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A test for two Fokker–Planck modellings of a master equation*

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Abstract. The kind of two Fokker–Planck equation modellings of a non-equilibrium system, defined by a two-variable master equation, is studied. We compute explicitly their associated stationary potentials in the weak noise limit, and we compare them with the exact one coming from the master equation. We find that a recently proposed Fokker–Planck equation is far better than the other coming from the commonly used Kramers–Moyal expansion.

1. Introduction

A Fokker–Planck equation (FPE) is a second-order partial differential equation in which the unknown is the probability to find a system in any given configuration at any given time. Usually, these kinds of equations are built by performing a continuum limit of some microscopic dynamical equation, by breaking some expansion of these, or simply by directly writing one with some desired properties. In most of the cases, the resulting FPE is weakly connected with the original microscopic system. Nevertheless, this type of modelling of physical systems has proven to be very useful for the description of different non-equilibrium phenomena [1–4]. In particular, the understanding of how the systems relax to the equilibrium state near a critical point has been achieved mainly by using these kinds of equations [5]. This indicates that in some cases the FPE modellings contain the key ingredients which are needed in order to describe these systems' behaviour. In general, the latter seems to be true whenever the system properties under consideration are almost independent of the microscopic dynamics details and they depend only on general system features as symmetries, dimensions, number of ground states, etc. However, when we deal with properties which depend on these microscopic details, the kind of FPE scheme considered can only be checked *a posteriori* by comparing the results that it yields with the exact ones coming from the underlying microscopic system definition. For example, microscopic dynamics dependent magnitudes are mean first passage times, exit rates from a metastable state [6, 7] or stationary properties of non-equilibrium systems [8].

An approach to the problem of how to model a given system by means of a FPE has been recently proposed by the authors in order to deal with some non-equilibrium systems defined by a master equation [9]. The FPE is constructed in such a way that it is *a priori* guaranteed that its associated stationary probability distribution is almost the exact one around the most probable configuration.

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There are in the literature several ways to build a FPE from a master equation. A strategy similar to ours was considered before by Hanggi *et al* [6, 7]. Their technique allowed them to deal only with systems with a known stationary probability distribution. There are also perturbative schemes which manage to reduce a master equation to a simplified FPE in the vicinity of a bifurcation point [10, 11].

From a purely theoretical point of view the new FPE constitutes an improvement with respect to other previous approaches. However, when dealing with properties that depend not only on the local form of the stationary probability distribution around their extrema, but on the global shape of the same, the new method has to be tested and compared with others in order to analyse the degree of accuracy that it yields.

To achieve this goal in a particular example, we consider a simple non-equilibrium model with two degrees of freedom and with a rich behaviour which has been studied previously [12]. By using some well known techniques [13–17], we compute and compare numerically its exact stationary non-equilibrium distribution and also the ones coming from the new FPE and from a currently used FPE. We found that the new FPE reproduces the exact distribution much more accurately than the other one. The outline of the paper is the following. In section 2 we define the model and we review some of its properties. Section 3 is devoted to obtaining the exact stationary non-equilibrium distribution while explaining, with some detail, how to do it. In section 4 FPE modellings are defined, their associated stationary solutions are obtained and they are compared with the exact one.

2. The model

The model was introduced in [12], and we refer the reader to there for a motivation and a more detailed construction. In order to fix notation, let us briefly recall its definition and some properties. In each point x of a d-dimensional lattice with N nodes, there is a spin variable, s_x which can take values $+1$ or -1. A stochastic dynamics governs the time evolution of the spins. This dynamics is constructed as a linear superposition of two different mechanisms: one attempting to drive the system to a ferromagnetic state, and the other to an antiferromagnetic one, defined in each case by a Gibbsian weight with a mean-field Hamiltonian. A system state is completely characterized by the ferromagnetic and antiferromagnetic order parameters: m_F and m_A ($|m_F| + |m_A| \leqslant 1$). The probability to find the system in a state with given values of m_F and m_A at time t, say $P_N(m_F, m_A; t)$, evolves following the Markovian master equation:

