-k'} - \eta \beta g V \delta_{|k|=1}\,. \tag{2.9}$$

(3) Eqs.(2.5) can be regarded as equations for $\mathbf{S}_n, n \ge 1$: if $\mathbf{S}_1 \equiv \binom{0}{\widetilde{\sigma}_0}$ (*i.e.* if $\widetilde{\sigma}_0$) is known, then all $\mathbf{S}_n$, $n \ge 3$, can be immediately computed. To this end, $\mathbf{S}_1$ and $\overline{\sigma}_1$ are computed from Eqs.(2.5) ($\overline{\sigma}_0 = 1$), together with $x_{2,k}$; then, from the pair $(\mathbf{S}_1, \overline{\sigma}_1)$ and $x_{2,k}$, we compute $\mathbf{S}_2, \overline{\sigma}_2$ and x_3, by Eq.(2.5), hence $\mathbf{S}_3, \overline{\sigma}_3$ and x_4 follow &tc.
(4) Eqs.(2.2) and its Fourier transform (2.3) will be considered as equations for $\mathbf{S}_{n,k}$ for $n \ge 2$ to be solved under the condition that $\mathbf{S}_2 = \binom{\widetilde{\sigma}_2}{0}$. The condition that the second component of $\mathbf{S}_2$ be 0 is the only condition to impose *a priori* and to use in the construction.

3 Perturbation expansion

Consider the expansion in g by writing

$$\begin{aligned} \widetilde{\sigma}_n(q) =& g\widetilde{\sigma}_n^{[1]}(q) + g^2 \widetilde{\sigma}_n^{[2]}(q) + \dots\,, \\ \overline{\sigma}_n =& \overline{\sigma}_n^{[0]} + g\overline{\sigma}_n^{[1]} + g^2 \overline{\sigma}_n^{[2]} + \dots\,, \end{aligned} \tag{3.1}$$

and, correspondingly, $F = F^{[0]} + gF^{[1]} + \dots$.

Eqs.(2.5) become a recursive relation for the the real constants $\overline{\sigma}_n^{[r]}$ and for the vectors $\mathbf{S}_{n,k}^{[r]} \stackrel{def}{=} \binom{\widetilde{\sigma}_{n,k}^{[r]}}{\widetilde{\sigma}_{n-1,k}^{[r]}}$, $k > 0$, keeping in mind the c.c. symmetry $\widetilde{\sigma}_{n,k}^{[r]} = \overline{\widetilde{\sigma}_{n,-k}^{[r]}}$. The order $r = 0$ is simply $\widetilde{\sigma}_n^{[0]} = 0$, $\overline{\sigma}_0 = 1$ and for $r \ge 0$ the recursion will be conveniently written in matrix form for $n \ge 0$

$$\begin{aligned} \mathbf{S}_{n+1,k}^{[r]} =& M_{n+1,k}\Big(\mathbf{S}_{n,k}^{[r]} + x_{n+1,k}^{[r]} \begin{pmatrix} 0 \\ 1 \end{pmatrix}\Big), \qquad \mathbf{S}_{0,k}^{[r]} = y_{0,k}^{[r]} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \stackrel{def}{=} \mathbf{Y}_k^{[r]}\,, \\ \overline{\sigma}_{n+1}^{[r]} =& -\beta\tau \overline{\sigma}_n^{[r]} + v_{n+1}^{[r]}, \quad \overline{\sigma}_n^{[0]} = (-\beta\tau)^n, \end{aligned} \tag{3.2}$$

where $y^{[r]}_{0,k}\equiv\widetilde{\sigma}^{[r]}_{0,k}$ (so that, by Eq.(1.8),(2.8), $\mathbf{S}^{[r]}_{1,k}=\begin{pmatrix}0\\ y^{[r]}_{0,k}\end{pmatrix}$) and $v^{[r]}_n, x^{[r]}_{n,k}$ are given by

$$
\begin{aligned}
x^{[r]}_{n+1,k}&\stackrel{def}{=}-\frac{\beta V}{ia_k}\Big(\overline{\sigma}^{[r-1]}_{n-1}\delta_{|k|=1}+\sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}^{[r-1]}_{n-1,k-k'}\Big),\qquad n\ge 0\,,\\
v^{[r]}_{n+1}&\stackrel{def}{=}-\sum_{k'=\pm1}\beta V\,ik'\widetilde{\sigma}^{[r-1]}_{n,-k'},\qquad n\ge0,\qquad \mathbf{S}^{[r]}_{1,k}=\begin{pmatrix}0\\ y^{[r]}_{0,k}\end{pmatrix}\,,\\
x^{[r]}_{2,k}&=\frac{-\beta V}{ia_k}(\delta_{|k|=1}\delta_{r=1}+\sum_{k'=\pm1}\frac{k'}{k}\widetilde{\sigma}^{[r-1]}_{0,k-k'})\,,
\end{aligned}
\tag{3.3}
$$

and depend on quantities of order lower than r. Here, quantities of order lower than 0 are interpreted as 0.

Therefore, at order r, all coefficients are determined in terms of the constants $\widetilde{\sigma}^{[r]}_{0,k}\equiv y^{[r]}_{0,k}$ and of the $\mathbf{S}^{[r']}_{n,k'}$ with $r'<r$; since the only harmonics in $U(q)$ are $k=\pm1$, it can be supposed that $\widetilde{\mathbf{S}}^{[r]}_{n,k}\equiv0$ for $|k|>r$ and all n.

Furthermore, the harmonics $\widetilde{\sigma}^{[r]}_{0,k}$ and $\widetilde{\sigma}^{[r]}_{0,-k}$ are complex conjugate, so it is possible to always suppose $k>0$ and to interpret harmonics with negative values of k as complex conjugate of the corresponding harmonics with $k>0$.

