Short note on problems with the matrix continued fraction method for solution of coupled Kramers equations describing a noisy classical shuttle

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In this note I summarize the theoretical formulation of the matrix continued fraction method as applied to our problem of the noisy classical shuttle and illustrate the numerical problems encountered in its implementation.

I. THEORY

The ultimate goal is to be able to solve the set of two coupled Kramers equations for the classical noisy shuttle, more precisely, their stationary solution (and consequently also solution with a suitable right hand side to get the noise spectrum — however, I will skip this part of the task in this note since all the problems appear already at the level of the stationary state and it seems that the solution at this level would also solve the other tasks). These equations read

$$\begin{aligned}\partial_t W_0(x,v;t) =& -v\,\partial_x W_0(x,v;t) + \omega_0^2\big(x+d/2\big)\partial_v W_0(x,v;t)\\ &+\gamma\partial_v v W_0(x,v,t) + \gamma k_B T/m\,\partial_v^2 W_0(x,v,t)\\ &-\Gamma_L e^{-\frac{2x}{\lambda}} W_0(x,v;t) + \Gamma_R e^{\frac{2x}{\lambda}} W_1(x,v;t)\ , \qquad (1)\\ \partial_t W_1(x,v;t) =& -v\,\partial_x W_1(x,v;t) + \omega_0^2\big(x-d/2\big)\partial_v W_1(x,v;t)\\ &+\gamma\partial_v v W_1(x,v,t) + \gamma k_B T/m\,\partial_v^2 W_1(x,v,t)\\ &-\Gamma_R e^{\frac{2x}{\lambda}} W_1(x,v;t) + \Gamma_L e^{-\frac{2x}{\lambda}} W_0(x,v;t)\ . \qquad (2)\end{aligned}$$

Here, $W_i(x,v,t)$ is the probability density of the shuttle being either charged ($i=1$) or empty ($i=0$) at the position x with the velocity v.

For the simplicity, I will demonstrate the derivation of the matrix continued fraction representation on a scalar Kramers equation of a Brownian particle in a general potential

$V(x)$ reading

$$\begin{aligned}\partial_t W(x,v;t) = -v\,\partial_x W(x,v;t) + \frac{V'(x)}{m}\partial_v W(x,v;t) + \gamma\partial_v v W(x,v,t) \\ + \gamma\frac{k_B T}{m}\partial_v^2 W(x,v,t) \equiv \mathcal{L}_K W(x,v,t)\end{aligned} \tag{3}$$

for the probability density in the phase space of coordinate and velocity $W(x,v,t)$. The differences in the shuttle case will be highlighted at the end of the derivation.

Since the Kramers operator $\mathcal{L}_K$ only contains at maximum quadratic terms in v and ∂_v it is possible, after a suitable similarity transformation specified below, to express the velocity part of the operator in terms of creation and annihilation operators $a_v^\dagger$, a_v known from the quantum mechanical treatment of harmonic oscillator [1] (note, however, that I use slightly different scaling factor in the velocity basis; this shouldn't influence the behavior significantly) as

$$\mathcal{L}_\mathcal{K} = -\gamma a_v^\dagger a_v - a_v D_x - a_v^\dagger \hat{D}_x \tag{4}$$

with $D_x, \hat{D}_x$ being still operators in the coordinate space. In the oscillator basis for the velocity the above equation (4) takes on a (operator/matrix) tridiagonal form since

$$a_v = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \ddots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \ddots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} , a_v^\dagger = a_v^T \ . \tag{5}$$