$$\frac{\partial}{\partial t} P_N(m_F, m_A, t) = \sum_{\mu_F, \mu_A = \pm 1} \left[c\left(\mu_F, \mu_A; m_F + \frac{\mu_F}{N}, m_A + \frac{\mu_A}{N}, \frac{2}{N}\right) \times P_N\left(m_F + \frac{\mu_F}{N}, m_A + \frac{\mu_A}{N}; t\right) - c(\mu_F, \mu_A; m_F, m_A, 0)\, P_N(m_F, m_A; t) \right] \tag{2.1}$$

where

$$c(\mu_F, \mu_A; m_F, m_A, \Delta) = \tfrac{1}{2} N (1 + \mu_F m_F + \mu_A m_A + \Delta) \left\{ p \exp\left[-K\left(2 m_F \mu_F + \Delta - \frac{1}{N}\right)\right] + (1-p) \exp\left[-K\left(2 m_A \mu_A + \Delta - \frac{1}{N}\right)\right]\right\} \tag{2.2}$$

where K is the inverse temperature and $p \in [0, 1]$ is the relative velocity between both mechanisms. In the limiting cases $p = 0$ and $p = 1$ a detailed balance condition (DBC) is satisfied, and the system stationary state is an equilibrium one. For general p values DBC does not hold and therefore, the stationary distribution is expected to be non-Gibbsian. In the deterministic limit $N \to \infty$, in which fluctuations are completely ignored, (2.1) reduces to

$$\frac{dv_{F(A)}}{dt} = A_{F(A)}(v_F, v_A) \equiv \sum_{\mu_F, \mu_A = \pm 1} \mu_{F(A)} c_0(\mu_F, \mu_A; v_F, v_A) \tag{2.3}$$

where $v_{F(A)}$ and $c_0(\mu_F, \mu_A; v_F, v_A)$ are the leading terms in the N^{-1}-expansion of $m_{F(A)}$ and (2.2), respectively. Because of the invariance of the equations under the transformations $v_{F(A)} \to -v_{F(A)}$ we will limit ourselves from now on to considering only positive order parameter values, i.e. $v_{F(A)} \geqslant 0$.

A deterministic stationary state $\underline{v}^* = (v_F^*, v_A^*)$ is a solution of (2.3) equated to 0. Its qualitative behaviour is as follows. When $K \to 0$ there is a unique stable solution $\underline{v}_0^* = (0, 0)$. When K is above a certain critical value, $K_c^{(1)}(p)$, the solution $\underline{v}_0^*$ becomes unstable and there appears a new stable solution in which one of the order parameters is non-vanishing. There is a second critical point, $K_c^{(2)}(p) > K_c^{(1)}(p)$, above which two solutions of the following forms coexist: $\underline{v}_I^* = (v_F^*, 0)$, and $\underline{v}_{II}^* = (0, v_A^*)$. Both of them are locally stable under the dynamics given by (2.3), and they have a definite domain of attraction. It is clear that one of them should be a metastable state but this can only be precisely determined by knowing the system non-equilibrium stationary distribution.

3. Computing the exact stationary distribution

Let us suppose that for the master equation (2.1) a stationary probability distribution exists, it is unique, and that in the weak noise limit, i.e. for large N values, it can be written in the asymptotic form,

$$P_N^{st}(v_F, v_A) \propto \exp[-NV_0(v_F, v_A) - \Theta(N^0)] \tag{3.1}$$

where $V_0(v_F, v_A)$ is the stationary non-equilibrium potential. This assumption is not mathematically rigorous for generic parameter values but it can be used, in any case, as useful ansatz to construct the stationary probability distribution [13]. To get a closed equation for $V_0(v_F, v_A)$, we substitute (3.1) into the stationary master equation (2.1), i.e. $(\partial/\partial t) P_N(v_F, v_A, t) = 0$, and we perform a N^{-1} expansion of it. The leading order of this expansion reads

$$H\left(v_F, v_A, \frac{\partial V_0(v_F, v_A)}{\partial v_F}, \frac{\partial V_0(v_F, v_A)}{\partial v_A}\right) \equiv \sum_{\mu_F, \mu_A = \pm 1} c_0(\mu_F, \mu_A; v_F, v_A) \times \left[1 - \exp\left[-\mu_F \frac{\partial V_0(v_F, v_A)}{\partial v_F} - \mu_A \frac{\partial V_0(v_F, v_A)}{\partial v_A}\right]\right] = 0. \tag{3.2}$$