4 The expansion coefficients

The recursion can be reduced to an iterative determination of $x^{[r]}_{n,k}$ and $\overline{\sigma}^{[r]}_n$ starting from $r=1$, as the case $r=0$ has been already evaluated at the end of Sec.2, namely $x^{[0]}_{n,k}=0$, $\overline{\sigma}^{[0]}_n=(-\beta\tau)^n$ and $\mathbf{S}^{[0]}_n=0$, since $\widetilde{\sigma}^{[0]}_n\equiv0$.

For $r\ge1$ it is, see Eqs.(2.9) and (3.3),

$$
\begin{aligned}
&\mathbf{S}^{[r]}_0\stackrel{def}{=}\mathbf{Y}^{[r]}=\begin{pmatrix}y^{[r]}\\0\end{pmatrix},\quad \mathbf{S}^{[r]}_1\stackrel{def}{=}\begin{pmatrix}0\\y^{[r]}\end{pmatrix},\\
&\mathbf{S}^{[r]}_2\stackrel{def}{=}\begin{pmatrix}i\,a_k\,\eta\,(y^{[r]}+x^{[r]}_2)\\0\end{pmatrix},\qquad \overline{\sigma}^{[r]}_0=0\,,
\end{aligned}
\qquad r\ge1\,.
\tag{4.1}
$$

Eqs.(3.2), for $r\ge1$, are related to the general r-independent equations for

$n \geq 2$, conveniently written by means of the inverse matrix $M^{-1}_{n+1,k}$ as

$$\begin{aligned}
&M^{-1}_{n+1,k} \stackrel{def}{=} \begin{pmatrix} 0 & 1 \\ \frac{1}{i\,n\,a_k\,\eta} & -\frac{1}{k\,a_k} \end{pmatrix}, \\
&\mathbf{S}_n = M^{-1}_{n+1,k}\mathbf{S}_{n+1} - \mathbf{X}_{n+1}, \qquad \mathbf{S}_2 = y' \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\
&\overline{\sigma}_n = (-\beta\tau)\overline{\sigma}_{n-1} + v_n, \quad \overline{\sigma}_0 = w, \quad \mathbf{X}_n = x_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \; x_0 = x_1 = 0\,.
\end{aligned} \tag{4.2}$$

This is inhomogeneous in the unknowns $(\mathbf{S}_n, \overline{\sigma}_n)_{n\geq 2}$, imagining $\mathbf{S}_2, \mathbf{X}_n, v_n, w$ (*i.e.* $y\,, x_n\,, v_n\,, w$) as known inhomogeneous quantities depending on the orders r and k, as prescribed by Eqs.(3.3). In the following, Eqs.(4.2) will be considered for different orders r. Moreover, $w = 0$ if $r \geq 1$ and $w = (-\beta\tau)^n$ if $r = 0$.

A few properties of products of matrices $M_{n,k}$ will be needed.
Let $(M^{-1}_p)^{*s} \stackrel{def}{=} M^{-1}_p \cdots M^{-1}_{p+s-1}$ for $s \geq 1$, $(M^{-1}_p)^{*0} \stackrel{def}{=} 1$ and define

$$\begin{aligned}
&\boldsymbol{\xi}_n \stackrel{def}{=} -\sum_{h=n}^{\infty} (M^{-1}_{n+1})^{*(h-n)}\mathbf{X}_{h+1}\,, \\
&\overline{\sigma}_n \stackrel{def}{=} \sum_{s\geq 1}^{n} (-\beta\tau)^{n-s} v_s + w\,,
\end{aligned} \qquad n \geq 2\,, \tag{4.3}$$

then $M^{-1}_{n+1}\boldsymbol{\xi}_{n+1} = \boldsymbol{\xi}_n + \mathbf{X}_{n+1}$, if the series converges and if y' is left free. Eq.(4.3) is thus a special solution of the recursion (4.2) ($n \geq 2$).

To proceed, we introduce some notation; given k, let

$$\begin{aligned}
&|\uparrow\rangle \stackrel{def}{=} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |1\rangle, \qquad |\downarrow\rangle \stackrel{def}{=} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |0\rangle, \\
&\Lambda_{\nu,\nu'}(n,h) \stackrel{def}{=} \langle \nu | (M^{-1}_{n+1})^{*(h-n)} | \nu' \rangle, \qquad \nu, \nu' = 0, 1\,, \\
&\Lambda(n,h) \stackrel{def}{=} \Lambda_{0,0}(n,h), \qquad \Lambda(n,n) = 1 \equiv \langle \downarrow | \downarrow \rangle\,, \\
&\zeta(n,h) \stackrel{def}{=} \frac{\langle \uparrow | (M^{-1}_{n+1})^{*(h-n)} | \downarrow \rangle}{\Lambda(n,h)}, \qquad \zeta(n,n) = 0 \equiv \langle 1 | 0 \rangle\,.
\end{aligned} \tag{4.4}$$