To see this, one takes the irreversible (Fokker-Planck) part of the Liouvillean

$$\mathcal{L}_{\rm irr} \equiv \gamma\left(\frac{\partial}{\partial v} v + \frac{v_0^2}{2}\frac{\partial^2}{\partial v^2}\right) , \qquad (v_0^2 = 2k_B T/m) \tag{6}$$

with the stationary solution $P_{\rm stat}(v) \propto \exp(-(v/v_0)^2)$ ($\mathcal{L}_{\rm irr} P_{\rm stat}(v) = 0$) and performs the standard similarity transformation $\mathcal{L}_K \to \left(\sqrt{P_{\rm stat}(v)}\right)^{-1} \mathcal{L}_K \sqrt{P_{\rm stat}(v)}$ which yields (due to $v \to v; \partial/\partial v \to \partial/\partial v - v/v_0^2$) the transformed irreversible part $\mathcal{L}_{\rm irr}$ in the hermitian form which is, moreover, equivalent to (minus) the Hamiltonian of the quantum-mechanical harmonic oscillator, i.e.

$$\begin{aligned}\left(\sqrt{P_{\rm stat}(v)}\right)^{-1} (\mathcal{L}_{\rm irr}/\gamma) \sqrt{P_{\rm stat}(v)} &= -\frac{1}{2}\left(-\frac{\partial^2}{\partial V^2} + V^2\right) + \frac{1}{2} \\ &= -\frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial V} + V\right)\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial V} + V\right) \\ &= -a_v^\dagger a_v\end{aligned} \tag{7}$$

with $V \equiv v/v_0$ (note that I scale the velocity differently compared to Risken [1] who prefers $v_{\rm th} = v_0/\sqrt{2}$). The reversible part of the Liouvillean $\mathcal{L}_{\rm rev} \equiv -v\,\partial_x + \frac{V'(x)}{m}\partial_v$ is after the similarity transformation expressed in the form of the last two terms of Eq. (4) with

$$\begin{aligned} D_x &= \frac{1}{\sqrt{2}} v_0 \frac{\partial}{\partial x} \\ \hat{D}_x &= \frac{1}{\sqrt{2}} \left(v_0 \frac{\partial}{\partial x} + \frac{2V'(x)}{v_0 m} \right) . \end{aligned} \tag{8}$$

The similarity transformation corresponds to looking for the solution in the form $W(x,v,t) = \psi_0(V) \sum_{n=0}^{\infty} c_n(x,t)\psi_n(V)$, where $\psi_n(V)$ are eigenfunctions of the operator $a_v^\dagger a_v$, in particular $\psi_0(V) \propto \sqrt{P_{\rm stat}(v)} \propto \exp(-\frac{v^2}{2v_0^2})$. Higher order eigenfunctions are given by the well-know oscillator functions which can be expressed as $\psi_n(V) = \frac{(a_v^\dagger)^n}{\sqrt{n!}}\psi_0(V) = \frac{1}{\sqrt{2^n n!}}(V - \frac{\partial}{\partial V})^n \psi_0(V) = H_n(V)\exp(-V^2/2)/\sqrt{\sqrt{\pi} 2^n n!}$ where $H_n(V)$ are Hermite polynomials. When this ansatz for the form of the probability density is inserted into Eq. (4) we obtain a hierarchy for coefficients $c_n(x,t)$ (so called Brinkman hierarchy)

$$\partial_t c_n(x,t) = -\sqrt{n}\hat{D}_x c_{n-1}(x,t) - n\gamma c_n(x,t) - \sqrt{n+1} D_x c_{n+1}(x,t) \ , \qquad c_n \equiv 0 \ (n<0). \tag{9}$$

This represent a tridiagonal recurrence functional equation for c_n's which can be solved by a matrix continued fraction method after suitable truncation in the position space [1].

For the shuttle described by Eq. (1), the only formal difference from the above is that the coefficients $c_n(x,t)$ become two-component vectors $\mathbf{c}_n(x,t) = (c_n^0(x,t), c_n^1(x,t))^T$ representing the two charge states. Correspondingly, the equation (9) changes into

$$\partial_t \mathbf{c}_n(x,t) = -\sqrt{n}\hat{\mathbf{D}}_x \mathbf{c}_{n-1}(x,t) - (n\gamma + \mathbf{\Gamma}(x))\mathbf{c}_n(x,t) - \sqrt{n+1}\mathbf{D}_x \mathbf{c}_{n+1}(x,t) \tag{10}$$