In order to solve (3.2) we can interpret it as a Hamilton–Jacobi type of equation [18] where H is the Hamiltonian which defines the dynamics of a system with two coordinates, say v_F and v_A, and its two respective conjugate momenta

$$p_{F(A)}(v_F, v_A) = \frac{\partial V_0(v_F, v_A)}{\partial v_{F(A)}}. \tag{3.3}$$

In this interpretation $V_0(v_F, v_A)$ becomes the system action, and it can be evaluated by integrating (3.3) along any path that connects a generic point of the form $P = (v_F, v_A, p_F(v_F, v_A), p_A(v_F, v_A))$ with a potential local minimum, $(v_F^*, 0, 0, 0)$ or $(0, v_A^*, 0, 0)$. The functional dependence of $p_{F(A)} = p_{F(A)}(v_F, v_A)$ is obtained in parametric form from the *equations of motion* defined as the Hamilton equations associated with the Hamiltonian H, that is, by solving

$$\frac{dv_{F(A)}}{dt} = \frac{\partial H(v_F, v_A, p_F, p_A)}{\partial p_{F(A)}} = \sum_{\mu_F, \mu_A = \pm 1} \mu_{F(A)} c_0(\mu_F, \mu_A, v_F, v_A) e^{-\mu_F p_F - \mu_A p_A} \tag{3.4}$$

$$\frac{dp_{F(A)}}{dt} = -\frac{\partial H(v_F, v_A, p_F, p_A)}{\partial v_{F(A)}} = \sum_{\mu_F, \mu_A = \pm 1} \left(\frac{\partial}{\partial v_Y} c_0(\mu_F, \mu_A, v_F, v_A) \right) \left[e^{-\mu_F p_F - \mu_A p_A} - 1 \right] \tag{3.5}$$

with initial conditions $p_{F(A)}(0) = 0$ at the deterministic stationary states. Because of (3.3), these boundary conditions are necessary to guarantee that potential $V_0(v_F, v_A)$ will have a local minimum in the deterministic attractors, a local maximum in deterministic repellors and saddles in saddles of (2.3).

All the trajectories going through a given potential minimum, are confined in one of two different two-dimensional invariant manifolds. One of them is the deterministic one, defined by (2.3), and $p_{F(A)} = 0$. It is a stable manifold, and its associated potential $V_0(v_F, v_A) =$ constant is a spurious trivial solution of (3.2). The other manifold is the unstable one, or so-called *separatrix*. Therefore, curves confined to the separatrices of each deterministic attractor are the interesting ones in order to calculate the potential.

The latter scheme seems to be simple and powerful but, in practice, it can only be rigorously applied when the unknown potential, $V_0(v_F, v_A)$, is a twice continuously differentiable and monovaluated function. This is the case, for example, in equilibrium situations and, in general, for integrable Hamiltonians, H. In particular, our model is exactly solvable, i.e. integrable, in the equilibrium limits, $p = 0$ and 1, as well as for $p = 0.5$ for which a DBC holds. However, when dealing with non-equilibrium systems, multivaluated potentials are expected to arise. Then, in order to define a monovaluated function V_0 it is necessary to introduce an additional ansatz: from all the branches we only keep at each point, (v_F, v_A), the one giving the mimimum value, because it gives the dominant contribution to (3.1).

Let us now describe, in detail, the numerical procedure to determine the potential $V_0(v_F, v_A)$ from (3.4) and (3.5) and the considered boundary conditions. For the sake of conciseness and without loss of generality, we consider a particular set of parameter values, $p = 0.6$ and $K = 3$, which correspond to a situation in which two different stable solutions of the stationary deterministic equations coexist (see last paragraph on section 2). The procedure is as follows:

(i) We locate the solutions of the stationary deterministic equations, $(v_F^*, 0)$ and $(0, v_A^*)$ in our case. We will call them from now on *fixed points* or *attractors*.