Notice that, by explicitly computing the vectors $\langle \nu | M^{-1}_{n+1}$ and $M^{-1}_h | \nu' \rangle$, the general relation (due to the special form, Eq.(4.2), of M^{-1}_j) is

$$\langle \nu | (M^{-1}_{n+1})^{*(h-n)} | \nu' \rangle = \frac{\Lambda(n+\nu, h-\nu')}{(i\eta a_k (h-1))^{\nu'}}, \quad \nu, \nu' = 0, 1\,, \tag{4.5}$$

which, provided $\Lambda(n,h)\neq 0$, implies the identities

$$\begin{aligned}&\boldsymbol{\zeta}(n,h)\overset{def}{=}\begin{pmatrix}\zeta(n,h)\\ 1\end{pmatrix},\ \zeta(n,h)=\frac{\Lambda(n+1,h)}{\Lambda(n,h)},\qquad 2\le n\le h\,,\\ &(M_{n'+1}^{-1})^{*(n-n')}\boldsymbol{\zeta}(n,n')=\frac{\Lambda(n',N)}{\Lambda(n,N)}\boldsymbol{\zeta}(n',N),\quad n+1>n'\,.\end{aligned}\tag{4.6}$$

with $\zeta(n,n)=0$. Here, the second relation will be called the *eigenvector property* of the $\zeta(n,h)$. Eq.(4.5) also implies the recurrence

$$\begin{aligned}\varphi(n,h)\overset{def}{=}&-\frac{\zeta(n,h)}{ka_k}=\frac{1}{1+\frac{z}{n}\varphi(n+1,h)}\\ &=\frac{1}{1+\frac{z}{n}\frac{1}{1+\frac{z}{n+1}}\cdots\frac{1}{1+\frac{z}{h-2}}},\qquad h-2\ge n,\qquad z\overset{def}{=}\frac{a_kk^2}{i\eta}\end{aligned}\tag{4.7}$$

and $\varphi(n-1,n)=1,\varphi(n,n)=0$, representing the ζ's as continued fractions and showing that $\zeta(n,h)$ and the limit $\zeta(n,\infty)$ are analytic in z for $|z|<\frac{1}{4}$, [7, p.45].

The continued fraction for $\varphi(n,\infty)$ is the S-fraction $\frac{n-1}{z}\,\mathbf{K}_{m=n-1}^{\infty}(\frac{z/m}{1})$, following [7, p.35], and defines an holomorphic function of z in the complex plane cut along the negative real axis (see [7, p.47,(A)]). The $\varphi(n,h)$ is also a (truncated) S-fraction obtained by setting $m=\infty$ for $m\ge h-1$ in the previous continued fraction. Hence, by [7, p.47,(B)], $\varphi(n,h)$ has the same holomorphy properties as $\varphi(n,\infty)$. Furhermore, $\varphi(n,h)$ is holomorphic for $|z|<\frac{1}{4}$, continuous and bounded by $\frac{1}{2}$ in $|z|\le\frac{1}{4}$, [7, p.45].

Relevant inequalities can be derived from the inequality in [7, p.138], see Sec.6.

The definitions imply $\boldsymbol{\xi}_n\equiv-\sum_{h=n}^{\infty}x_{h+1}\Lambda(n,h)\boldsymbol{\zeta}(n,h)$ (see Eq.(4.3)). Furthermore, if the limits $\lim_{N\to\infty}\frac{\Lambda(2,N)^{-1}}{\Lambda(n,N)^{-1}}$ exist, and are symbolically denoted $\frac{\Lambda(2,\infty)^{-1}}{\Lambda(n,\infty)^{-1}}$, then

$$\mathbf{T}_n^0=\frac{\Lambda(2,\infty)^{-1}}{\Lambda(n,\infty)^{-1}}\boldsymbol{\zeta}(n),\qquad \boldsymbol{\zeta}(n)\overset{def}{=}\boldsymbol{\zeta}(n,\infty)\tag{4.8}$$

is a solution of Eq.(4.2) with $\mathbf{X}=0$ and some initial data for $n=2$.

A solution to the r-th order equations will thus have the form

$$\mathbf{S}_n=\boldsymbol{\xi}_n+\lambda\mathbf{T}_n^0\,,\tag{4.9}$$

where the constant λ will be fixed to match the data at $n = 2$, *i.e.* null $\mathbf{S}_2$ second component, see Eqs.(2.8),(3.2). Concerning the r-th order equation, the initial data of interest are $\overline{\sigma}_1^{[r]}$ and $y_{2,k}^{[r]}$ and $\mathbf{X}_{n,k}^{[r]}, v_n^{[r]}$ are given by Eq.(3.3), in terms of quantities of order $r-1$.

Therefore there seems to be no freedom, because we expect that the condition that $\mathbf{Y}$ is proportional to $|\uparrow\rangle$, *i.e.* that its second component is 0, fixes the free constant λ. Thus the (unique) solution to the recursion with initial data $\mathbf{S}_2^{[r]} = y|\uparrow\rangle$ has necessarily the form

$$\mathbf{S}_{2,k}^{[r]} = -\sum_{h=2}^{\infty} x_{h+1,k}^{[r]} \Lambda(2,h)(\boldsymbol{\zeta}(2,h) - \boldsymbol{\zeta}(2)) \tag{4.10}$$

which is proportional to $|\uparrow\rangle$, because the second components of $\boldsymbol{\zeta}(2,h)$ and $\boldsymbol{\zeta}(2)$ are 1; hence in Eq.(4.9)

$$\lambda = \sum_{h=2}^{\infty} x_{h+1,k}^{[r]} \Lambda(2,h)\,. \tag{4.11}$$

Proceeding formally, for $n > 2, \mathbf{S}_n^{[r-1]}$ will be given by applying the recursion. Since $\boldsymbol{\xi}_n$ is a formal solution and $\boldsymbol{\zeta}(n)$ has the eigenvector property Eq.(4.6), it is

$$\begin{aligned}\mathbf{S}_{n,k}^{[r]} = &\sum_{h=2}^{n-1} x_{h+1,k}^{[r]} \frac{\Lambda(2,h)\Lambda(n,\infty)}{\Lambda(2,\infty)} \zeta(n) \\ &- \sum_{h=n}^{\infty} x_{h+1,k}^{[r]} \Big(\Lambda(n,h)\zeta(n,h) - \frac{\Lambda(2,h)\Lambda(n,\infty)}{\Lambda(2,\infty)} \zeta(n) \Big)\,.\end{aligned} \tag{4.12}$$

It should be stressed that the series in Eq.(4.3) might diverge; nevertheless, cancellations may (and will) occur in Eq.(4.12), so that Eq.(4.3) would still be a solution, if the series in Eq.(4.12) converges (as can be checked by inserting it in the equation Eq.(4.2)).