where the operators $\mathbf{\Gamma}(x), \mathbf{D}_x, \hat{\mathbf{D}}_x$ have the 2-by-2 block structure reading

$$\mathbf{\Gamma}(x) = \begin{pmatrix} \Gamma_L e^{-\frac{2x}{\lambda}} & -\Gamma_R e^{\frac{2x}{\lambda}} \\ -\Gamma_L e^{-\frac{2x}{\lambda}} & \Gamma_R e^{\frac{2x}{\lambda}} \end{pmatrix} \tag{11}$$

$$\mathbf{D}_x = \frac{1}{2}\begin{pmatrix} a_x - a_x^\dagger & 0 \\ 0 & a_x - a_x^\dagger \end{pmatrix} \tag{12}$$

$$\hat{\mathbf{D}}_x = \frac{1}{2}\begin{pmatrix} 3a_x + a_x^\dagger + \frac{d\omega_0\sqrt{2}}{v_0} & 0 \\ 0 & 3a_x - a_x^\dagger - \frac{d\omega_0\sqrt{2}}{v_0} \end{pmatrix} \tag{13}$$

where $a_x,\ a_x^\dagger$ are the annihilation and creation operators analogous to $a_v, a_v^\dagger$ but acting on the coordinate space. The physical difference between the shuttle and a simple scalar Kramers

equation is quite deep — while in the scalar case the full stationary state (not only its velocity part) is usually (depending on the boundary conditions) the Maxwell-Boltzmann distribution $W_{\mathrm{stat}}(x,v) \propto \exp(-(\frac{mv^2}{2}+V(x))/k_BT)$ which identically satisfies the Brinkman hierarchy (for the zero-flux boundary condition), in the shuttle case already finding the stationary state is a highly nontrivial task. This may somehow leak into technical details and convergence issues (purely my conjecture).

II. IMPLEMENTATION

In practice, it turns out that the implementation of the matrix continued fraction algorithm in a "poor man's way" (i.e. exactly as presented here so far) results in a highly unstable and not convergent routine. I will demonstrate this behavior here by a couple of figures for the shuttle (Figs. 1, 2). When the coefficients $\mathbf{c}_n(x,t)$ are expanded in the oscillator basis as $\mathbf{c}_n(x,t) = \sum_{m=0}^{N} \mathbf{b}_{n,m}(t)\psi_m(X)$ with $X \equiv x\omega_0/v_0$ (note that only the N lowest states are retained) the relevant operators acting in the coordinate space are truncated to the dimension $2N \times 2N$, in particular the creation and annihilation operators are given by N-dimensional truncation of the matrix (5). When the matrix continued fraction method is implemented to find the solution of the Brinkman hierarchy the continued fraction does not converge. Therefore, I only present here the results of a fixed length recurrence (of the length of $10N$) which sometimes shows reasonable behavior but is highly unstable with respect to changing N — see Figs. 1 and 2.

The naive implementation thus fails. However, it's possible to perform additional similarity transformation in the coordinate space analogous to the one in the velocity space (for the case of the scalar Kramers equation this method is described in Risken [1]). For the shuttle, we use the stationary state of a particle in harmonic potential (corresponding to the solution of the shuttle in the limit $d = 0$, $\Gamma_{L,R} = 0$) which is proportional to $\exp(-(\omega_0 x/v_0)^2)$ for both charge states, i.e. the transformation acts as unity on the charge label. In the transformation only the operators D_x, $\hat{D}_x$ will change since only these contain the derivatives $\partial/\partial x$. In the dimensionless form with $X \equiv x\omega_0/v_0$ we get $\partial/\partial X \to \partial/\partial X - X$ and, therefore, the