(ii) We determine the unstable invariant manifold associated with each attractor. An extensive discussion about technicalities in the evaluation of invariant manifolds can be found in [19]. Because the non-equilibrium nature of the problem, both manifolds do not coincide and the process that follows has to be repeated for each deterministic attractor.

The first step is to linearize equations (3.4) and (3.5) around the fixed point and then to calculate the eigenvalues and eigenvectors for the associated matrix. The pair

of eigenvectors corresponding to positive eigenvalues determine a basis in the tangent space of the unstable invariant manifold at this point. In order to define an accurate local approximation to the separatrix, we consider a set of different linear combinations of these eigenvectors, with a fixed small modulus. From this local approximation it is possible to reconstruct the complete separatrix by leaving all the different initial points to evolve with the Hamiltonian flow (3.4) and (3.5). The integration of these equations of motion is carried out by a fourth-order Runge–Kutta algorithm. Working with small enough integration steps, the Hamiltonian value is conserved up to the required precision (four decimal digits), therefore, a more elaborate symplectic algorithm is not necessary to deal with this dynamical system. The main difficulty at this point is that it is not possible to know *a priori* how to distribute the initial points to explore all the separatrix. We have considered homogeneously distributed initial points and, once the main structure of the separatrix is known, we interpolate new initial conditions between the previous ones in order to fill as uniformly as possible the separatrix with these trajectories. In this way we have a set of curves whose enveloping surface is the separatrix. The first approximation to the non-equilibrium potential at any point at the separatrix of each attractor is then calculated by evaluating the integral

$$V_0(v_F(t), v_A(t)) - V_0(v_F(0), v_A(0)) = \sum_{Y=F,A} \int_0^t \mathrm{d}\tau \; p_Y(\tau) \frac{\mathrm{d}v_Y}{\mathrm{d}\tau} .$$

Notice that $V_0(v_F(0), v_A(0))$ can be replaced by a constant which depends on the attractor: C_1 for $(v_F{}^*, 0)$ and C_2 for $(0, v_A{}^*)$. The error we make by doing that is of the order ε^2, ε being the distance from the initial point to the attractor. Considering ε values small enough the error can be kept below the precision we work with. Finally, for each point (v_F, v_A) where two or more trajectories overlap, the minimum value of $V_0(v_F, v_A)$ has to be selected. Technically it is done by projecting the trajectories over a discrete set of values (v_F, v_A) that define a lattice, and then by keeping the minimum value at each node.

(iii) The last step, once both local pieces of the potential have been determined, is to join them and to fix their relative depths, i.e. by evaluating the constants C_1 and C_2. The general principle which allows us to fix the constants is the balance between the incoming and outgoing fluxes of the stationary probability distribution from each domain of attraction [2, 16]. The logarithm of the exit rate from an attractor M can be written in the weak noise limit as $V_0(M) - \min_P V_0(P)$ where the minimum is taken in the set of points P belonging to the curve which limits the domains of attraction, under the deterministic equations (2.3), of the attractor M. In our case, the minima for both attractors coincide and are located at the deterministic saddle point. Therefore at this point both local potential values have to be equal. For the considered choice of parameters we obtain $C_2 = 0.2934\cdots + C_1$. This indicates that a fluctuation carrying the system from $(0, v_A{}^*)$ to $(v_F{}^*, 0)$ appears to be much more likely than the opposite one. Therefore, the solution $\underline{v}_{\mathrm{II}}^*$ is a metastable state. The remaining free constant can be fixed by normalizing the stationary probability distribution.