To compute the first component of $\mathbf{S}_{n,k}^{[r]}$, we left multiply Eq.(4.12) by $\langle\uparrow|$, considering that $\zeta_k(n,m) = \frac{\Lambda(n+1,m)}{\Lambda(n,m)}$ by the first of the (4.6) and that

$\Lambda(n+1,n)=\zeta_k(n,n)\Lambda(n,n)\equiv 0$. Setting $\Lambda(n,m)=0\,,\forall\, m<n$, we obtain

$$\begin{aligned}
\widetilde\sigma^{[r]}_{n,k}=&\sum_{m=2}^{n} x^{[r]}_{m+1,k}\Lambda(2,m)\frac{\Lambda(n,\infty)}{\Lambda(2,\infty)}\boldsymbol{\zeta}(n)\\
&-\sum_{m=n+1}^{\infty} x^{[r]}_{m+1,k}\Big(\Lambda(n,m)\boldsymbol{\zeta}(n,m)-\Lambda(2,m)\frac{\Lambda(n,\infty)}{\Lambda(2,\infty)}\boldsymbol{\zeta}(n)\Big)\\
\equiv&\sum_{m=2}^{n} x^{[r]}_{m+1,k}\Big(\prod_{j=2}^{m-1}\frac{\zeta(j,\infty)}{\zeta(j,m)}\Big)\Big(\prod_{j=m}^{n}\zeta(j,\infty)\Big)\\
&-\sum_{m=n+1}^{\infty} x^{[r]}_{m+1,k}\Big(\prod_{j=n+1}^{m-1}\frac{1}{\zeta(j,m)}\Big)\Big(1-\prod_{j=2}^{n}\frac{\zeta(j,\infty)}{\zeta(j,m)}\Big),
\end{aligned}\tag{4.13}$$

for $n\ge 2$. From $\widetilde\sigma^{[r]}_{2,k}$ and $x^{[r]}_{2,k}$ (derived from Eq.(3.3)) and using $\widetilde\sigma^{[r]}_{1,k}=0$ (see Eq.(4.1)) the "main unknown" $y^{[r]}_{0,k}$, *i.e.* $\sigma^{[r]}_{0,k}$, is computed.

As stressed above, Eqs.(4.10),(4.13) are acceptable if the series converge. When $r=1$, they do for $\beta\tau$ small enough using $x^{[1]}_{n,k}=-\frac{\beta V}{ia_k}(-\beta\tau)^{n-1}\,\delta_{|k|=1}$, since (i) the squared norm of $M_{n+1,k}$ in C^2 is equal to

$$\frac12(1+\frac{1}{\eta^2n^2|a_k|^2}+\frac{1}{k^2|a_k|^2})\Big(1+\Big(1-\frac{4\frac{1}{\eta^2|a_k|^2n^2}\frac{1}{k^2|a_k|^2}}{(1+\frac{1}{\eta^2n^2|a_k|^2}+\frac{1}{k^2|a_k|^2})^2}\Big)^{\frac12}\Big)\tag{4.14}$$

i.e. to the square root of the maximum eigenvalue of $M^{-1\,*}_{n+1,k}M^{-1}_{n+1,k}$ and (ii) the convergence condition of the first of Eqs.(4.3) is $\beta\tau||M^{-1}_{2,1}||<1$, meaning that $\beta\tau$ should be small enough. As it will be seen from the estimates of Sec.6, this restriction on $\beta\tau$ can be removed, because of the cancellations that occur between the two addends in Eq.(4.10)). Therefore, it will be possible to try an iterative construction, $\forall\,\eta,\beta\tau,r>0$.

5 A constructive algorithm

If $x^{[r]}_{n,k},\overline\sigma^{[r]}_n$ are known, it is possible to compute $\widetilde\sigma^{[r]}_{n,k}$ from Eqs.(3.3),(4.13) for all $n\ge 0$. In particular,

$$\begin{aligned}
\widetilde\sigma^{[r]}_{2,k}=&x^{[r]}_{3,k}\zeta(2,\infty)-\sum_{m=3}^{\infty}x^{[r]}_{m+1,k}\Lambda(3,m)\Big(1-\frac{\Lambda(2,m)\Lambda(3,\infty)}{\Lambda(2,\infty)\Lambda(3,m)}\Big)\,,\\
\widetilde\sigma^{[r]}_{0,k}=&\frac{1}{i\eta a_k}\widetilde\sigma^{[r]}_{2,k}+\frac{\beta V}{ia_k}\Big(\delta_{|k|=1}\delta_{r=1}+\sum_{k'=\pm1}\frac{k'}{k}\widetilde\sigma^{[r-1]}_{0,k-k'}\Big)\Big),\qquad \widetilde\sigma_1\equiv 0
\end{aligned}\tag{5.1}$$