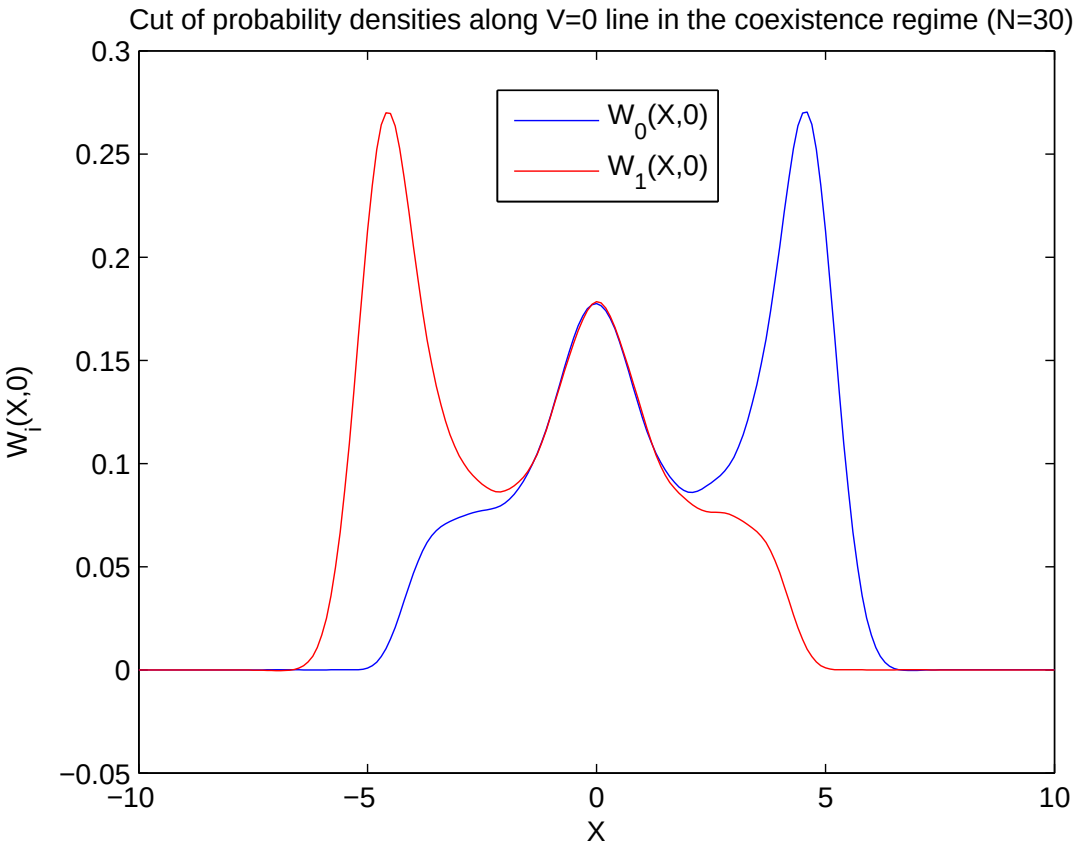

FIG. 1: The cut through the two probability densities (occupied $W_1(X,0)$ and empty $W_0(X,0)$) along the line $V = 0$ for the parameters $\Lambda \equiv \lambda\omega_0/v_0 = 1$, $\gamma = 0.0035\omega_0$, $\Gamma_{L,R} = 0.015\omega_0$, $D \equiv d\omega_0/v_0 = 0.05$ which corresponds to the coexistence regime. The size of the retained basis is $N = 30$. These results look OK and are very likely almost correct.

transformed $\tilde{D}_x$, $\hat{\tilde{D}}_x$ read

$$\begin{aligned} \tilde{D}_x &= \frac{\omega_0}{\sqrt{2}}\left(\frac{\partial}{\partial X} - X\right) = -\omega_0 a_x^\dagger \\ \hat{D}_x &= \frac{\omega_0}{\sqrt{2}}\left(\frac{\partial}{\partial X} + X\right) = \omega_0 a_x \end{aligned} \tag{14}$$

and in the whole matrix form

$$\tilde{\mathbf{D}}_x = -\omega_0 \begin{pmatrix} a_x^\dagger & 0 \\ 0 & a_x^\dagger \end{pmatrix} \tag{15}$$

$$\hat{\tilde{\mathbf{D}}}_x = \omega_0 \begin{pmatrix} a_x + \frac{d\omega_0\sqrt{2}}{v_0} & 0 \\ 0 & a_x - \frac{d\omega_0\sqrt{2}}{v_0} \end{pmatrix} . \tag{16}$$