The potential calculated following the above three steps has been represented in figure 1. The main feature we want to stress is that it is continuous, but there is a line in configurational space in which it is not differentiable. This line corresponds to the boundary in which the minimum is transferred from one local piece of the potential to the other. Roughly it goes parallel to the axis v_A crossing at $v_F = 0.27$. This effect is shown

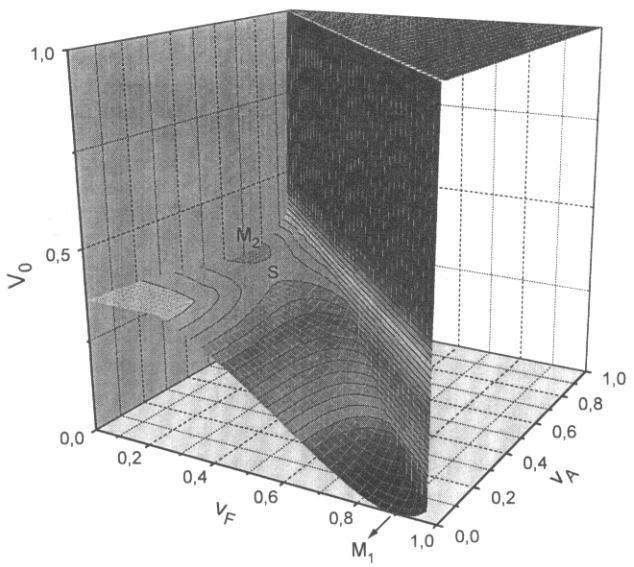

Figure 1. Effective stationary potential calculated in section 3 is represented versus (v_F, v_A). Pairs (v_F, v_A) with $v_F + v_A \geqslant 1$ are meaningless. For these values we draw $V_0(v_F, v_A) = 1$. The presence of two minima, M_1 and M_2, and the saddle point, S, are clearly shown.

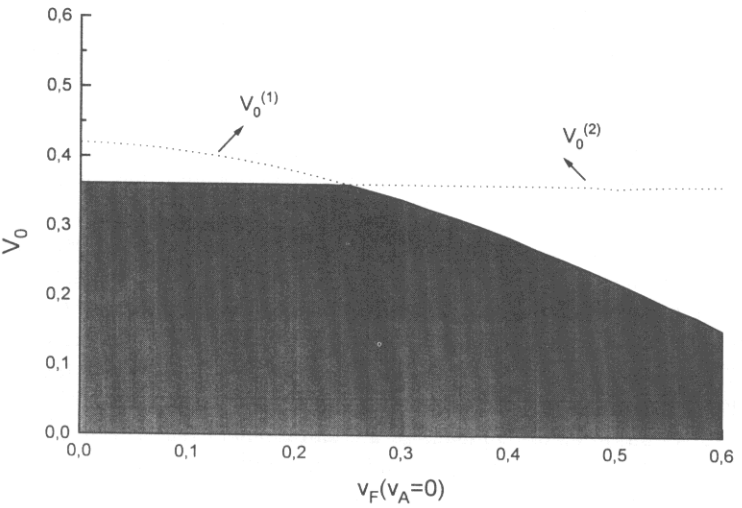

Figure 2. The lower area corresponds to a section of the potential $V_0(v_F, v_A)$ with $v_A = 0$. This is obtained by taking the minimum of the two different branches, $V_0^{(1)}$ and $V_0^{(2)}$ which are built from the minima M_1 and M_2 respectively. Close to $v_F = 0.25$, the minimum of the potential is transferred from one branch to the other. At this point the resulting potential is clearly non-differentiable.

more clearly in figure 2, where a section, $v_A = 0$, of the two local pieces of the potential is represented versus v_F. It is clear that the minimization procedure is responsible for the presence of non-differenciabilities in the resulting potential.

4. Two FPE modellings and their stationary solutions

As we said in the introduction, it is our purpose to take advantage of the knowledge we have of the exact stationary potential in order to test two different FPE modellings of this systems. The first one is the FPE coming from the N^{-1} expansion of the master equation (2.1) (Kramers–Moyal expansion) truncated up to second-order derivatives. This is the most frequently used method to obtain a FPE from a master equation [3, 4]. In our case, this FPE (from now on FPE–KM) reads

$$\frac{\partial}{\partial t}P_N(v_F, v_A, t) = -\sum_{Y=F,A}\frac{\partial}{\partial v_Y}\Bigg[A_Y(v_F, v_A)P_N(v_F, v_A, t) - \frac{1}{2N}\sum_{Z=F,A}\frac{\partial}{\partial v_Z}(B_{YZ}(v_F, v_A)P_N(v_F, v_A, t))\Bigg] \tag{4.1}$$

where A is given by (2.3) and

$$B_{YZ}(v_F, v_A) = \sum_{\mu_F,\mu_A=\pm 1} c_0(\mu_F, \mu_A; v_F, v_A)\mu_Y\mu_Z\,. \tag{4.2}$$