The order $r=1$ is therefore known because $x^{[1]}_{m+1,k}=\frac{-\beta V}{ia_k}(-\beta\tau)^{m+1}\delta_{k,1}$, provided the series in Eqs.(5.1),(4.13) converge. It is convenient to introduce the kernels $\vartheta_k(n;m)$ to abridge the Eqs.(4.13),(5.1) into the form:

$$\begin{aligned}
\widetilde\sigma^{[r]}_{n,k}=&\sum_{m=0}^\infty\vartheta_k(n;m)\,x^{[r]}_{m+1,k},\quad n\ne1,\quad \vartheta_k(n;0)=0,\quad\forall n\ge2\,,\\
\vartheta_k(n;m)=&\Big(\prod_{j=2}^{m-1}\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}\Big)\Big(\prod_{j=m}^{n}\zeta_k(j,\infty)\Big),\quad 2\le m\le n\,,\\
\vartheta_k(n;m)=&\Big(\prod_{j=n+1}^{m-1}\frac{1}{\zeta_k(j,m)}\Big)\Big(\prod_{j=2}^{n}\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}-1\Big),\quad 2\le n<m\,,\\
\vartheta_k(0,m)\stackrel{def}{=}&\frac{\vartheta_k(2,m)}{i\eta a_k}\delta_{m\ge2}-\delta_{m,1},\qquad \vartheta_k(1;m)\equiv0\,,
\end{aligned}\tag{5.2}$$

where products over an empty set of labels are interpreted as 1.

Consider the sequences $\mathbf{Z}=\binom{\widetilde\sigma_{n,k}}{\widetilde\sigma'_{n,k}}$, $n=0,1,\ldots,\ k=\pm1,\pm2,\ldots$, in the particular cases $\mathbf{Z}^{[r]}=\binom{\widetilde\sigma^{[r]}_{n,k}}{\widetilde\sigma^{[r-1]}_{n,k}}$, $n=0,1,\ldots,\ k=\pm1,\pm2,\ldots$. Remark that $\mathbf{Z}^{[1]}_{n,k}=\begin{pmatrix}\widetilde\sigma^{[1]}_{n,k}\\0\end{pmatrix}$ and $\widetilde\sigma^{[1]}_{n,k}$ is known (see comment after Eq.(5.1) and remark that $\widetilde\sigma^{[0]}=0$), if the series defining it converges. Then Eqs.(4.13),(5.2) can be rewritten as

$$\mathbf{Z}^{[r]}=\mathcal{B}\mathbf{Z}^{[r-1]},\qquad r\ge2,\qquad \mathbf{Z}^{[1]}_{n,k}=\begin{pmatrix}\widetilde\sigma^{[1]}_{n,k}\\0\end{pmatrix},\tag{5.3}$$

with the map $\mathcal{B}$ defined by taking into account the above relations and also Eqs.(3.3),(4.2), which yield

$$\begin{aligned}
\overline\sigma^{[r]}_n=&\Big((-\beta\tau)^n\delta_{r,0}-\beta V\sum_{k'=\pm1}ik'\sum_{h=0}^{n-1}(-\beta\tau)^h\widetilde\sigma^{[r-1]}_{n-1-h,-k'}\Big),\quad n\ge1\,,\\
x^{[r]}_{n,k}=&-\frac{\beta V}{ia_k}\Big(\overline\sigma^{[r-1]}_{n-2}\delta_{|k|=1}+\sum_{k'=\pm1}\frac{k'}{k}\widetilde\sigma^{[r-1]}_{n-2,k-k'}\Big),\qquad n\ge2\,,\\
x^{[r]}_{2,k}=&-\frac{\beta V}{ika_k}(\delta_{|k|=1}\delta_{r=1}+\sum_{k'=\pm1}k'\widetilde\sigma^{[r-1]}_{0,k-k'})\,,
\end{aligned}\tag{5.4}$$

$\forall n\ne1,|k|\le r$. Therefore, if $\widetilde\vartheta_k(n;m)\stackrel{def}{=}\sum_{h=0}^\infty(-\beta\tau)^h\vartheta_k(n,m+h+1)\,\delta_{m\ge1}$

and the kernels $t_k(n;m), \widetilde{t}_k(n;m)$ are defined as

$$\begin{aligned}
t_k(n,m) &\stackrel{def}{=} \frac{-\beta V}{ika_k}\,\vartheta_k(n;m)\,\delta_{m\ge 2}\,, \quad n\ge 2\\
\widetilde{t}_k(n,m) &\stackrel{def}{=} \frac{(\beta V)^2}{a_k}\,\widetilde{\vartheta}_k(n;m)\,, \quad n\ge 2\\
t_k(0,m) &= \frac{t_k(2,m)}{i\eta a_k}\delta_{m\ge 2}+\delta_{m,0}\frac{\beta V}{ika_k}\,, \quad \widetilde{t}_k(0,m)=\frac{\widetilde{t}_k(2,m)}{i\eta a_k}\delta_{m\ge 1}\,,\\
t_k(1,m) &= \widetilde{t}_k(1,m)=0\,,
\end{aligned} \tag{5.5}$$

the map $\mathcal{B}$ acquires the form $\binom{y'_{n,k}}{z'_{n,k}}=\mathcal{B}\binom{y_{n,k}}{z_{n,k}}$, with

$$\begin{aligned}
y'_{n,k} &= \sum_{m=1}^{\infty}\sum_{k'=\pm 1} k'\Big(t_k(n,m)y_{m-1,k-k'}+\delta_{|k|=1}\widetilde{t}_k(n,m)z_{m-1,-k'}\Big)\,,\\
z'_{n,k} &= y_{n,k}\,,
\end{aligned} \tag{5.6}$$

In conclusion, if
(i) $\mathbf{Z}^{[1]}$ is given,
(ii) the series over m converge,
the map $\mathcal{B}$ determines $\mathbf{Z}^{[r]}$ for $r\ge 2$. Convergence will be studied in Sec.6.

Remark: an interesting check is that, if $\tau=0$, the recursion gives $\overline{\sigma}_n^{[r]}\equiv 0, \forall n\ge 1, r\ge 0$ and $\widetilde{\sigma}_{2,k}^{[r]}=0,\forall r>0$ and this leads, as expected, to $\sigma_n\equiv 0,\forall n>0$ and $\sigma_0(q)=Z^{-1}e^{-\beta\, 2\, g\, V\,\cos q}$, after some algebra and after summation of the series in g.