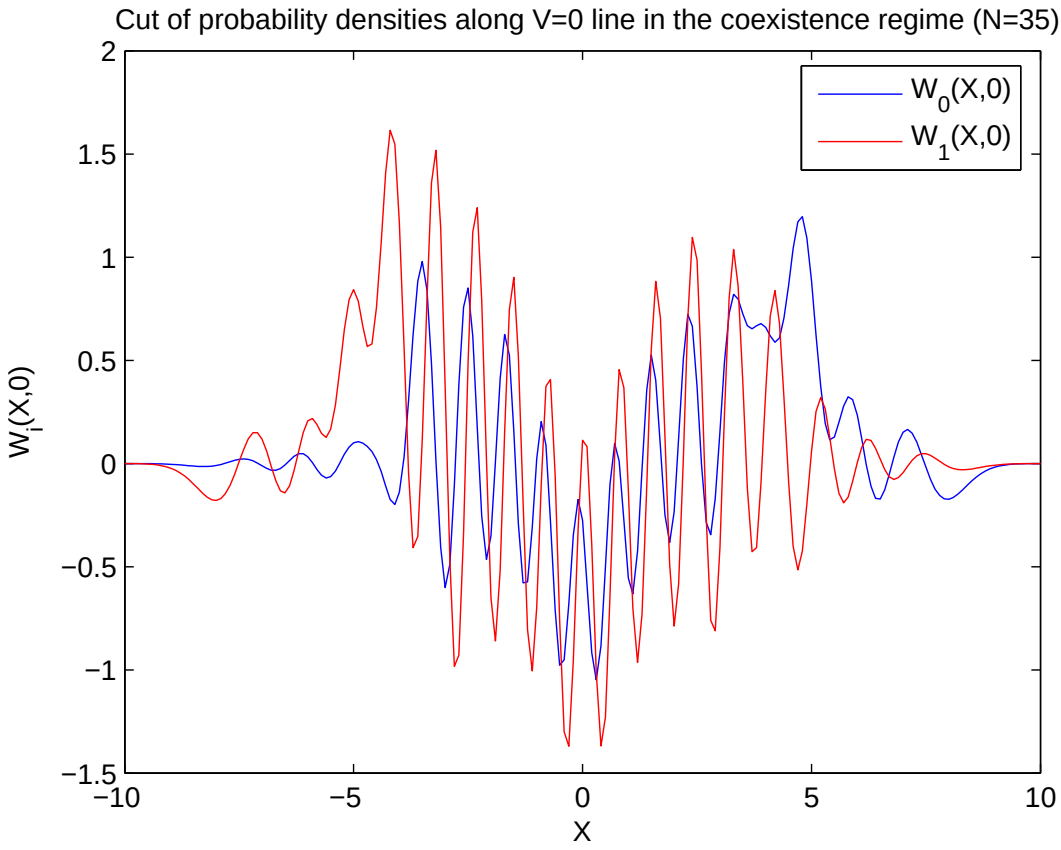

FIG. 2: The cut through the two probability densities (occupied $W_1(X,0)$ and empty $W_0(X,0)$) along the line $V=0$ for the same parameters as in Fig. 1 but for $N=35$. In the run through the recurrence Matlab issues warnings that results might be inaccurate due to matrix being close to singular. The results are obviously wrong since $W_i(X,V)$ should be always non-negative.