The second FPE is the one proposed in [9] which in our case reads

$$\frac{\partial}{\partial t}P_N(v_F, v_A, t) = -\sum_{Y=F,A}\frac{\partial}{\partial v_Y}\Bigg[A_Y(v_F, v_A)P_N(v_F, v_A, t) - \frac{1}{N}\sum_{Z=F,A}L_{YZ}(v_F, v_A)\frac{\partial}{\partial v_Z}P_N(v_F, v_A, t)\Bigg] \tag{4.3}$$

with

$$L_{YZ}(v_F, v_A) = \frac{c_0(-1,-1; v_F, v_A) - c_0(1, 1; v_F, v_A)}{\log\left[c_0(-1,-1; v_F, v_A)/c_0(1, 1; v_F, v_A)\right]} \pm \frac{c_0(-1, 1; v_F, v_A) - c_0(1,-1, v_F, v_A)}{\log\left[c_0(-1, 1; v_F, v_A)/c_0(1,-1; v_F, v_A)\right]}$$

where the plus (minus) sign stands for Y equal (different) to Z. By construction, it is guaranteed that this new FPE (FPE–N) reproduces the exact stationary potential in the equilibrium limits, as well as in the vicinity of the deterministic attractors [9].

Substitution of (3.1) in (4.1) and (4.3) respectively leads to two different Hamilton–Jacobi-type equations. Each them is analogous to (3.2). The procedure to obtain the stationary potential for each equation follows the same lines as we have already explained in section 3. The main results can be summarized as follows:

(i) The qualitative form of the stationary potential, V_0, the location of the extrema, the saddle point, and the curvatures around the minima, coincides in both approximations with their master equation counterparts.

(ii) The potential associated with the FPE–KM, V_0^{KM}, is qualitatively similar to the one shown in figure 1 for the exact potential V_0. However, V_0^{KM} presents quantitative systematic deviations with respect to V_0. In particular: (i) $V_0^{\mathrm{KM}}(v_F, v_A) \leqslant V_0(v_F, v_A)\ \forall(v_F, v_A)$, (ii) $\max_{(v_F,v_A)}|V_0^{\mathrm{KM}}(v_F, v_A) - V_0(v_F, v_A)|/V_0(v_F, v_A) \simeq 0.05$, and (iii) $\langle|V_0^{\mathrm{KM}}(v_F, v_A) - V_0(v_F, v_A)|\rangle \simeq 0.004$, where $\langle\cdot\rangle$ is the average over the phase space.

Table 1. The values of the exact and approximate potentials are shown for different values of (v_F, v_A). The associated error is 5×10^{-4}. In all the points the FPE–N modelling yields better results than the FPE–KM.

Point	Exact	FPE–N	FPE–KM
M_1	0.0	0.0	0.0
M_2	0.293	0.293	0.284
(0, 0)	0.362	0.362	0.352
S	0.304	0.304	0.294