6 Bounds and theorem proof

Let $z=\frac{k^2 a_k}{i\eta}\equiv(1+\frac{\beta\tau}{ik})\frac{k^2}{\eta}$. If $z=|z|e^{2i\alpha}$, $|\alpha|<\frac{1}{2}\mathrm{arctg}\frac{\beta\tau}{|k|}<\frac{\pi}{4}$ (so that $|\cos\alpha|>\frac{1}{\sqrt{2}}$), let $\lambda^{\alpha}_{\ell,\pm}\stackrel{def}{=}\sqrt{1+\frac{4|z|}{(\ell-1)\cos^2\alpha}}\pm 1$; then from the inequality in [7, p.138] we derive that

$$|\varphi(j,\infty)-\varphi(j,h)|\le 2\sqrt{2}\prod_{\ell=j}^{h-2}\frac{\lambda^{\alpha}_{\ell,-}}{\lambda^{\alpha}_{\ell,+}}\stackrel{def}{=}\Delta(j,h)\,, \tag{6.1}$$

for $h \ge j+1$ and $\varphi(j,j+1)=1, \varphi(j,j)=0$. Furthermore, the recursion for $\varphi(j,h)$ implies $|\arg(\frac{z\varphi(j+1,h)}{j})| \le |\arg(\frac{z}{j})| \le 2\alpha$, and

$$\begin{aligned}&\Big|\varphi(j,h)-1\Big| \equiv |\frac{z\varphi(j+1,h)}{j+z\varphi(j+1,h)}| \le 1\,,\\ &\Big|\varphi(j,h)^{-1}-1\Big| \equiv |\frac{z}{j}\varphi(j+1,h)| \le 2\frac{|z|}{j}\,,\end{aligned} \qquad h \ge j+2\,, \tag{6.2}$$

therefore

$$\Big|\frac{\varphi(j,\infty)}{\varphi(j,h)}-1\Big| \le \Big(1+2\frac{|z|}{j}\Big)\,\Delta(j,h), \qquad h \ge j+2\,. \tag{6.3}$$

These inequalities are useful to estimate the kernels $\vartheta_k(n;n')$ appearing in Eqs.(5.2) (*i.e.* in Eqs.(4.13) written as $\widetilde\sigma^{[r]}_{n,k} = \sum_{m=0}^\infty \vartheta_k(n;m)\, x^{[r]}_{m+1,k}$) and, using $\frac{\sqrt{1+x}-1}{\sqrt{1+x}+1} \le \frac{x}{1+x}$, imply

$$\begin{aligned}\frac{1}{1+\frac{2\sqrt2|z|}{j}} \le&\Big|\frac{\zeta_k(j,\infty)}{ka_k}\Big| \le 2\,,\\ \Big|\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}-1\Big| \le& \Big(1+\frac{2\sqrt2|z|}{j}\Big)2\sqrt2\prod_{\ell=j}^{m-2}\frac{\sqrt{1+\frac{8|z|}{\ell-1}}-1}{\sqrt{1+\frac{8|z|}{\ell-1}}+1}\\ \le& 8\Big(1+\frac{|z|}{j}\Big)\prod_{\ell=j}^{m-2}\frac{8|z|}{\ell-1+8|z|}, \qquad m \ge j+1\,.\end{aligned} \tag{6.4}$$

Hence (as $|1-X| = |e^{\log X}-1| \le e^{|\log X|}-1$)

$$\Big|1-\prod_{j=2}^{n}\frac{\zeta_k(j,\infty)}{\zeta_k(j,m)}\Big| \le \Big[e^{\sum_{j=2}^n \log\left(1+8\left(1+\frac{|z|}{j}\right)\prod_{\ell=j}^{m-2}\frac{8|z|}{\ell-1+8|z|}\right)}\Big]-1\,. \tag{6.5}$$

Sacrificing better bounds for simpler ones, for $n \ge 2$ and $m < n$, it is

$$\begin{aligned}&|\prod_{j=2}^{m-1}\frac{\zeta(j,\infty)}{\zeta(j,m)}| \le e^{\sum_{j=2}^{m-1} 8(1+|z|)\frac{(8|z|)^{-(m-1-j)}}{(m-1-j)!}} \le e^{8(1+|z|)e^{8|z|}}\,,\\ &|\prod_{j=m}^{n}\zeta(j,\infty)| \le (2|ka_k|)^{n-m+1}, \qquad |\vartheta(n;m)| \le |2\,k\,a_k|^{n-m+1}e^{8e^{9|z|}}\,.\end{aligned} \tag{6.6}$$

and, for $m \ge n$, using $e^X - 1 \le e^X X, \forall X \ge 0$

$$\begin{aligned}\frac{|\vartheta_k(n;m)|}{|ka_k|^{n-m+1}} &\le \Big(\prod_{j=n+1}^{m-1}(1+\frac{4|z|}{j})\Big)\Big(e^{\sum_{j=2}^n\left(1+\frac{8|z|}{j}\right)\prod_{\ell=j}^{m-1}\frac{8|z|}{\ell-1+|z|}}-1\Big)\\ &\le e^{4|z|(\log m-\log n)}\Big((1+8|z|)\sum_{j=2}^n\frac{(8|z|)^{m-j}}{(m-j)!}-1\Big)\\ &\le e^{4|z|(m-n)}\Big(e^{(1+8|z|)\frac{(8|z|)^{m-n}}{(m-n)!}\sum_{j=2}^n\frac{(8|z|)^{n-j}}{(n-j)!}}-1\Big)\\ &\le e^{4|z|(m-n)}\Big(e^{8e^{9|z|}\frac{(8|z|)^{m-n}}{(m-n)!}}-1\Big)\le 8e^{9|z|}e^{8e^{9|z|+8|z|}}\frac{(8|z|e^{4|z|})^{m-n}}{(m-n)!}\,.\end{aligned}\tag{6.7}$$