In the new representation the matrix continued fraction reasonably converges up to $N \sim 100$. The results for the mean current and Fano factor (zero-frequency noise power normalized by the mean current) around the shuttling transition as functions of the damping γ are shown in Fig. 3 together with the semi-analytical results based on Kramers rate theory. We see a rather nice match but the numerical results become more and more noisy for lower damping, i.e. deeper in the shuttling regime which needs higher N's, and eventually the numerics breaks down for $N \sim 150$. The routine does not converge for too high N in a similar way as for the naive implementation. It seems to me that the stabilizing factor of the transformed representation compared to the naive one is the fact that the finite size representations of $\tilde{\mathbf{D}}_x$, $\tilde{\tilde{\mathbf{D}}}_x$ are *singular* matrices while in the naive case at least one of

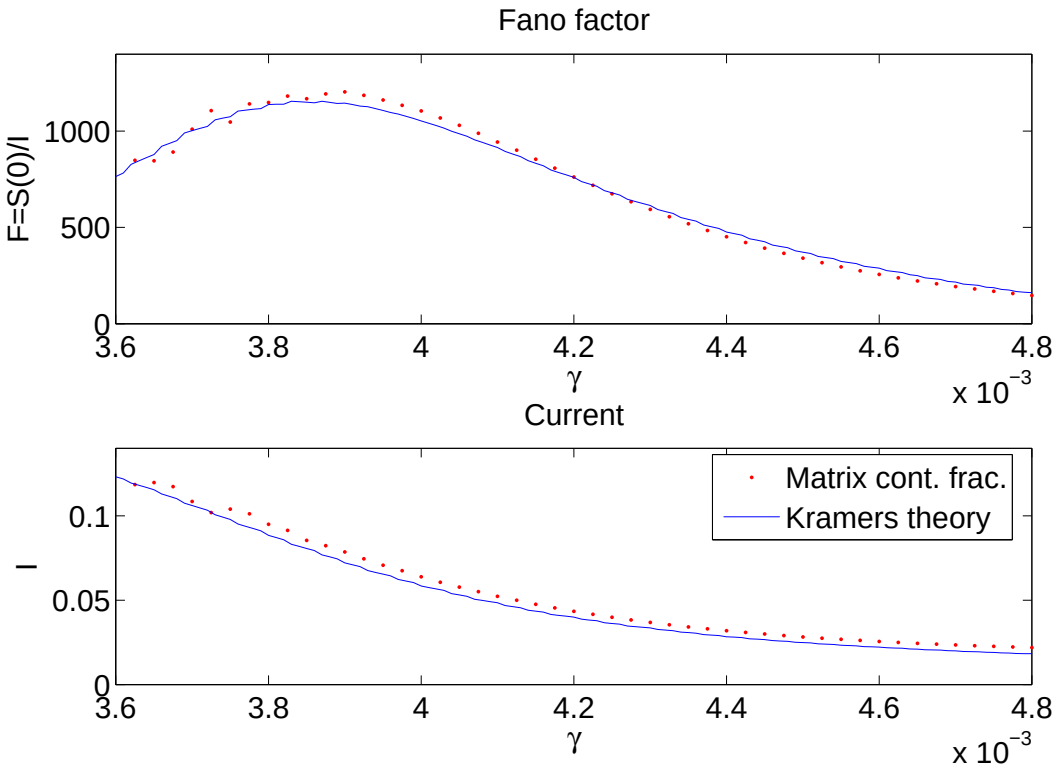

FIG. 3: Comparison of the results for the Fano factor $F = S(0)/I$ (upper panel) and mean current I (lower panel) around the shuttling transition calculated by the (modified version of the) matrix continued fraction method (dots) and by the semi-analytical Kramers rate theory (line). The number of states used was $N = 100$ and, apparently, the numerical method stops working reliably for low enough damping.

$\mathbf{D}_x$, $\hat{\mathbf{D}}_x$ is regular.

Thus, we are still looking for a stable routine which would work reliably even further into the shuttling regime, i.e. for N up to around 200. Also the basic understanding of the cause of the encountered problems is missing so far.

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[1] H. Risken, *The Fokker-Planck equation: Methods of solution and applications* (Springer, Berlin, 1996), 2nd ed.