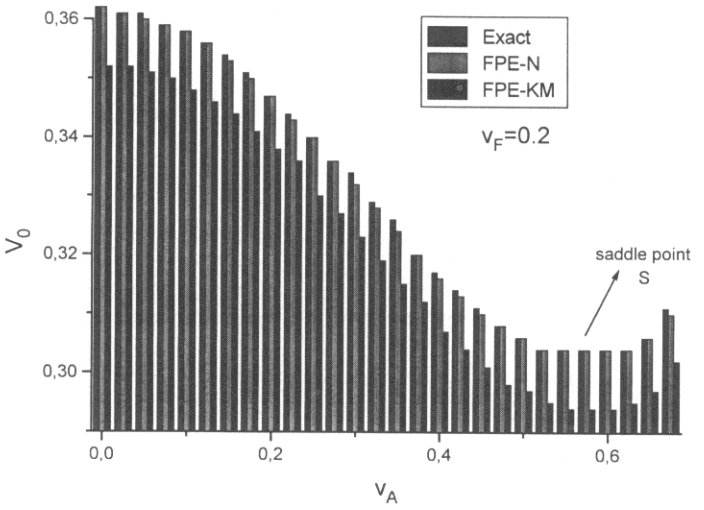

Figure 3. Potentials section for $v_F = 0.2$. The differences between the exact potential and the approximate ones, corresponding to the Kramers–Moyal and the new Fokker–Planck equation modellings, are put forward.

(iii) The potential solution of the FPE–N, V_0^N, has a much better behaviour than V_0^{KM}. It has no systematic deviations with respect to the exact potential. It fluctuates around the exact solution along the phase space. The averaged amplitude of this fluctuation is $\langle |V_0^N(v_F, v_A) - V_0(v_F, v_A)| \rangle \simeq 7 \times 10^{-5}$. That is, two orders of magnitude less than the deviations associated to V_0^{KM}. In fact, within the precision degree we are working with, we can conclude that our FPE gives an almost exact result.

(iv) In order to compare both approximations we present table 1, and show in figures 3 and 4 two different sections of the different potentials (in figure 3 we fix $v_F = 0.2$ and, in figure 4: $v_F + v_A = 0.775$). As can be seen in both figures, the differences between the master equation potential and V_0^N are small at all points, and less than the numerical error in any case. On the other hand, it is clear that V_0^{KM} presents systematic differences with respect to the exact potential. In particular, in the saddle point, S, we have $V_0 - V_0^{\mathrm{KM}} = 0.01$ (see table 1) which means that this approximation overestimates the exit rate from the deeper (ferromagnetic) minima. In contrast, the FPE–N reproduces correctly the potential value at the saddle point. Analogously, as can be deduced from the data in table 1, the FPE–KM overestimates the exit rates from $(v_F^*, 0)$ to $(-v_F^*, 0)$ and from $(0, v_A^*)$ to $(0, -v_A^*)$, while FPE–N gives the correct results.

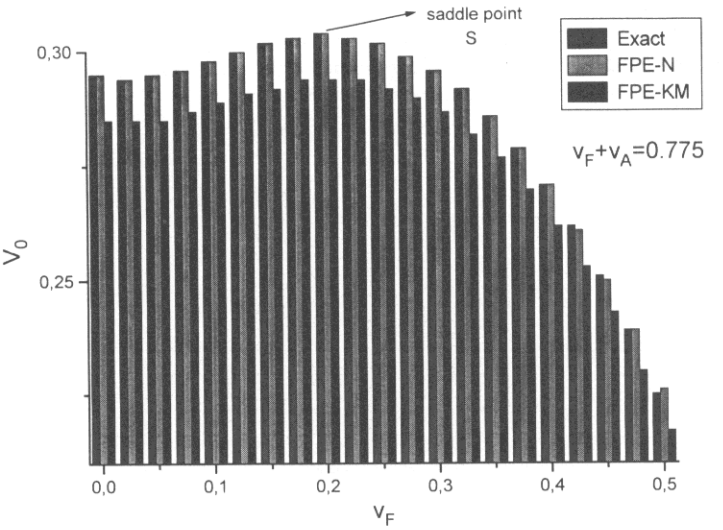

Figure 4. A different section of the three potentials. The potential associated to FPE–N compares far better with the exact one than the one associated with the FPE–KM.

5. Conclusions

We have suggested that a recently proposed FPE modelling of non-equilibrium master equations, FPE–N, gives better results in the low noise limit than the conventional approach based on a truncated Kramers–Moyal expansion, FPE–KM. In the vicinity of the deterministic extrema it is guaranteed by construction that FPE–N reproduces the exact stationary distribution [9]. What we have verified in a particular exactly solvable model is that, even far from the extrema, where there is no *a priori* rigourous justification of this modelling, it reproduces the low noise stationary potential much better than the usual Kramers–Moyal modelling.

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