Therefore, $\forall z$ such that $|\arg z| < \frac{\pi}{4}$

$$\frac{|\vartheta_k(n;m)|}{|2\,k\,a_k|^{n-m+1}} \le C(z)\Big(\frac{(2^4e^{5|z|})^{m-n}}{(m-n)!}\Big)^{\delta_{m>n}}, \qquad C(z)\le 8e^{9|z|}e^{2^4e^{2^5|z|}}\,. \tag{6.8}$$

This implies that the common bound on $\vartheta_k(n;m)$ and $\widetilde{\vartheta}_k(n;m)$ is

$$\begin{aligned}&\le C(z)(2|ka_k|)^{n-m+1}\Big(\delta_{n\ge m}+\frac{D(z)^{m-n}}{(m-n)!}\delta_{m>n}\Big)e^{D(z)} \qquad \text{with}\\ &z=\frac{k^2a_k}{i\eta}, \qquad \frac{\beta\tau}{2|ka_k|}\le\frac12, \quad D(z)\stackrel{def}{=}(2^4e^{5|z|})\end{aligned}\tag{6.9}$$

The case $n = 0$ can be likewise checked to lead to the bounds Eq.(6.9) with $n = 0$, possibly adapting the definition of $C_1(k)$.

The latter inequalities can be used in the estimate of $|\widetilde{\sigma}^{[r]}_{n,k}|$, $r > 1$ and also for $r = 1$, because the "extra term" $\delta_{|k|=1}\delta_{r=1}$ in Eq.(5.4), *i.e.* the only non trivial term in $x^{[1]}_{n,k}$, does not affect the bounds, up to a redefinition of the constants.

If $r = 1$, then $|k| = 1$ and, if $n \ge 2$

$$\begin{aligned}|\widetilde{\sigma}^{[1]}_{n,k}| &\le \sum_{m\ge2}(\beta\tau)^m|\vartheta_k(n,m)|\\ &\le\frac{\beta V}{|a_1|}C(z)\left[\frac{(\frac{2|ka_k|}{\beta\tau})^n-1}{\frac{2|ka_k|}{\beta\tau}-1}+e^{D(z)}\right]2|ka_k|\,(\beta\tau)^n\\ &\le\delta_{|k|=1}C_1(k)|ka_k|^n\,,\end{aligned}\tag{6.10}$$

with $C_1(k)$ suitably chosen, poorly bounded in k, but bounded independently of the value of τ, as τ varies in any prefixed bounded interval (at η fixed).

The case $n = 0$ can be likewise checked to lead to the bounds in Eq.(6.10) with $n = 0$, possibly adapting the definition of $C_1(k)$.

Define the kernels

$$T_{k,n,\alpha;\widetilde{k},\widetilde{n},\widetilde{\alpha}} = \begin{cases} \frac{-\beta V}{ika_k}\vartheta_k(n,\widetilde{n})\delta_{|\widetilde{k}-k|=1} & \alpha=1,\ \widetilde{\alpha}=1 \\ \frac{(\beta V)^2}{a_k}\widetilde{\vartheta}_k(n,\widetilde{n})\delta_{|\widetilde{k}-k|=1} & \alpha=1,\ \widetilde{\alpha}=2 \\ \delta_{n,\widetilde{n}}\delta_{k,\widetilde{k}} & \alpha=2,\ \widetilde{\alpha}=1 \\ 0 & \alpha=2,\ \widetilde{\alpha}=2 \end{cases}, \tag{6.11}$$

and consider $\binom{\widetilde{\sigma}^{[r]}_{n,k}}{\widetilde{\sigma}^{[r-1]}_{n,k}}$, as a vector with components $\sigma^{[r]}_{n,k,1} \stackrel{def}{=} \widetilde{\sigma}^{[r]}_{n,k}$ and $\sigma^{[r]}_{n,k,2} \stackrel{def}{=} \widetilde{\sigma}^{[r-1]}_{n,k}$. It is thus possible to write the general expression for $\sigma^{[r]}_{n,k,\alpha}$

$$\sigma^{[r]}_{n,k,\alpha} = \sum_{m;k';\alpha'} T_{n,m;k,k';\alpha,\alpha'}\sigma^{[r-1]}_{m,k',\alpha'}\,, \tag{6.12}$$

and bound it by

$$\sum_{\{n_i\},\{k_i\},\{\alpha_i\}} \delta_{|k_{r-1}|=1}\prod_{i=1}^{r-1}|T_{n_{i-1},n_i;k_{i-1},k_i;\alpha_{i-1},\alpha_i}||\widetilde{\sigma}^{[1]}_{n_{r-1},k_{r-1}}|\,, \tag{6.13}$$

with $n_0 = n, k_0 = k, \alpha_0 = \alpha$.

Inserting the bounds (6.9) and (6.10) into Eq.(6.13)[1], taking into account that $|k_j| \le r - j$, summing a few elementary (geometric and exponential) series, the bound $|\sigma^{[r]}_{n,k}| \le A_r(B_r)^n$, $r > 1$, for suitable A_r, B_r follows and the theorem is proved.

7 Weak small scale dissipation. Conclusions

The bounds on $|\rho^{[r]}_{n,k}|$ hold with a suitable choice of the constants A_r, B_r which are positive if $\eta, \beta\tau > 0$. Therefore a formal asymptotic series at $g = 0$ is $\forall R \ge 0$:

$$\rho^{[\le R]}(q,p) = \sum_{r=0}^{R} g^r \sum_{k=-R}^{R}\sum_{n=0}^{\infty} e^{iqk}\rho^{[r]}_{n,k} : p^n : \tag{7.1}$$

[1]Remark that the summation over the labels k_i involves at most 3^r choices (as there are only three choices for $k_i - k_{i+1}$ in Eq.(6.13)), while the summation over the labels α_i involves 2^r choices (due to the two possibilities for the labels α_i)

is bounded by (using the bound on Hermite functions, [6, 8.954.2])

$$\begin{aligned}|\rho^{[\le R]}(p,q)| &\le \sum_{r=0}^{R}\sum_{k=-R}^{R}\sum_{n=0}^{\infty}\overline{A}_r g^r B_r^n \frac{1}{n!}\frac{\sqrt{n!}2^{1-n/2}}{\xi\sqrt{\eta^n}}e^{+\frac{\beta}{4J}p^2}\\ |F^{[\le R]}(p,q)| &\le e^{-\frac{\beta}{4J}p^2}B'_R\end{aligned}\tag{7.2}$$

with a suitably chosen B'_R. A natural question is whether having obtained non convergent bounds is due to a poor estimate or to a singularity at $g=0$.

The mechanical system has two qualitatively different motion regimes: if $\tau>0$ is fixed then for g small ($\tau\gg gV$) the pendulum will in the average rotate on a time scale of order $\frac{J\tau}{\xi}$; if, instead, g is fixed and τ small ($\beta\tau\ll g\beta V$), the pendulum will oscillate, very rarely performing full rotations.

Our theory, however, gives a formal power series with estimates uniform in $\beta\tau$, for $|\beta\tau|$ in a bounded interval, thus the power series would be the same for g in an interval where motions with $\tau\gg gV$ or $\tau\ll gV$ take place. Therefore we think that our series is really only formal and resummations have to be devised that would treat differently the large τ and large g regimes.

Remarks: (1) If the series for F could be shown to converge (in "any" sense) it could be concluded that the coefficients that have been formally computed are indeed the coefficients of the Hermite expansion for F, as even the positivity of F could be derived by the following simple argument. Adapting the proof in [5], any $0\le f\in L_1\cap L_\infty$ function with $\int f dpdq=1$ has the property that $\lim_{t\to+\infty}e^{\mathcal{L}^*t}f=F_\infty>0$ with $\mathcal{L}^*F_\infty=0$ and F_∞ is the unique smooth, positive, integrable, normalized solution of $\mathcal{L}^*F_\infty=0$. Hence if f_+,f_- denote the positive and negative parts of F it will be

$$F\equiv e^{\mathcal{L}^*t}F\equiv e^{\mathcal{L}^*t}f_+-e^{\mathcal{L}^*t}f_-\xrightarrow[t\to+\infty]{}(a-a')F_\infty\tag{7.3}$$

if $\int f_+=a,\int f_-=a'$. Therefore $a-a'=1, F=F_\infty, a=1, a'=0$ and this would prove that $F>0$ and that it is the unique stationary probability density in $L_1\cap L_2$ for the process with generator $\mathcal{L}^*$, *i.e.* for the stochastic equation Eq.(1.1).
(2) The algorithm in Sec.4 can be implemented numerically, by computing with prefixed precision a prefixed number of coefficients $\rho_n^{[r]}(q)$, and programming the recursion in Eq.(5.6).
(3) The overdamped case, see Sec.1, can be treated in the same way: in this case $\rho_n\equiv0$ for $n\ne0$ and $\rho_0(q)$ is analytic in g for g small: it is possible to

study the distribution ρ_0 in great detail and for all g, obtaining interesting results on large fluctuations of several observables: see [4].
(4) The continued fractions in Eq.(4.7) are really remarkable and a natural question is whether they are related to known special functions or, alternatively, which are their properties near the negative real axis.

Acknowledgements: *This work has been partially supported by the European Advanced Grant* Macroscopic Laws and Dynamical Systems *(MALADY) (ERC AdG 246953). GG is grateful to INFN-Roma1, Rutgers University and CNRS for support.*

giovanni.gallavotti@roma1.infn.it, iacob@ceremade.dauphine.fr, olla@ceremade.dauphine.fr

References

[1] A. Iacobucci, F. Legoll, S. Olla, and G. Stoltz. Negative thermal conductivity of chains of rotors with mechanical forcing. *Physical Review E*, 84:061108 +6, 2011.

[2] B. Derrida, J. L. Lebowitz, and E. R. Speer. Exact free energy functional for a driven diffusive open stationary nonequilibrium system. *Physical Review Letters*, 89:030601, 2002.

[3] L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, and C. Landim. Fluctuations in stationary nonequilibrium states of irreversible processes. *Physical Review Letters*, 87:040601, 2001.

[4] A. Faggionato and G. Gabrielli. A representation formula for large deviations rate functionals of invariant measures on the one dimensional torus. *Annales de l' Institut H. Poincaré, (Probabilité et Statistique)*, 48:212–234, 2012.

[5] J. C. Mattingly and A. M. Stuart. Geometric ergodicity of some hypoelliptic diffusions for particle motions. *Markov Processes and Related Fields*, 8:199–214, 2002.

[6] I.S. Gradshtein and I.M. Ryzhik. *Table of integrals, series, and products.* Academic Press, New York, 1965.

[7] A. Cuyt, V. Petersen, B. Verdonk, H. Waadeland, and W. Jones. *Handbook of Continued Fractions for Special Functions.* Springer, Berlin, 2004.